ICASP-7 / 7th International Conference on Advances in Solidification Processes

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Abstract booklet

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Phase-field modeling of far-from-equilibrium solidification processes: from additive manufacturing to ice templating

Alain Karma

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This talk will discuss recent advances in phase-field modeling of microstructure development during alloy solidification concomitant with the breakdown of local thermodynamic equilibrium at the solid-liquid interface. For metallic alloys with atomically rough interfaces, breakdown of chemical equilibrium typically occurs at high interface velocity, a regime of renewed interest for additive manufacturing. Breakdown can also occur even at low velocity when a faceted phase grows with a large kinetic undercooling, as exemplified by freeze casting of porous polymeric or ceramic materials. Recently developed phase-field modeling approaches will be discussed that quantitatively model the departure from local equilibrium at a spatially diffuse rough or faceted interface while, at the same time, enabling simulations on experimentally relevant length and time scales. Selected large-scale simulation results will be presented to illustrate both quantitative comparisons with experimental observations and new insights into microstructural pattern formation during rapid solidification and ice templating. The talk will conclude with an outlook of future challenges for phase-field modeling.

In situ dynamics of directionally solidified irregular eutectic alloys

Sabine Bottin-Rousseau, Ashwin Shahani, Samira Mohagheghi, Melis Şerefoğlu, Kamal Sbargoud, Bumedijen Raka, Eliane Farhi, Georges Salloum-Abou-Jaoudé, Christine Nardin, Philippe Jarry and Silvere Akamatsu

Sorbonne University & CNRS (France); University of Michigan (USA); Istinye University (Turkey); Marmara University (Turkey)

Many eutectic alloys of significant industrial value solidify by forming irregular multiphased microstructures, often made of one (or several) faceted solid phase(s) such as silicon, graphite, or intermetallics, dispersed in a nonfaceted matrix (e.g., aluminum or austenite). In this talk, I will present an overview of experimental results obtained during in situ directional solidification of various faceted/non-faceted alloys in thin samples. Two kinds of real-time observation methods were employed, depending on the model system on focus, namely, optical microscopy and synchrotron X-ray nano-imaging. We studied first several two-phased binary alloys: (i) the AMPD-SCN transparent organic system, which offers the advantage of allowing a complete optical visualization of the interfaces, and (ii) the Al-Al3Ni and Al-Si eutectics, which are both model binary irregular eutectic alloys and closer to metallic systems of practical importance in a variety of applications. Surprisingly enough, we found striking similarities between all those alloys, in spite of their contrasting chemical nature. At very low solidification velocity (in the 1 μm/s range, or below), the growth is decoupled, and the faceted crystals grow ahead of the non-faceted solidification front with an inclination angle and a tip undercooling that depends on their orientation with respect to the main growth axis. This can lead to fibre-like, tubular or C-shaped patterns that are frequently found as frozen microstructures in many materials. When the velocity is increased, a transition from decoupled to (partly) coupled growth takes place involving mobile facets and/or non-crystallographic branching mechanisms. Importantly, the dynamic stability of the trijunctions is discussed based on the observations made with the transparent alloy. More specific features of the Al-Al3Ni and Al-Si alloys will also be presented. In the last part of the presentation, I will show some recent results on the three-phased Al–Si eutectic system (is an Fe-rich intermetallic) of concentration close to the nonvariant point in the Al-Si-Fe phase diagram. These fundamental results open the route towards laboratory studies aiming at a better understanding of the formation of irregular-eutectic microstructures of industrial aluminum-based alloys in the framework of the optimization of recycling.

Fast directional solidification enabling the design of novel alloys for additive manufacturing

Ulrike Hecht, Ivan Cazic, Niloofar Navaeilavasani and Parham Anvari

Access e.V. (Germany)

The economic benefits of additive manufacturing are substantial and diverse, offering manufacturers a competitive advantage through cost savings by reduced tooling requirements, accelerated product development and customized design, while also having positive environmental impact due to low amounts of material waste. After the disruptive onset, AM is now maturing, while remaining a strong innovation driver (http://epo.org/trends-3dp) providing advanced 3D printers, new lasers and more versatile software. The most fascinating asset however, remains the outreach to novel materials with truly unique microstructures and properties. We will review some of the most successful developments, featuring metallic alloys for Laser Powder Bed Fusion (LPBF). They take advantage of the fast directional solidification in the travelling melt pool and / or of texture manipulation through grain selection across neighboring melt pools. We will further account on two recent in-house developments which explore eutectic alloy systems, specifically in the hypo-eutectic alloy composition range, i.e. Ni-21Fe-19.6Cr-15.4Al (at. %) and Ni-32Co-28Cr-3.5Hf-0.25C (wt.%). For these alloys post-build heat treatments are the key step for microstructure control using as the starting point the unique and far-from equilibrium microstructure achieved during LPBF solidification.

Additive manufacturing of fully amorphous Fe-based metallic glasses for soft magnetics

María Teresa Pérez-Prado, Marcos Rodríguez, Saumya Sadanand, Amirhossein Ghavimi, Ralf Busch, Paola Tiberto, Enzo Ferrara, Gabriele Barrera, Lena Thorsson, Alexander Elsen and Isabella Gallino

IMDEA Materials (Spain); Saarland University (Germany); National Institute for Research in Metrology (Italy); Heraeus AMLOY (Germany); TU Berlin (Germany)

Advancing technologies that minimize energy losses in electric motors is key to decarbonize the transportation sector. The primary sources of these losses, which are electrical and magnetic in nature, arise from the relatively high coercivity of the silicon steel currently used to manufacture key components like rotors and stators. Additionally, conventional manufacturing techniques are incapable of producing parts with the intricate geometries needed to optimize magnetic field guidance. Fe-based metallic glasses (MGs) have extraordinary soft-magnetic properties, which greatly surpass those of silicon steel. However, their widespread commercial application is hindered by their low glass forming ability. The cooling rate needed to produce fully amorphous Fe-based MG specimens is in the order of 10^6 K/s, which limits the viable manufacturing routes to melt-spinning of thin ribbons, powder atomization, and suction casting of thin rods. Even though additive manufacturing methods, particularly laser powder bed fusion (LPBF), have recently shown promise for producing large MG components, Fe-based MG parts produced via LPBF so far exhibit glassy-crystalline composite microstructures due to unavoidable crystallization during solidification and thermal cycles from adjacent layer deposition. Moreover, these components are frequently plagued by cracks that must be addressed before large-scale commercialization is feasible. Achieving crack-free, high-density, fully amorphous Fe-based MG components with intricate geometries remains an unsolved challenge. This talk will review the state of the art on LPBF of Fe-based metallic glasses, highlighting potential avenues towards the solution to this outstanding problem.

Modeling assisted workflows for single-crystal Ni-based superalloy processing: Adaptations from Directional solidification to Additive

Swapnil Bhure, Divya Nalajala and Abhik Choudhury

Indian Institute of Science, Bengaluru (India)

Single crystalline Ni-base superalloys are employed as turbine blades in the high-pressure compressor stages of jet engines to increase the operating temperatures and thereby maximize efficiency. This endeavor entails metallurgical and production challenges, given the complicated design of the cooling channels and the variable geometries of a typical turbine blade. Given these challenges, additive manufacturing is a viable alternative as long as the parameters can be determined, which results in defect-free single-crystal production. In this talk, I will present a modeling-assisted workflow for determining the appropriate parameter space that involves a complimentary utilization of experiments and simulation studies. In this direction, a novel multi-physics model was formulated that can be used to simulate the thermal histories during the Direct energy deposition (DED) process. The thermal histories derived from the simulations are integrated with a Potts-based microstructure evolution model for a quick estimate of the grain structure that emerges during solidification. While the modeling framework allows for validating the experimental microstructures, it also enables the determination of the suitable parameter space. The results reveal that the epitaxial builds from single-crystal substrates can be achieved by controlling the shape of the solidification interface much in the same manner as in the classical Bridgman setup. The parameters that lead to flatter solidification interfaces directly lead to builds with the appropriate texture in the IN718/CMSX4 superalloys. These conditions change with the shape, size, and geometry of the part to be built, making it essential for prior feedback from simulation studies. Further, the simulations can also be utilized for programming the dynamic change of parameters during additive manufacturing, which is necessary for single-crystal manufacturing of complicated geometries.

Parallel sessions

Day 1 / Tuesday June 10, 2025

Session Tue-A-I / Microgravity I

The effect of fluid flow on microstructure evolution in Al-alloys within the framework of the ESA project MICAST

Sonja Steinbach, Laszlo Sturz, Gerhard Zimmermann, András Roósz, Zsolt Veres, Arnold Rónaföldi, Olga Budenkova, Sadik Dost, Gerd Ulrich Grün, Nils Warnken and Wim Sillekens

DLR - Institute of Materials Physics in Space (Germany); ACCESS e.V. (Germany); University of Miskolc (Hungary); Université Grenoble Alpes, SIMAP (France); University of Victoria (Canada); Speira GmbH (Germany); University of Birmingham (UK); ESA-ESTEC(Netherlands)

The ESA research program MICAST (Microstructure Formation in CASTing of Technical Alloys under Diffusive and Magnetically Controlled Convective Conditions) focuses on a systematic analysis of the effect of convection on microstructure evolution in cast Al-alloys. Questions are, for example, how intensity of convection and flow direction act on the evolution of the mushy zone, on macro- and micro-segregations, on dendrite morphology, on the growth mode and on spatial distribution of intermetallic precipitates. In order to simplify the complex interactions between heat and mass transport and microstructure evolution, the experiments performed by the MICAST team are carried out under well-defined thermally and magnetically controlled convective boundary conditions using directional solidification. They are analysed using advanced diagnostics and theoretical modelling, involving micro-modelling and global simulation of heat and mass transport. The MICAST team uses binary, ternary and technical (hypoeutectic, eutectic, hypereutectic) alloys of the industrially relevant AlSi cast alloys family (enriched with Fe and Mn). In the frame of the MICAST project solidification experiments were performed on the International Space Station in the ESA payload Materials Science Laboratory with a low gradient furnace (LGF) and a high(er) gradient one (solidification and quenching furnace SQF) to complement the scanning of a range of solidification times. The samples were directionally solidified under both purely diffusive and stimulated convective conditions induced by a rotating magnetic field. This contribution gives an overview on recent experimental results of MICAST Batch-3a Set1 and theoretical modelling of the MICAST team and gives an outlook for Batch-3a 2nd Set and the questions to be addressed with future experiments. Acknowledgements: The MICAST team gratefully acknowledges financial support by ESA under contract No. 14347/00/NL/SH within the ESA-MAP project MICAST' AO-99-031, CNES, DLR and the Hungarian Space Office. This work was supported by Speira GmbH (D), Inotal (HU), Alcoa-Köfém (HU) and Nemak (HU)

Analysis of Microgravity and Hypergravity Observations of Equiaxed Solidification of Al-Cu Alloys in Parabolic Flight Campaigns

Dudu Geng, Sinéad Uí Mhurchadha, David J. Browne and Andrew G. Murphy

South East Technological University (Ireland); University College Dublin (Ireland)

Understanding the solidification behavior of high-performance light metal alloys is pivotal for tailoring microstructures and achieving desired thermomechanical properties, which can be effectively predicted using advanced numerical solidification models. Gravity-induced thermosolutal natural convection apparent during solidification significantly influences grain growth, morphology, and chemical segregation within the microstructure. Sophisticated experimental validation is required to ensure the accuracy of simulation predictions. Real-time in-situ X-radiography has been used extensively to provide exceptional insight into solidification phenomena. Microgravity-based experiments eliminate the influence of gravity, providing diffusion-limited solidification conditions which can substantially reduce the complexity of mathematical models. This work presents analysis of microgravity and hypergravity solidification experiments performed on board the 58th and 60th ESA Parabolic Flight Campaigns, wherein g-level was varied from ~0.0 g to 1.8 g at various stages of solidification. A Bridgman-type gradient furnace (XRMON-GF) was used to melt and solidify grain-refined Al-20wt.%Cu alloy test specimens and in-situ X-ray diagnostic equipment used to record the equiaxed solidification in real time. Equiaxed grains nucleated in microgravity were observed to oscillate in the field-of-view (FOV) in synchronization with g-level fluctuations. Relative grain position was maintained with grain growth slowing due to the interaction of advancing solute fields surrounding each equiaxed grain (soft impingement). Once hypergravity was established the semi-solid mush moved rapidly downwards in the FOV causing the equiaxed crystals to impinge on each other. The hard impingement of the equiaxed grains on each other, as well as the crucible wall, prevented any further primary phase growth, with the remainder of the phase transformation being related to coarsening. The results of this experimental analysis are currently being used to develop a multiscale solidification model that can be used to predict the influence of g-level variation on microstructural evolution, which has applications in both terrestrial and space-based liquid metal processing.

Determination of the effect of convections and Fe-containing intermetallic phases on the permeability of technical aluminum alloys

Golo Zimmermann, Sonja Steinbach and Florian Kargl

RWTH Aachen University (Germany); Deutsches Zentrum für Luft- und Raumfahrt, DLR (Germany)

In this work the effect of convections and the precipitation of Fe-containing phases on the permeability of directionally solidified technical aluminum alloys is investigated. Samples from Al-Si 6 wt.%-Cu 4 wt.% alloys with an addition of 1 wt.% or 2 wt.% Fe were processed in microgravity on the International Space Station in the Materials Science Laboratory using the LFG furnace. Purely diffusive mass transport conditions and forced melt flow conditions induced by a rotating magnetic field were studied. The fully solidified rod-samples were non-destructively analyzed by X-ray computed tomography (CT) and on sections of the samples using conventional light microscopy. From the obtained 3D and 2D images microstructure parameters like the primary dendrite spacing were obtained and based on these static structures the permeability of the interdendritic space was calculated. The focus of the investigation was on the interplay of the 3D-network formed by AlFeSi-phases in the interdendritic space and its impact on the permeability of the dendritic network due to changes in the solidification sequence and the volume of the intermetallic phases. Further, we show results of a correlation analysis of the shape parameters and the volume fractions with the permeability. This work contributes to a better understanding of the solidification process of Fe-containing intermetallic phases in technical aluminum-based casting alloys through the investigation of the influence of high iron content on their castability.

Mesoscale Front Tracking Simulation of a Microgravity-based Near-Isothermal Equiaxed Solidification Experiment of an Al-20wt/%Cu Alloy performed on board the MASER 13 Sounding Rocket

Andrew Murphy and David Browne

South East Technological University (ireland); University College Dublin (Ireland)

The ability to accurately predict microstructural evolution in response to metallic alloy composition and thermal processing parameters is of critical importance in preventing defects and maximising sustainability in advanced liquid metal processing manufacturing, e.g., casting, welding, and additive manufacturing. Sophisticated solidification models are used widely in industry to optimise mould designs and processing parameters. To ensure validity of simulation predictions, similarly sophisticated solidification experiments are required. Since its development, real-time in situ X-ray radiography of solidification has become the benchmark for solidification experimentation, providing significant insight into nucleation, primary phase evolution, solutal rejection, soft and hard impingement, and isothermal transformations. The compact nature of lab-based X-ray diagnostic equipment and solidification furnaces has further resulted in metal alloy solidification being observed in real time under microgravity conditions. One such experiment was performed on board the MASER 13 sounding rocket showing, for the first time, near-isothermal equiaxed solidification Al-Cu alloy in microgravity. In this work, mesoscale Front Tracking (FT) was used to simulate the near-isothermal solidification of a grain refined Al-20wt.% alloy performed in microgravity on board the MASER 13 sounding rocket. Experimental data was used to initialise the FT algorithm with grain envelope development predicted based on the applied cooling rate. Latent heat release during solidification was shown to have a negligible impact on solidification overall, owing to the small volume of metal and the relatively low cooling rate. Soft impingement, i.e., solutal awareness, of neighbouring grains was shown to be the dominant mode of primary dendrite growth restriction and inoculant particle poisoning.

Structures in grain-refined directionally solidified hypoeutectic Al-Cu alloys: Benchmark experiments under microgravity on-board the International Space Station

Laszlo Sturz, Gerhard Zimmermann, Christoph Pickmann, Elke Schaberger-Zimmermann, Andras Roósz, Arnold Ronaföldi, Zsolt Veres, Charles-André Gandin, Guillaume Reinhart, Henri Nguyen-Thi, Nathalie Mangelinck-Noël, Shaun McFadden, Gerd-Ulrich Grün and Wilhelmus Sillekens

Access e.V. (Germany); RWTH Aachen (Germany); University of Miskolc (Hungary); Mines Paris PSL & CNRS, CEMEF (France); Aix Marseille Univ. & CNRS, IM2NP (France); Ulster University (UK); Speira GmbH (Germany); European Space Agency ESTEC (Netherlands)

Benchmark solidification experiments were successfully performed under microgravity conditions on-board the International Space Station (ISS) within the ESA programme CETSOL (Columnar-to-Equiaxed Transition in SOLidification Processing). Cylindrical samples of grain-refined Al-4wt.%Cu, Al-10wt.%Cu and Al-20wt.%Cu alloys were directionally solidified in a gradient furnace to investigate columnar and equiaxed dendritic growth structures, as well as the columnar to equiaxed transition under diffusive conditions. The determination of temperature gradients; interface velocities; and cooling rates at liquidus, solidus, and eutectic front positions provides well-defined thermal experimental characterization. The evaluation of these Batch-3 flight samples demonstrates that no significant macrosegregation along the sample axis occurred and no radial effects were observed. Therefore, purely diffusive solidification behaviour without any residual melt convection can be assumed for these microgravity experiments. The analyses of the microstructure in longitudinal cross-sections show dendritic structures without any pore formation and the averaged eutectic fraction is largely constant along the sample. The samples of refined Al-4wt.%Cu alloy show a sharp CET from columnar dendrites to a fine equiaxed steady-state grain structure whereas in the samples of refined Al-10wt.%Cu and Al-20wt.%Cu alloy, only equiaxed dendritic grain growth is observed. A quantitative analysis of the equiaxed grain morphology shows, that the shapes of the equiaxed dendrites depend on the applied temperature gradient, but the grain sizes in radial and longitudinal directions are identical. Therefore, a fully equiaxed dendritic growth structure without dendrite elongation was obtained. Compared to experiments in microgravity with non-refined Al-Cu alloys the average equiaxed grain size is about three times smaller.

Comparison of the grain structure of grain refined hypoeutectic Al-Cu alloys directionally solidified on ground base (1g) and under microgravity on board the International Space Station

András Roósz, Arnold Rónaföldi, Zsolt Veres, Maria Svéda, Laszlo Sturz, Christoph Pickmann, Elke Schaberger-Zimmermann, Charles-André Gandin, Guillaume Reinhart, Henri Nguyen-Thi, Nathalie Mangelinck-Noël, Shaun McFadden, Gerd-Ulrich Grün, Wim Sillekens and Gerhard Zimmermann

University of Miskolc (Hungary); HUN-REN-ME Materials Science Research Group (Hungary); ACCESS e.V. (Germany); RWTH Aachen University (Germany); Mines Paris PSL & CNRS, CEMEF (France); Aix Marseille Univ. & CNRS, IM2NP(France); Ulster University (UK); Speira GmbH (Germany); European Space Agency ESTEC (Netherlands)

One of the aims of solidification experiments in microgravity environments is to investigate the effect of melt flow on the solidified microstructure by comparing their results with those of terrestrial (1g) and forced flow experiments. Within the ESA programme CETSOL (Columnar-to-Equiaxed Transition in SOLidification Processing) cylindrical samples of grain-refined Al-4wt.%Cu, Al-10wt.%Cu and Al-20wt.%Cu alloys were directionally solidified in a gradient furnace to investigate columnar and equiaxed dendritic growth structures, as well as the columnar to equiaxed transition under diffusive conditions (0g samples). In the laboratory of Miskolc University, these experiments were reproduced under similar solidification parameters (temperature gradient, solid/liquid front velocity, Rotation Magnetic Field induction). The grain structure, amount of eutectic, secondary dendrite arm spacing and macrosegregation were investigated and compared with the results of 0g samples. The grain structure of Al-4 %Cu alloy is similar in the three samples (0g, 1g, RMF), after a columnar structure fine equiaxed structure formed. The grain structure of the Al-10 wt% and 20wt%Cu was equiaxed in all samples, but in the Al-20wt% Cu alloy, both 1g and RMF samples strong macrosegregation was formed.

Sessions Tue-A-II & Tue-A-III / Special Symposium in memory of Markus Rettenmayr

Stability of solidification fronts and formation of two-phase mushy zone

Peter Galenko and Stephanie Lippmann

University of Jena (Germany)

An overview on recent developments in stability of solidification fronts in undercooled liquids as well as during the directional solidification of alloys controlled by heat and mass-transport is presented. The discussion focuses on (i) the impact of convective and conductive boundary conditions on the stability of solid-liquid interfaces, (ii) an appearance of cellular and dendritic crystals with the formation of the two-phase mushy zone, (iii) crystals nucleation ahead of the mushy zone, and (iv) the analysis of theoretically predicted and experimentally measured kinetic relationships for the morphologically selected crystal scales / interface velocities / thermal gradients / undercooling. Theoretical predictions are used for interpretation of experimentally observed propagation of the recalescence fronts in droplets solidified in electromagnetic levitation facility (EML) on the Ground, under reduced gravity during parabolic flights, and in microgravity conditions onboard the International Space Station.

Meshless methods for multiphase, multiphysics and multiscale problems

Božidar Šarler, Izaz Ali, Tadej Dobravec, Umut Hanoglu, Qingguo Liu, Boštjan Mavrič, Katarina Mramor and Gašper Vuga

University of Ljubljana (Slovenia)

This paper presents an overview of the progress of meshless methods used in metallurgical process models developed in the last two decades. The models encircle melting in an alloying furnace to solidification in different casting techniques, reheating and heat treatment furnaces to rolling, and controlled cooling. The overview is divided into fluid dynamics and solid dynamics developments. The fluid dynamics models range from simple laminar flow models to non-Newtonian models and large-eddy turbulence simulations. The solid mechanics models range from simple elastic to highly non-linear elastic-visco-plastic models and crack propagation. The multiscale models range from phase-field and point automata models to macroscopic models and reduced models for automating the production process steps. The inclusion of external field influences like electrohydrodynamics and acoustofluidics is outlined. The common future of the listed models is a direct strong-form formulation of the governing equations and approximation of the involved fields on differently constructed overlapping subdomains by polynomial-augmented radial basis shape functions or fundamental solutions. The approximation can range from collocation and weighted least squares to moving least squares. The order of shape functions, subdomain size, and quadtree and octree manipulations can influence accuracy and efficiency. The advantage of the presented numerical technique is basically the same node generation, refinement, and de-refinement manipulations in two or three dimensions, as well as simple numerical implementation that does not require any space integration. The listed meshless method elements are shown on a spectrum of industrial liquid-solid phase-change problems. The existing research gaps and the direction of future developments are outlined.

Solutal Melting

Julien Zollinger and Benoît Appolaire

Université de Lorraine, CNRS, IJL (France)

Markus Rettenmayr have performed a pioneering work on solutal melting since the early 2000's based on both experiments and numerical modeling. It has triggered the work that will be presented here, started 10 years later with many interactions with Markus over the years. First some experimental results on solutal melting will be presented on the Cu-Ni and Ag-Au systems, revealing some unusual behaviour of the solid/liquid interface. A model will be presented to give better insight on the melting kinetics and interface properties. Finally, open questions and prospects will be given.

A X-ray view on solutal melting in Cu-Pd

Nagarjuna Remalli, Julien Zollinger and Florian Kargl

Institute of Materials Physics in Space, German Aerospace Center, DLR (Germany); Université de Lorraine, Institut Jean Lamour (France)

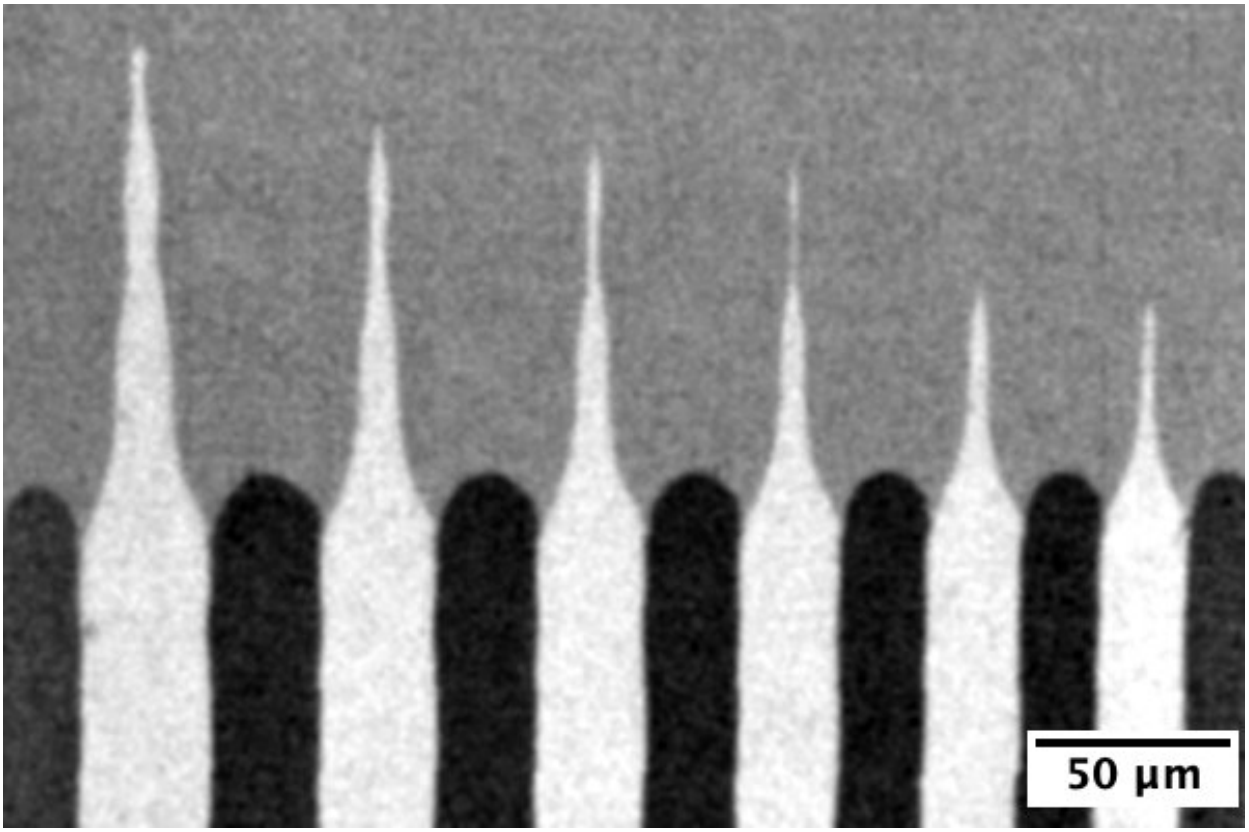
We present solute-driven, i.e. solutal melting, experiments on isomorphous Cu-Pd melting couples to better understand the kinetics of the solid-liquid (s-l) interface evolution. In-situ monitoring of the melting process with a sub-second time-resolution by X-radiography (XRR) is key to identify the evolution of the concentration fields during the process. The samples used, were concentric. They have been fabricated by casting Cu into a BN-coated steel-mold under an inert Argon atmosphere. The mold contained a short 3 mm diameter Pd-rod at its center around which the Cu did freeze. For the XRR experiments thin samples of 200 µm and 500 µm thickness, respectively were manufactured by slicing 1 mm discs from the as-cast Cu-Pd rod and grinding. The samples have been processed in an isothermal furnace by rapid heating with approximately 19.5 °C/min followed by annealing at holding temperatures slightly above the melting point of Cu (1085 °C) but far below the melting point of Pd (1555 °C). Consequently, the thermally melted liquid Cu was in contact with solid Pd. Since the liquid and solid compositions at the s-l interface were out of equilibrium, solutal melting of Pd was uniformly observed in real-time. At the same time fast diffusion of Cu into solid Pd was observed. We compare our data with observations made on Cu-Ni and Ag-Au isomorphous systems and solutal melting experiments. In our study particular attention was paid to the effect of temperature and specimen height on the s-l interface velocity. Furthermore, post-mortem analysis was performed using SEM to investigate the radial composition gradients of Cu in the re-solidified Cu-Pd alloy for comparison with the in-situ measurement results and to serve for calibration of the real-time experiments.

Real-time Investigation of Melting Dynamics in Two-Phase Eutectics

Ayşe Ecem Yürük, Didem Kaplan, Gizem Doğan, Endercan Süslü and Melis Şerefoğlu

Marmara University (Turkey)

The dynamics of melting remain significantly less understood than those of solidification in eutectic systems. With the advent of additive manufacturing, the importance of understanding melting phenomena has become increasingly evident. While controlled solidification of a homogeneous liquid can produce intricate microstructures, the challenge intensifies when dealing with non-homogeneous liquids formed due to melting kinetics and subsequent (re)solidification. Furthermore, in industrial multicomponent, multiphase alloys, the cyclic melting and solidification processes lead to even more complex microstructures. These can only be comprehended through fundamental scientific investigations involving highly controlled, systematic, and model experiments. This study investigates the melting dynamics of the In-Bi eutectic system in real time using a Bridgman-type directional solidification and melting setup. Eutectic microstructures with varying spacings and crystal/crystal interphase anisotropy are melted at different velocities to quantitatively examine the effects of eutectic spacing, phase width, anisotropy, and velocity on melting behavior. The study reports various melting morphologies and intriguing instabilities, including oscillatory behaviors.



In situ directional melting of eutectic microstructures in transparent alloys

Silvere Akamatsu, Kamal Sbargoud, Bumedijen Raka and Sabine Bottin-Rousseau
Sorbonne University & CNRS (France)

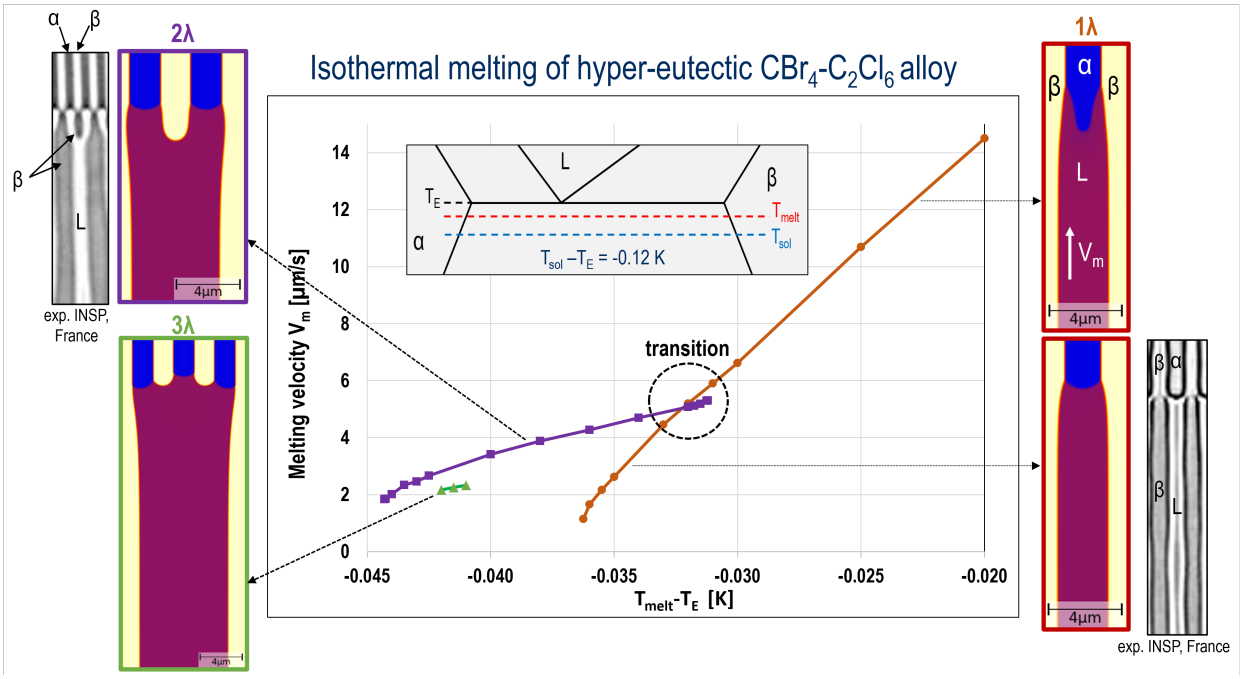
In contrast to the dynamics of eutectic solidification, little is known on the reverse process: eutectic melting. In an attempt to fill this knowledge gap, and contribute to a fundamental understanding of multiphase melting/solidification processes that are at play in novel material elaboration techniques, we endeavoured an in situ experimental study of the directional melting of eutectic microstructures in model transparent alloys. This permits the optical observation of the solid-liquid interface in real time. In the experiments, a regular lamellar microstructure is first created by directional solidification, with an average interphase spacing that is determined, at least in order of magnitude, by the solidification velocity. The thus frozen microstructure is melted by reversing the motion of the sample in the temperature field. Our observations actually reveal a complex sensitivity of the eutectic melting dynamics on the alloy concentration, the melting velocity, and the interphase spacing. A discussion will be initiated on the basis of a comparison with recent numerical simulations.

Phase-field simulations of eutectic melting

Rahul Nellissery Rajan and Guillaume Boussinot

Access e.V. (Germany)

In the recent years, the development of additive manufacturing techniques has renewed the attention paid by scientists to the melting phenomenon. Fundamental questions relative to the melting kinetics in alloys, particularly in eutectic systems, are less understood than for solidification. Using the multi-phase-field software MICRESS, we investigate pattern formation during the melting of the initially solidified structure of a hyper eutectic alloy. Directional melting simulations were performed under Bridgman conditions at various velocities and were complemented by simulations under isothermal conditions. The simulation results demonstrate a good agreement with recent experiments, providing insights into the melting dynamics in eutectic systems.

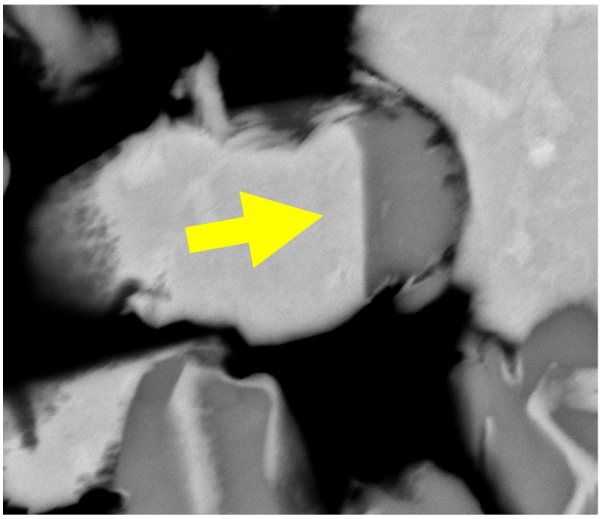


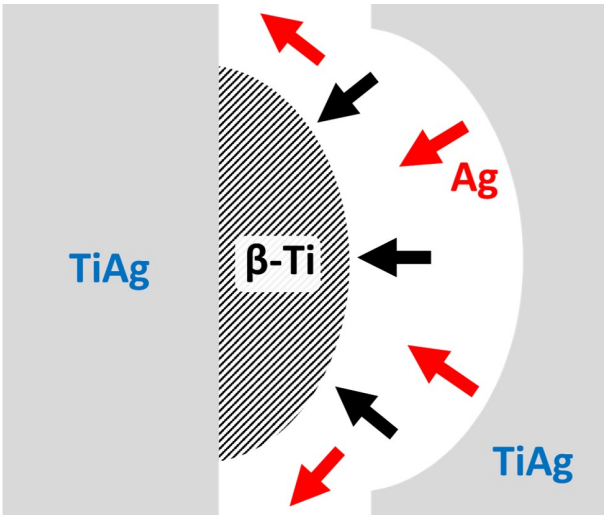
Formation mechanism of bicontinuous structure during peritectic melting of TiAg

Zhongyang Li, Lukas Lührs, Tobias Krekeler and Jörg Weissmüller

Hamburg University of Technology (Germany); Helmholtz-Zentrum Hereon (Germany)

Fine-scale porous or bicontinuous microstructures may be prepared by liquid-metal dealloying (LMD). Reverse peritectic reactions, and specifically the peritectic melting of TiAg, have been proposed as dealloying-like processes that produce quite similar microstructures but avoid the restrictions on sample size inherent in LMD. Here, studies of the microstructure evolution during peritectic melting of TiAg suggest a formation mechanism that is not LMD-like but rather relies on the migration of liquid films. The process starts with wetting of the TiAg grain boundaries by the alloy melt. Successively, both Ti and Ag continue to dissolve from one side of, while β-Ti deposits on the other side and the liquid film sweeps the pristine TiAg crystal. TiAg-Ti interfaces with well-defined orientation relationship and with concentration gradients support this picture, as does the phase morphology in partly decomposed samples. The process generates a bicontinuous structure with a solid Ti skeleton, interpenetrated by the Ag-rich melt, which is conserved even after coarsening. Upon quenching, the Ti phase transforms to α-Ti. This study clarifies the mechanism of peritectic melting in TiAg, and it may provide a basis for identifying other alloy systems suitable for producing bicontinuous microstructures by that process.





Session Tue-B-I / Facetted interfaces and intermetallics

Phase-field modeling of dendritic growth in crystals with strongly anisotropic surface free energies

Enugala Sumanth Nani, Thomas Philippe and Mathis Plapp

Tata Institute of Fundamental Research, Bangalore (India); CNRS & Ecole Polytechnique, PMC (France)

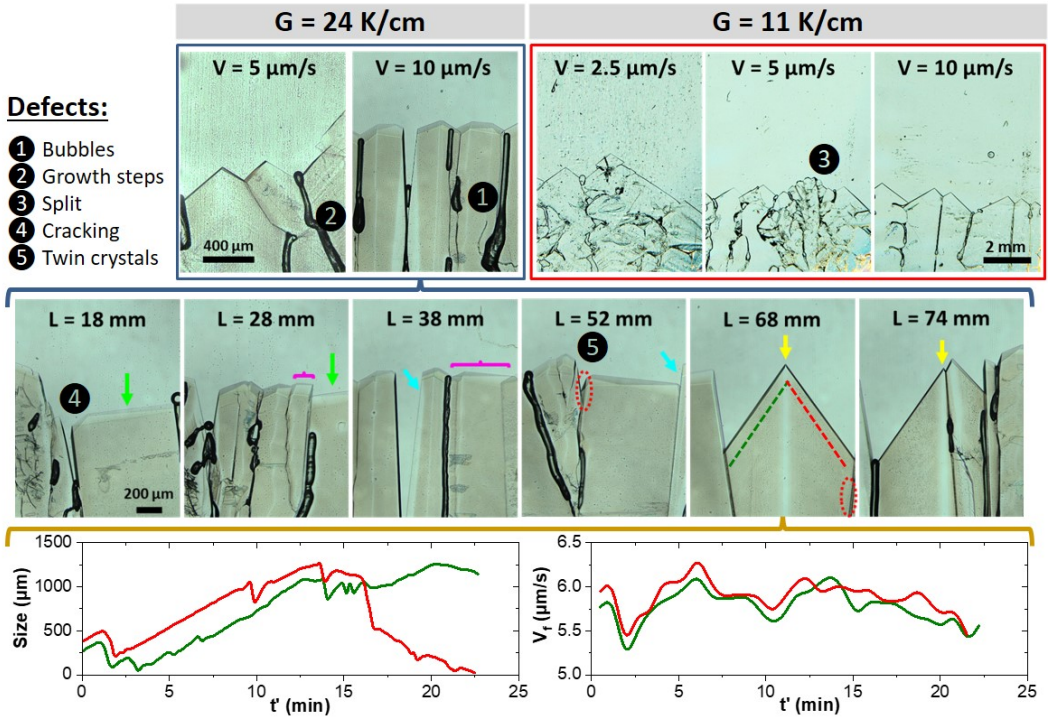
Dendritic crystals form in many different substances when growth is limited by diffusion. For dendritic monocrystals, the directions of the main branches are determined by the anisotropy of the surface free energy, which is linked to the crystallographic structure. A well-developed theory for dendritic growth is available for small and smooth interfacial anisotropy. For strongly anisotropic interfaces, two different types of singularities of the equilibrium crystal shape can occur: facets and missing orientations. A facet is linked to the presence of a cusp-like local minimum in the polar plot of the surface energy. For missing orientations, the interface stiffness is negative, so that interfaces with this orientation are thermodynamically unstable against a capillary wrinkling instability and do not occur on the equilibrium crystal shape. The latter then exhibits sharp corners. We study crystal growth with missing orientations using a newly developed phase-field model, in which the corners are rounded by a Willmore regularization of the free energy, which introduces an energy penalty proportional to the square of the interface curvature. We show that, for a standard anisotropy function with cubic symmetry, we can simulate dendritic growth for arbitrary anisotropy strength. Three regimes can be distinguished: (i) for low anisotropy, the model reproduces the known growth laws, with an increase of the growth velocity for increasing anisotropy, (ii) this increase continues beyond the critical anisotropy value for corner formation, but then levels off for even stronger anisotropies, and a wrinkling instability occurs on the flanks of the dendrite trunk. Finally, (iii) the growth velocity starts to decrease with increasing anisotropy, and becomes oscillatory. This is due to a feedback of the wrinkling instability on the dendrite tip operating state.

Facet growth and defect dynamics during the solidification of pure salol

Anassya Raad, Nathalie Bergeon, Nathalie Mangelinck-Noël and Fatima Mota

Aix Marseille University & CNRS, IM2NP (France)

During solidification from the melt, the solid-liquid interface morphology depends on the material physical parameters and processing parameters. It is all the more important to characterize this interface as it plays a critical role in defining the final material properties. With this objective, directional solidification is highly effective as it allows precise control of process parameters. Faceted interfaces at the macroscopic scale are a typical interface morphology generated during solidification of many materials like semiconductors, quasicrystals, etc In this case, the atoms attachment from the liquid at the interface is anisotropic and slow, and its effect is dominant during growth. Crystals exhibit then smooth surfaces at the atomic scale. A clear understanding of the faceted morphology dynamics remains a challenge and requires key information that could only brought by in situ and real time observation of the process. In this work, focusing on achieving advances in the analysis of mechanisms involved during faceted interfaces growth, directional solidification experiments of an organic transparent material are used. We will report results obtained with pure salol that is orthorhombic in structure and grows from its melt with a marked macroscopic faceted interface because of its high degree of anisotropy. The experiments were carried out in a Bridgman-type furnace designed for thin rectangular samples, equipped with an optical microscope to observe solid-liquid interface dynamics in situ and real time. A series of experiments were performed with different thermal gradients and pulling velocities, which all display a highly faceted solid-liquid interface. Some of the most striking results regarding the facet growth dynamics will be presented. Defects, such as bubbles, growth steps or cracks, arise very frequently and their origin and time evolution will be detailed. The relationship between the facet velocity, its crystallographic nature and the undercooling will also be explored.

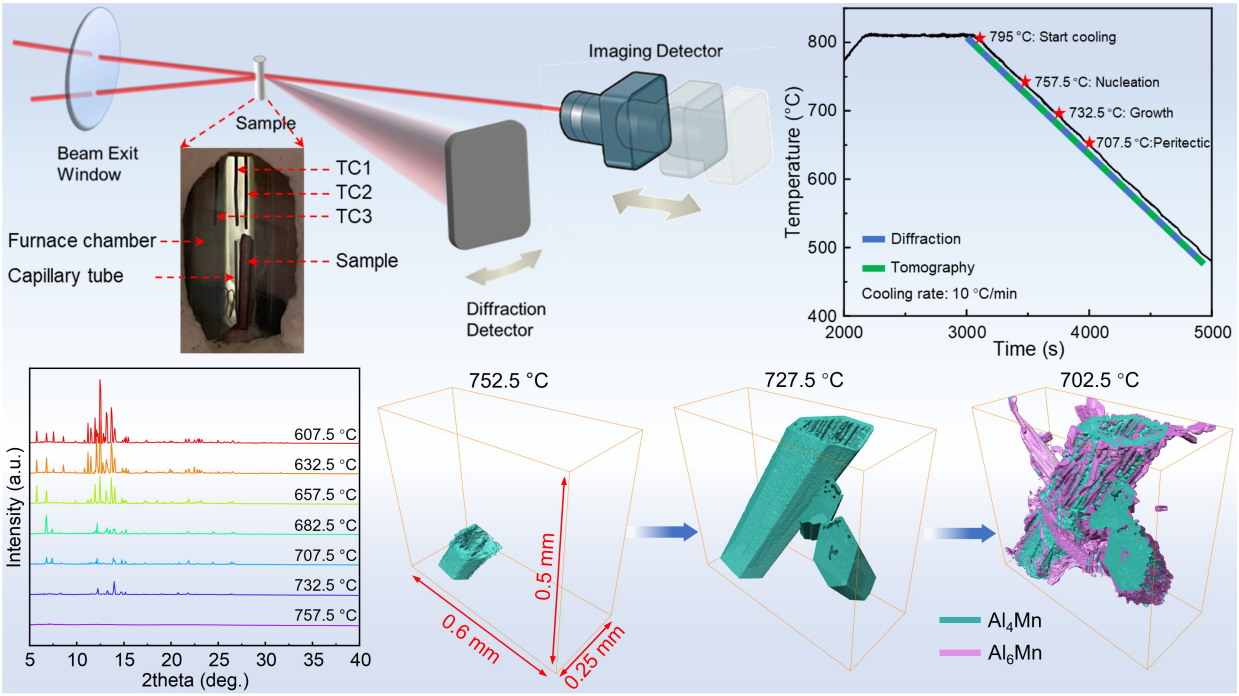


Operando study of the nucleation and co-growth dynamics of multiple intermetallic phases in solidification of Al-Mn alloys by simultaneous synchrotron X-ray diffraction and tomography

Kang Xiang, Shi Huang, Yueyuan Wang, Alberto Leonardi, Sharif Ahmed, Mohsen Danaie, Matthew Spink, Michal Klosowski, Mengnie Li and Jiawei Mi

University of Hull (UK); Diamond Light Source (UK); Research Complex at Harwell (UK); Kunming University of Science and Technology (China)

In most metal alloys, nm and/or μm intermetallic compounds (or phases) are often formed in the solidification and/or solid-state phase transformation processes. Controlling the chemistry, structure, size, morphology and distribution of the intermetallics in an alloy is the most important strategy to achieve the desired structural and functional properties. In this study, we focused on studying, in real-time and in operando conditions, the nucleation and co-growth dynamics of multiple intermetallic phases of Al-Mn based alloys through the peritectic and eutectic reactions during the solidification process. We used synchrotron X-ray dual imaging tomography and diffraction technique available at DIAD beamline of the Diamond Light Source, UK for the study. We have collected ~30 TB data via quasi-simultaneous diffraction and tomography operations. Through comprehensive data analyses, we have revealed and elucidated the nucleation ang growth dynamics of the multiple Al-Mn intermetallic phases. In particular, how the nucleated Al4Mn phases grew into hexagonal prism shape and transformed into orthorhombic Al6Mn phases with complicated cauliflower morphology though peritectic reaction. Combined with Scanning Transmission Electron Microscopy (STEM) and Electron Back Scattered Diffraction (EBSD), we have revealed for the first time the co-growth behaviour and the orientation relationship across the interface between the Al4Mn and Al6Mn phases. Possible strategies of how to tailor and control the multiphases growth dynamics to achieve the desired size and morphology were also discussed in detail.



Nucleation and growth of Al-Mn intermetallics in the solidification sequence of Mg-Al-Mn alloys

Chris Gourlay, Di Wang and Guang Zeng

Imperial College London (UK); Central South University (China)

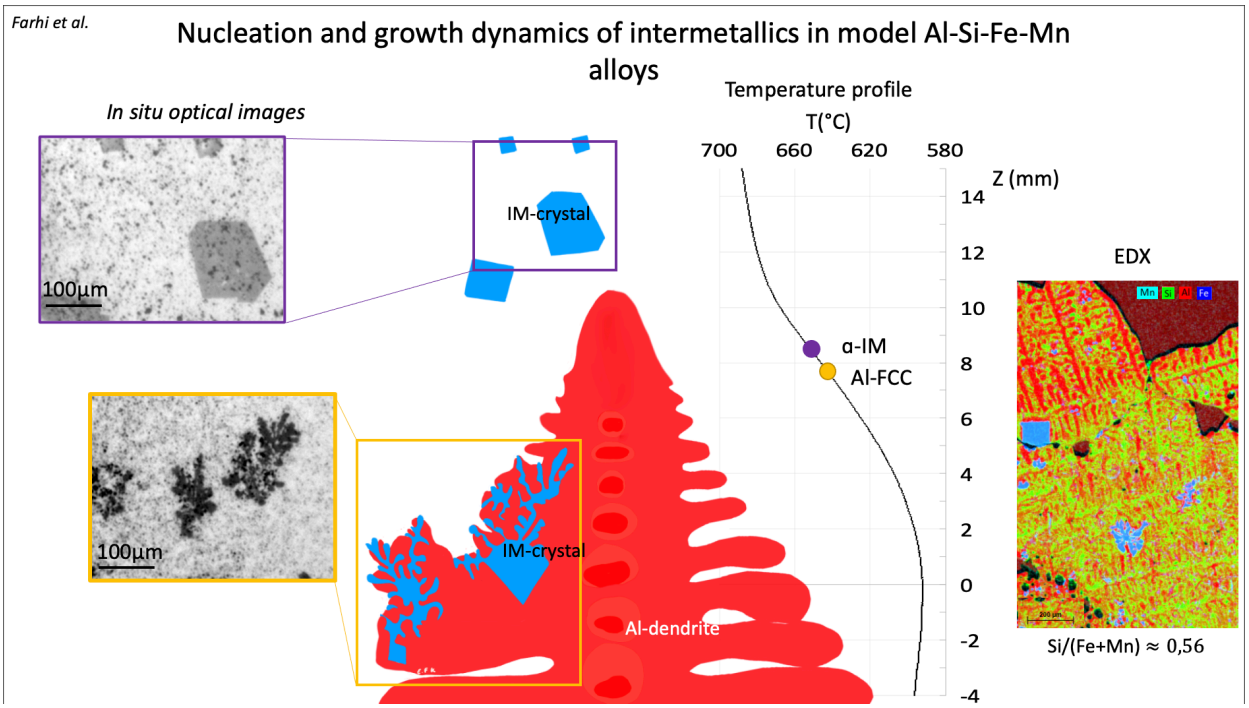
Most Mg-Al-based alloys also contain manganese to control corrosion resulting multicomponent alloys. The Mn addition causes a range on Al-Mn intermetallic compounds to form during solidification in a variety of solidification reactions that are rarely considered in detail. This presentation will overview research on the competitive nucleation and growth of Al-Mn intermetallics throughout the solidification sequence of Mg-9Al-0.7Zn-xMn alloys. We combine electron microscopy of the faceted growth crystallography with in-situ synchrotron X-ray imaging of the nucleation and growth dynamics of the Al-Mn particles. New insights will be presented into the factors affecting the faceted growth shape of Al8Mn5 and divorced eutectic solidification in this system, including interactions between α-Mg dendrites and Al8Mn5 faceted particles during their simultaneous but divorced growth.

Nucleation and growth dynamics of intermetallics in model Al-Si-Fe-Mn alloys

Eliane Farhi, Georges Salloum-Abou-Jaoude, Silvère Akamatsu, Philippe Jarry, Kamal Sbargoud, Bumedijen Raka, Christine Nardin and Sabine Bottin-Rousseau

Sorbonne University & CNRS, INSP (France); Constellium C-TEC (France)

Improving the recyclability of aluminum requires designing alloys that are more tolerant to Fe and Si impurities. Higher impurity concentrations result in an increased volume fraction of Al-Fe-Si intermetallics (IMs) formed during solidification, detrimental to formability properties of alloys. While the nature of IMs can be classified and distinguished by their morphologies and chemistry, our understanding of the physical phenomena governing the nucleation and growth of Al-Fe-Si IMs remains limited due to the lack of direct observations; and research on high recycled content alloys is still ongoing. This study presents an in situ experimental analysis of Al-Fe-Si-Mn model alloys based on the 6XXX series Al-alloys, utilizing directional solidification combined with real-time optical observations in thin-samples. These experiments capture the nucleation and growth of IM crystals under well-controlled solidification parameters. Chemical (EDX) and crystallographic (EBSD) analyses identify the different IM phases predicted by thermodynamic models and determine their orientations. For the first time, we provide direct evidence of distinct growth behaviors, demonstrating how solidification speed influences the solidification dynamics. Furthermore, we document a morphological transition from faceted polyhedral primary Fe-IM crystals in the liquid to coupled FCC-Al/Fe-IM growth in these alloys.

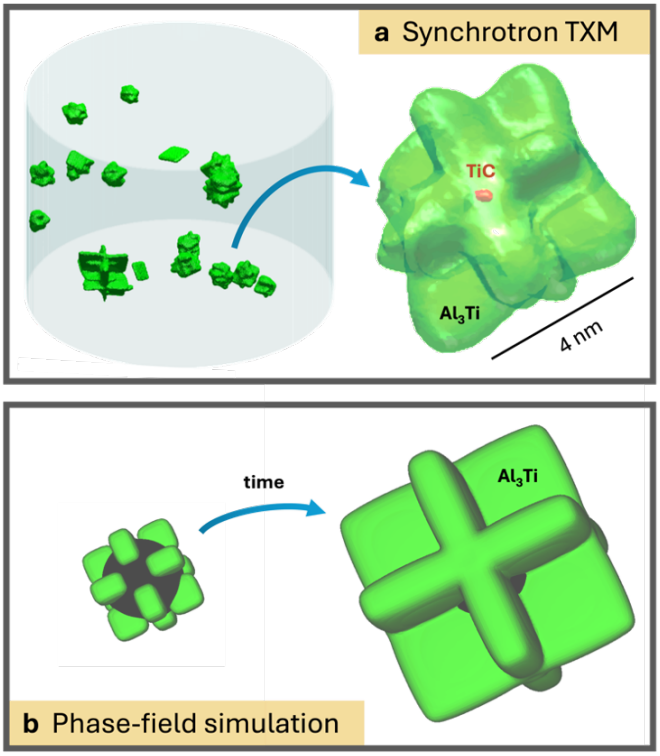


Capturing microstructure and its evolution in metal matrix nanocomposites

Ashwin J. Shahani

University of Michigan (USA)

Aluminum (Al)-based alloys are widely employed in automotive, aerospace, and defense applications due to their high strength-to-weight ratio, low cost, and excellent machinability. However, their mechanical properties deteriorate at elevated temperatures, limiting their use in high-temperature environments. One promising solution is the development of Al-based metal matrix nanocomposites (MMNCs) mixtures of Al and nanoscale reinforcements which offer enhanced mechanical properties at both ambient and elevated temperatures without sacrificing the lightweight benefits of Al. Despite this promise, critical gaps remain in our understanding of (i) how nanoparticles form in the Al melt, and (ii) how they interact with secondary phases during solidification. To address these fundamental questions, we investigate in unprecedented detail the formation mechanisms, morphologies, and microstructures of an Al/TiC MMNC produced via salt flux reaction. By integrating synchrotron-based X-ray nanotomography (TXM) with scanning and transmission electron microscopy, we visualize in over five orders-of-magnitude of length-scale the TiC nanoparticles, Al3Ti intermetallics, and their co-locations. Three-dimensional reconstructions from TXM reveal a surprising diversity of intermetallic morphologies including an orthogonal plate structure. Combining our experimental observations with phase-field simulations, we demonstrate that this exotic growth form arises when Al3Ti nucleates epitaxially on a TiC particle that is larger a critical size at a given undercooling. Yet the smaller TiC particles, which cannot independently nucleate Al3Ti, still influence intermetallic growth by splitting intermetallic plates during solidification. These insights into the dual effects of TiC nanoparticles on intermetallic nucleation and growth offer guidelines on microstructure control in MMNCs.



Tue-B-II / Machine Learning

Porosity prediction in investment casting parts using simulation and machine learning

Juergen Jakumeit, Youness Bami, Thomas Bähr, Gongyuan Zheng, Romuald Laqua, Sayan Chatteryjee, Chris Nicolae and Jan Schievenbusch

Access e.V. (Germany)

Microporosity in investment castings is difficult to avoid and limits the mechanical properties and fatigue behaviour of critical parts such as turbine blades. Its presence can lead to increased rejection rates and reduced component lifespans, and greater inspection requirements during operation. Traditional methods to minimize microporosity through casting trials are both time-consuming and expensive. Numerical simulations are increasingly used to accelerate the development process. However, the prolonged simulation times restrict the number of parameter configurations that can be affordably explored, thereby limiting their utility in optimization loops. In this paper, the combination of process and simulated data is used to achieve a fast prediction of microporosity adapted to material and process using machine learning (ML) methods. This approach enables three objectives: the calibration of microporosity criteria for a specific alloy and application, the derivation of new correlations between the temperature field and microporosity and the rapid estimation of microporosity based on process and material parameters. The differences between process and simulation data are a challenge: While in simulation the 3D porosity distribution is estimated using criteria functions (Niyama) based on physical models and their parameters, process data is often 2D (X-ray images and micrographs, 3D from CT) and represented by a grey or colour pattern that must be transferred into a 3D porosity distribution. ML methods from image recognition can be successfully used to close this gap between process and simulation data. The methodology was applied to a complex test bar assembly. Several casting trials were combined with the simulation of the full assembly and fast simulations of test bars to generate sufficient data for the training of ML-models. The results demonstrate that the integration of this ML approach into the casting development process led to a significant increase in efficiency and reduced number of costly casting trials.

Comparison of image analysis techniques based on deep learning for the solidification microstructure in different alloys

Alexandre Viardin, Angelos Theofilatos, Christoph Pickmann and Laszlo Sturz

Access e.V. (Germany)

This work explores advanced image analysis techniques applied to the study of solidification and microstructure in different distinct alloy systems: technical aluminum alloys and optically transparent model alloys. For aluminum alloys, Mask R-CNN is employed to detect, classify, and quantify Fe-containing intermetallic phases in alloys such as AlSi6Cu4Fe1 and AlSi6Cu4Fe2. Additionally, it is used to delineate strongly connected dendrites in serial sections of 3D CT images from AlCu alloys. For both cases, a 3D algorithm is proposed for reconstructing 3D microstructures, utilizing phase field simulations and traditional dataset preparation methods. In parallel, Faster R-CNN is applied to optically transparent alloys to automate the detection of dendritic growth under experimental conditions. Phase field simulations generate highly accurate datasets for training, enabling the algorithm in identifying loosely connected dendrites, particularly in microgravity and terrestrial environments where optical overlap challenges traditional methods. In the case of terrestrial gravity conditions, tracking methods are integrated to enhance the analysis. By merging deep learning methodologies with traditional image analysis, this work delivers new perspectives on microstructural evolution during solidification, offering a robust framework for the automated analysis of both 2D and 3D microstructures across diverse alloy systems. Acknowledgments: The authors thank financial support in the projects KICK-G and KIMi (BMWK/DLR projects under contracts 50WM2050 and 50WM2356B).

Neural Network Approximation of a Phase-Field Model for Dendritic Growth

Chih-Kang Huang, Ludovick Gagnon, Benoît Appolaire and Miha Založnik

Université de Lorraine, CNRS, IJL (France)

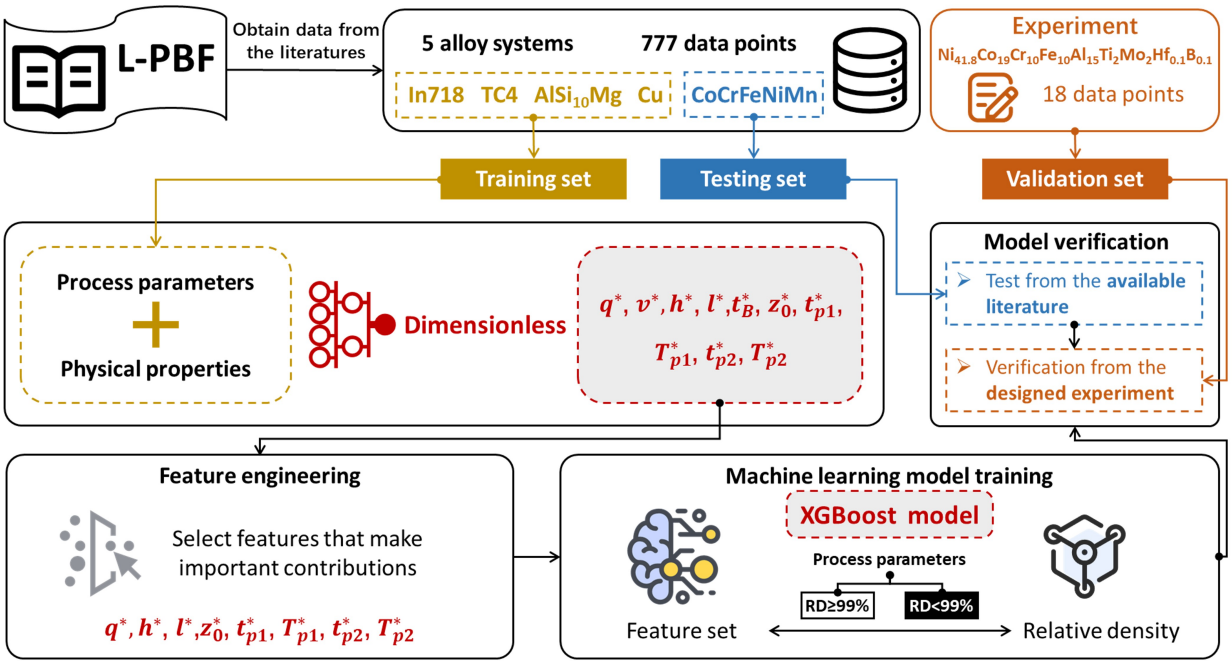
The multi-scale and non-linear nature of phase-field models of solidification requires fine spatial and temporal discretization, leading to long computation times. This could be overcome with artificial-intelligence approaches, which promise a paradigm shift for approximating solutions to partial differential equations. Surrogate models based on neural networks could have a much lower computational cost than conventional numerical discretization methods. They could therefore replace or accelerate them. We propose a new neural-network approach for approximation of phase-field models of solidification. It consists of a semi-implicit scheme leveraging the Deep Ritz method, where a neural network is trained to approximate a convex-concave minimization scheme for gradient flows. Such a scheme can be challenging to solve using conventional methods. We first apply the neural-network approach on the isotropic Allen-Cahn equation, and we demonstrate that energy-based physically-informed training provides better generalization in out-of-distribution evaluations compared to classical data-driven approaches. Inspired by splitting techniques in semi-implicit schemes, we introduce a Reaction-Diffusion neural network architecture, which outperforms standard models such as MLPs (multi-layer perceptrons), FNO (Fourier neural operator), and U-Net in our test cases. Finally, we apply our method to anisotropic dendritic growth simulations, achieving evaluation speeds about four times faster than conventional scalar-auxiliary-variable (SAV) type semi-implicit schemes.

Accurate identification of high relative density in laser-powder bed fusion across materials using a machine learning model with dimensionless parameters

Yiming Chen, Junjie Li and Jincheng Wang

Northwestern Polytechnical University (China)

Machine learning (ML) methods have been extensively applied to optimize additive manufacturing (AM) process parameters. However, existing studies predominantly focus on the relationship between processing parameters and properties for specific alloys, thus limiting their applicability to a broader range of materials. To address this issue, dimensionless parameters, which can be easily calculated from simple analytical expressions, were used as inputs to construct an ML model for classifying the relative density in laser-powder bed fusion. The model was trained using data from four widely used alloys collected from the literatures. The accuracy and generalizability of the trained model were validated using two L-PBF high-entropy alloys that were not included in the training process. It was found that the prediction accuracies for both cases exceeded 0.8. Moreover, the simple dimensionless inputs in the present model can be calculated conveniently without numerical simulations, thereby facilitating the recommendation of process parameters.



Machine learning for molten pool dynamic prediction in hybrid laser-MIG welding

Le Song and Xuyang Chen

National University of Singapore (Singapore); Karlsruhe Institute of Technology (KIT)

This study investigates the influence of process parameters on the dynamic behavior of the molten pool in hybrid Laser-MIG welding, particularly focusing on aluminum alloys commonly used in aerospace, marine engineering, heavy vehicles, and high-speed railway carbody. The research encompasses a comprehensive numerical modeling approach to simulate the thermal dynamics of molten pool, including factors like multiple reflection, Fresnel absorption, and the synergistic effects of laser and arc heat sources. Key parameters such as temperature field, flow field, element distribution, and solidification behavior are calculated and analyzed at different process parameters. It is indicated that scanning speed significantly impacts the dynamics of molten pool. The study reveals that higher scanning speeds result in lower temperatures and lower liquid velocities in the molten pool, influencing the penetration, width, and height of the molten pool. The distribution of magnesium, a critical element in the alloy, varies with the scanning speed. Then, the SVR method of machine learning is used to dig out the rules of melt pool behavior under different process parameters and make predictions. This research provides vital insights into optimizing welding parameters in hybrid Laser-MIG welding processes for aluminum alloys. It underscores the significance of scanning speed as a key factor in controlling the dynamic behavior of the molten pool, thereby influencing the quality and characteristics of the weld.

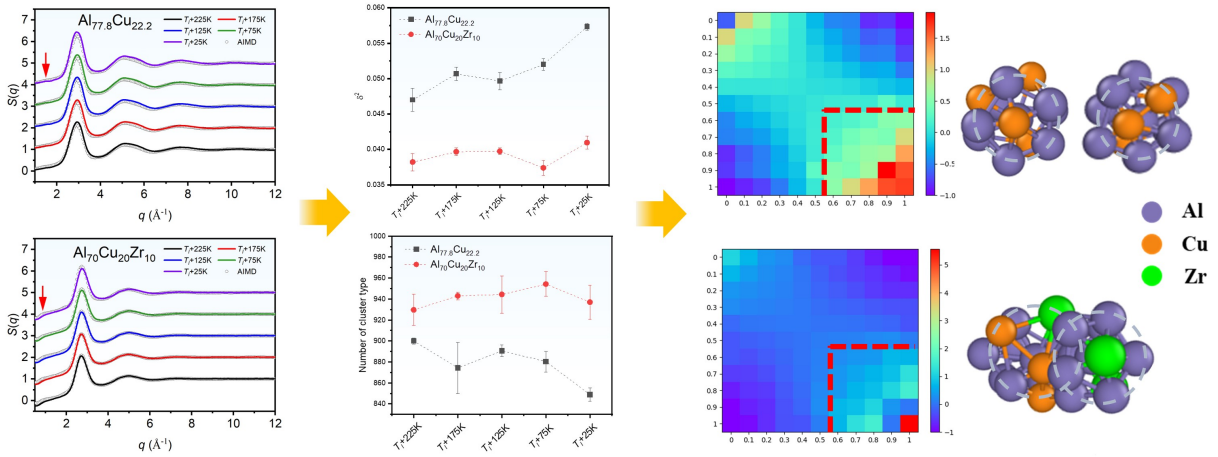
Tue-B-III / Glasses

Structural origin of the glass-forming ability of Al-Cu-Zr liquid alloy: experimental and simulation studies

Saichao Cao, Mingxu Xia and Noel Jakse

Shanghai Synchrotron Radiation Facility, Shanghai Advanced Research Institute, Chinese Academy of Sciences (China); Shanghai Jiao Tong University (China); University Grenoble Alpes & CNRS, SIMaP (France)

The relationship among chemical composition, structure and glass-forming ability in multicomponent alloys is a long-standing puzzle due to the complexity of compositions. In this work, Al-Cu and Al-Cu-Zr amorphous alloy liquids were investigated by combining high-energy X-ray diffraction at a synchrotron facility, abinitio molecular dynamics and reverse Monte Carlo simulations. The analysis of short- and medium-range order structures of two liquid alloys show that the addition of Zr element increases the number of cluster types and makes the distribution of cluster content more uniform, and enhances the structural heterogeneity and correlation of clusters with high five-fold symmetry. These findings reveal the influence of Zr element on the atomic structure of the Al-Cu liquid alloy and deepen the understanding of Al-based metallic glasses formation.



The effects of experimental casting parameters on crystalline and amorphous phase balance during casting of Mg-Zn-Ca alloys

Yanuar Rohmat Aji Pradana and David J. Browne

University College Dublin (Ireland)

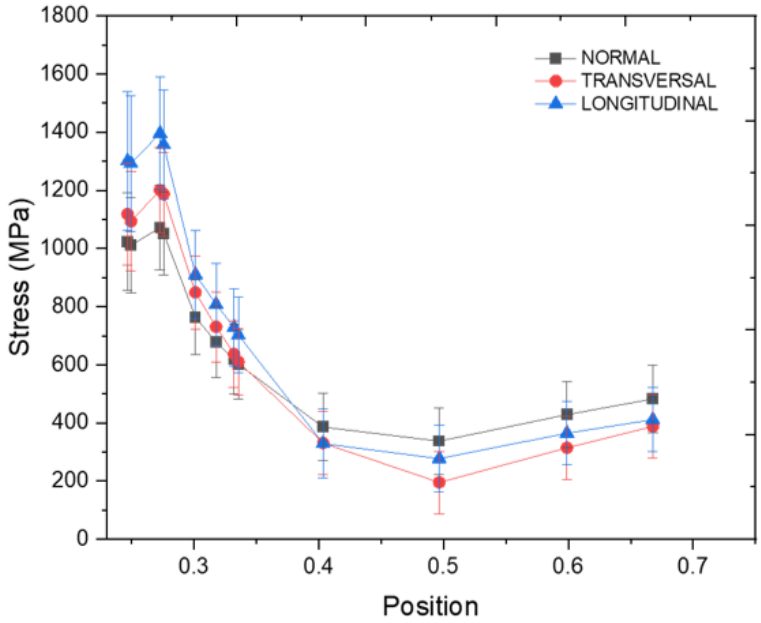
With a high enough cooling rate from above the liquidus, certain Mg-Zn-Ca alloys form Bulk Metallic Glasses. Here we study the cooling rate-driven crystalline-amorphous phase transformation is Mg-Zn-Ca alloys with limited glass-forming ability. We investigated the microstructural evolution of bioresorbable Mg-Zn-Ca alloys using induction melting in an inert atmosphere. Rods of Mg66Zn30Ca4 (at. %) with a diameter of 3 mm were fabricated using suction casting into a cylindrical copper mould, in which the cooling rate varies along the length. In parallel, a computer simulation was conducted using finite element-based software to calculate the temperature gradient and cooling rate in the alloy, based on the melt pouring and mould temperatures measured during the experiment. Structural and microstructural characterisations were carried out to reveal the effects of phase transformation kinetics on the degree of crystallinity in the resulting rods. These were done using X-ray diffraction and scanning electron microscopy-energy dispersive spectroscopy. The maximum rod length achieved was 100 mm. The structure varies along the rod length with the gradual crystalline-amorphous transformation from the top to the bottom of the rod. When the longest rod was produced, the region having a fully amorphous structure increased. The critical cooling rate mapping to cast a rod with a fully amorphous structure was determined using computer simulations. This finding will be useful in determining the required set-up for producing Mg66Zn30Ca4 bulk metallic glass and composites for biomedical applications.

Strain-Stress characterization of a bulk metallic glass by neutron scattering

Paula Rodriguez Gonzalez, Sandra Cabeza, Andreas Meyer and Ralf Busch

Institut Laue Langevin (France)

Bulk Metallic Glasses have gained significant attention due to their unique properties, including high specific strength, improved corrosion resistance and remarkable fracture toughness. Zr-based BMGs, the commercial alloy AMZ4 ($Zr_{59.3}Cu_{28.8}Al_{10.4}Nb_{1.5}$), are notable for their high glass-forming ability. Strain levels in AMZ4 significantly influence its mechanical properties, making Residual Stress (RS) characterization critical for optimizing treatments. We show that a non-destructive method with high penetration has proven effective for evaluating RS in BMGs. SALSA provides the highest lateral spatial resolution compared to other neutron instruments, thanks to the combination of high neutron flux from the steady reactor source and the optical setup with radial collimators of 0.6 x 0.6 mm horizontally and 2 mm vertically. AMZ4 samples (2 x 4 x 25 mm^3) were prepared from a single cast plate to ensure uniform cooling rates. Samples underwent different thermal treatments: as-cast (As-C) and annealed at 623 K for 45 h (AN). Tensor measurements were conducted to calculate the residual stress. Entry scans from the surface to the bulk were carried out with a spatial resolution layer thickness of 400 µm. A peak shift of the structure factor maximum is observed on SALSA at q = 2.6 $Å^{-1}$ for the As-C sample. In the bulk of the AN sample, no peak shift is observed. This value was used as the reference (d) to calculate the stress-strain profile of As-C. The As-C exhibits a high stress gradient, where tensile stress decreases gradually with depth from the surface (max. 1 GPa) until compressive stress emerges in the bulk. Even in the AN sample, a smaller stress gradient from the surface to the bulk. Significant strain variations in annealed BMG's from the surface to the bulk are somewhat unexpected. Further experiments on differently annealed samples are ongoing to clarify the origin of this behavior.



Stress results for AC sample with d0 averaged from annealed

Tue-C-I / Fluid flow I: Semi-solid flow

Evolution of dendritic morphology in a solidifying Ga-In-Bi alloy studied by in-situ synchrotron radiography

Natalia Shevchenko, Joerg Grenzer, Olga Budenkova, Tobias Lappan, Martins Sarma and Sven Eckert

Helmholtz-Zentrum Dresden-Rossendorf (Germany); Univ. Grenoble Alpes, CNRS, Grenoble INP, SIMAP (France)

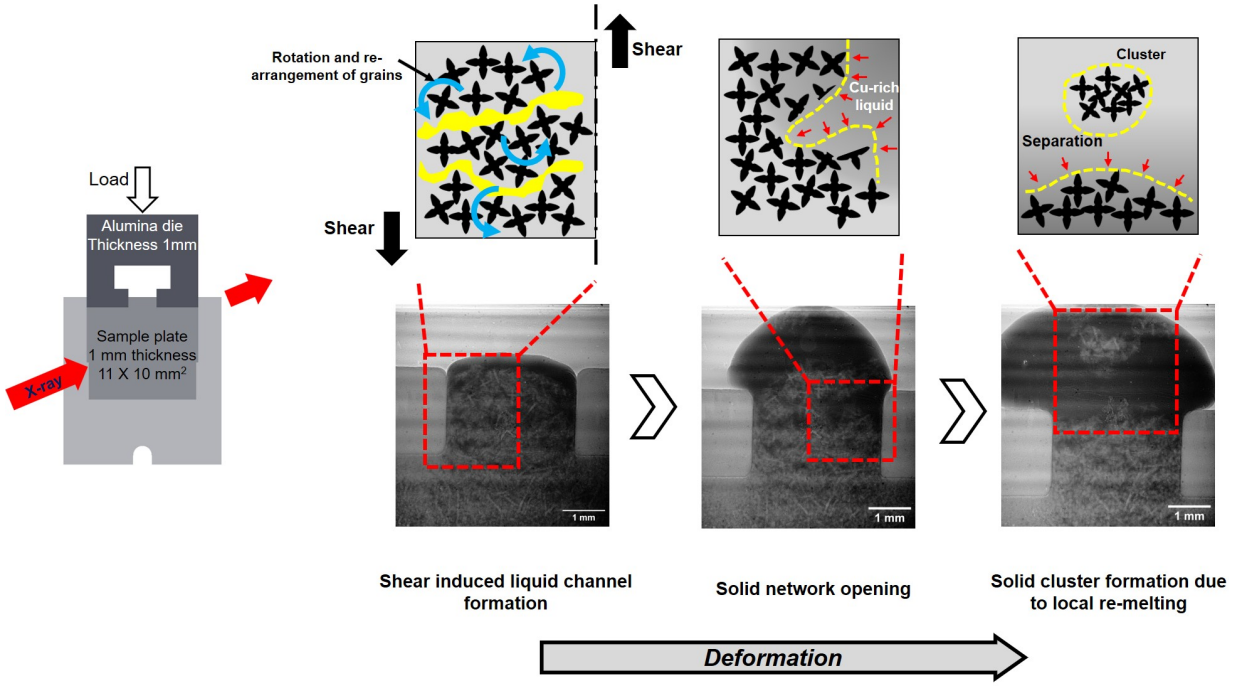
Previous studies of the solidification of a low-melting temperature ternary Ga-In-Bi alloy with a laboratory microfocus X-ray system demonstrated that the morphology of the growing indium dendrites was significantly altered by the presence of a small amount of bismuth (2.5wt%) [ICASP 2021 and TMS 2023 conference contributions]. Our observations revealed the formation of curved dendrites, multiple splitting events, and the development of branched or seaweed-like structures. We explained this phenomenon by the fact that the addition of bismuth as a third alloying element reduces the anisotropy properties of the phase boundaries, making them more susceptible to disturbances. This work uses X-ray synchrotron radiography to study the formation of a variety of solid phase morphologies in the same ternary system. The synchrotron imaging experiments were performed at the ID19 beamline (ESRF, France) with a spatial resolution of ~1 μm. The high spatial resolution allows us to analyse the shape of the dendrites' tips and local dynamics of splitting or branching in great detail. The preliminary analysis of the data clearly shows that the direction of the dendrite growth can deviate because of different mechanisms, e.g. branching or unstable tip growth. The ongoing data processing will provide further insights into the physics of the transition to branched growth in ternary alloys.

In situ X-ray imaging of defects and microstructural heterogeneity during semi-solid flow

Utkarsh Godwal, Shyamprasad Karagadde, Shishira Bhagavath, Bita Ghaffari, Mei Li, Sebastian Marussi, Chu Lun Alex Lueng and Peter D Lee

IIT Bombay (India); University College London (UK); Ford Research and Advance Engineering, Dearborn (USA)

Aluminium alloy castings are routinely used to manufacture complex automotive and aerospace components. However, the strength of cast components can be adversely affected by the microstructural inhomogeneities, including defects such as porosity and shear bands. The formation of shear bands in castings depends on the semi-solid flow patterns, solid fraction gradient normal to the bulk flow, die shape, and the applied pressure. A parametric study quantifying these effects is not available. In this study, we utilized fast synchrotron X-ray imaging to capture the effect of solid fraction and semi-solid flow patterns in different custom alumina die-pistons mounted on a bespoke thermo-mechanical rig. The effect of semi-solid flow through a narrow opening, creating liquid channels and porosity formation during deformation, were quantified using in situ radiography. Further, ex situ observations using optical and electron microscopy show evidence of microstructural heterogeneity in specific regions of the dies due to strain localization and increased local solute concentration. These observations elucidated the formation mechanisms of liquid channels and defects, allowing a more detailed understanding the formation of banded defects in large industrial castings.



Numerical modelling of extrusion of granular particles against gravity through an opening

Abhinesh Kumar, Utkarsh Godwal, S. Bhagavath, B. Ghaffari, M. Li, P. D. Lee and Shyamprasad Karagadde

Indian Institute of Technology Bombay (India); Research Complex at Harwell, Harwell (UK); Ford Research and Advanced Engineering, Dearborn (USA)

The High Pressure Die Casting (HPDC) process involves the flow of molten metals through complex geometries with sudden contractions, leading to the formation of small metal grains during solidification due to heat loss from the confining walls. In this study, a simplified rectangular domain with a sudden contraction at the exit and a moving plate at the bottom was used to simulate the extrusion of molten metal. The extrusion process and behavior of particulate bed has been analyzed using a CFD-DEM coupled approach implemented in the open-source software CFDEM-coupling. The formation of shear bands during particle extrusion have been examined for both spherical and non-spherical particle shapes across a range of extrusion velocities. The results demonstrate that apart from particle size, particle shape also significantly influences the formation and characteristics of shear bands. Additionally, the study characterizes both moving, transition layer (shear zone) and stagnant zones throughout the extrusion process. Simulations were conducted for various sizes of the sudden contraction opening to assess its impact on shear band formation. The simulated results were compared with experimental data and it is showing a reasonable agreement and similar flow behavior. These findings contribute to a better understanding of the impact of particle shape and contraction geometry on the shear band formation in HPDC processes.

Numerical modelling of flow through porous media to study shear bands

Ankit Tamrakar, Utkarsh Godwal, Shishir Bhagavath, Bita Ghaffari, Mei Li, Peter Lee and Shyamprasad Karagadde

Indian Institute of Technology Bombay (India); Research Complex at Harwell, Harwell (UK); University College of London (UK); Ford Research and Advanced Engineering, Dearborn (USA)

The semi-solid flow (SSF) of solidifying mixtures is of importance in manufacturing processes, such as high pressure die casting (HPDC), as well as natural phenomena, such as flow of lava and glacial ice. In HPDC, such flows can induce defects such as porosity, cracks, and shear bands. However, modeling these defects is complex due to the multiscale and multiphysics nature of SSF. Understanding the intricate interactions in solid-liquid movement, considering the effects of grain morphology, and tracking the evolution of permeability are essential for developing more realistic models to predict shear bands. This study aims to illustrate and quantify flow through a solidifying structure. We employed isotropic and anisotropic permeability models for flow through a pipe with a stationary porous zone. We quantified the flow with varying pressure gradient and solid fraction ratio along and across the length of the mushy zone, respectively. We observed the localized shear strain position to shift towards the wall with increase in order of solid fraction ratio. Also, the magnitude of shear strain increased with increasing pressure gradient. The model was validated with a previously developed anisotropic permeability model. Solid phase movement during the SSF can be further added in the present model to predict the location of shear bands more accurately, and to better mimic the movement of Externally Solidified Crystals.

Experimental Investigation on the Rheology of Suspensions Containing Dendritic-like Structures

Andreas Ludwig, Mihaela Stefan-Kharicha, Johann Mogeritsch and Abdellah Kharicha

Montanuniversitaet Leoben (Austria)

The relation of shear viscosity and solid fraction is a crucial input for volume-averaged multiphase solidification simulations. The relationship is typically derived from rheological studies of suspensions containing spheres of uniform size. In these experiments, both the shear viscosity and the normal viscosity arising from the so-called particle pressure are generally measured. Using 3D printing, we fabricated a large number of small, dendrite-like structures with six-fold symmetry. These structures were incorporated into a suspension and processed in the same rheometer previously used for sphere-based suspensions. The measured relationships between shear rate, momentum, normal force, and volume fraction will be presented and discussed.

Volume-Averaged Two-Phase Simulations of the Rheology of Suspensions

Christian Gomes-Rodrigues, Andreas Ludwig, Michaela Stefan-Kharicha, Menghuai Wu and Abdellah Kharicha

Montanuniversitaet Leoben (Austria)

The relationship between shear viscosity and solid fraction is a crucial input for volume-averaged multiphase solidification simulations. This relationship is typically derived from rheological studies of suspensions containing spheres of uniform size. In these studies, simplified assumptions about particle dynamics during shearing are often made. We have extended a standard volume-averaged two-phase simulation to account for particle pressure and applied it to the rheometer process. Our findings reveal that the suspension dynamics within the rheometer are highly sensitive to the drag law considered. However, in all cases, the motion of the particles under shear conditions is more complex than typically assumed in the literature.

Tue-C-II / Fluid flow II: External fields stirring

Solidification process in electromagnetic levitation with a superposed horizontal DC magnetic field

Olga Budenkova, Abdalmagid El Bakali, Ganesh Guggilla, Paul Chometon and Didier Chaussende

University Grenoble Alpes & CNRS, SIMaP (France); Institut Néel, CNRS (France)

Electromagnetic levitation is a prominent environment that allows materials' characterisation as well as materials' elaboration, with solidification of alloys among the processes that can be realised. The intense stirring inside the samples intrinsic to the EM levitation can be favourable, if uniformity of the microstructure is expected, or detrimental, if diffuse heat and mass transport is requested. It has been demonstrated that vertically directed DC magnetic field can effectively damp the fluid flow inside the levitating sample [1]. Since then, the EML levitation coupled with the DC magnetic field has been used for measurements of physical properties of liquid metals [2,3]. However, application of this technique to solidification processes remains rather exceptional, few examples can be found elsewhere [4]. In the present work, we study solidification of the Cu-Ni alloy in a setup where electromagnetic levitation can be coupled with a horizontally directed DC magnetic field. Details of the heat and mass transport are discussed and microstructure of the samples obtained without and with the application of the DC magnetic field is compared. Acknowledgement. Ganesh Gugilla gratefully acknowledge the financial support of LabEx Tec21 , UGA. The solidification setup was developed with the support of the CNES within the Material Science program. [1] H. Yasuda et al, J. Cryst. Gr. 260 (2004), 475-485 [2] M.Watanabe, J. Mol. Liquids, 324 (2021), 115138. [3] M. Watanabe et al., Thermochimica Acta, 708 (2022), 179119, 2022., [4] Y.K. Zhang et al., Scripta Mater., 59 (2008) 1002-1005

Time-Dependent Magnetic Field Impact on Laser Additive Manufacturing

Ivars Krastins, Xianqiang Fan, Harry Chapman, Catherine Tonry, Peter Soar, Koulis Pericleous, Peter Lee and Andrew Kao

University of Greenwich (UK); University College London (UK)

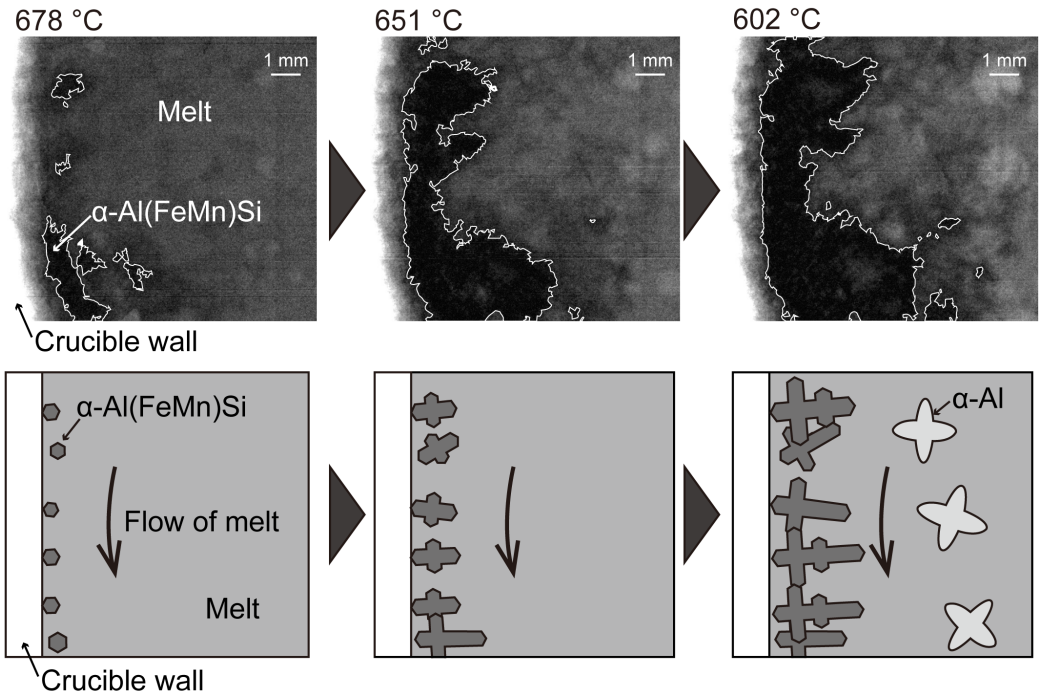
Studies have shown that relatively weak magnetic fields, ~0.1 T, achievable with permanent magnets, can significantly decrease pore formation in printed metal components during laser additive manufacturing (AM). The current understanding is that Thermoelectric Magnetohydrodynamic (TEMHD) flow transports the bubbles to the surface removing them from the melt. This phenomenon is further supported by experimental observations of how tracer particles segregate when the magnetic field is applied. By modulating the magnetic field further control can be attained, where the modulation is related to characteristic time and length scales of the process. Simulation results show how this can lead to the disruption of typical epitaxial growth of microstructures. Preliminary experimental results indicate that the modulated field corresponds to a modulated fluid flow and the underlying mechanism is TEMHD in nature. TEMHD in AM is still a relatively unexplored area and these results highlight its potential as a novel way to control the process and/or mitigate defect formation. To understand the underlying mechanisms, a bespoke parallel multi-physics numerical code TESA (Thermoelectric Solidification Algorithm) is used. TESA couples heat and mass transport with solidification, hydrodynamics and particle transport. Its modular nature allows each of the physics to use a different method so that TESA is a combination of finite difference, enthalpy-based and lattice Boltzmann methods together with Lagrangian particle tracking. The model provides insight into the melt pool dynamics during the metal alloy solidification and the interplay mechanism between the Marangoni and TEMHD flow. The application of a magnetic field offers means to control the flow behaviour and ultimately improve the mechanical properties like porosity in the final material. The results show that a successfully chosen magnetic field configuration can challenge the dominant Marangoni flow morphology in the melt pool and promote an upward motion for the trapped bubbles to escape.

Electromagnetic Stirring-Induced Macrosegregation in Aluminum Alloys Containing Iron

Keiji Shiga, Takeshi Fujiwara, Yuichiro Murakami and Naoki Omura

National Institute of Advanced Industrial Science and Technology, AIST (Japan)

This study investigates the effect of electromagnetic stirring (EMS) on the solidification of an Al-10Si-2Fe-2Mn alloy. To understand how EMS influences the growth and distribution of the primary intermetallic α-Al(FeMn)Si phase, we designed and implemented a novel X-ray imaging system. This system enables real-time observation of solidification under electromagnetic forces over an area exceeding 100 mm², several hundred times larger than conventional synchrotron X-ray imaging setups. In-situ X-ray imaging provides critical insights into the macrosegregation process during solidification in the presence of melt flow. Without EMS, α-Al(FeMn)Si grains are horizontally uniform but settle at the sample's bottom due to gravity. In contrast, EMS induces peripheral congregation and dendritic growth of these grains, significantly altering the microstructure. In-situ observations reveal that the area of the α-Al(FeMn)Si phase at the periphery expands toward the center of the melt under EMS, indicating grain coarsening induced by EMS. This phenomenon occurs because melt flow generated by EMS enhances solute transport and heat dissipation, accelerating grain coarsening. Electron backscatter diffraction measurements confirm a dominant single grain orientation of the α-Al(FeMn)Si phase under EMS, suggesting that grain coarsening, rather than random grain agglomeration, governs the observed behavior. Contrary to theories of electromagnetic separation, the peripheral macrosegregation results from enhanced grain growth, not the movement of grains caused by electromagnetic forces. Because the melt flow influences the solute and thermal fields, EMS expands the constitutional supercooling zone, promoting dendritic growth and morphological transformations in intermetallic grains. This study enhances the understanding of the macrosegregation mechanisms during the stir-casting of alloys and provides valuable insights into refining secondary aluminum alloys through EMS processes.



Comparison of the microstructure of Al12.6Si and Al18Si alloys solidified with and without rotating magnetic field

Zsolt Veres, Éva Kócsák, Arnold Rónaföldi and András Roósz

University of Miskolc (Hungary); HUN-REN-TKI Materials Science Research Group (Hungary)

The microstructure of Al-Si alloys plays a crucial role in determining their mechanical properties and performance in engineering applications. Among others, the natural and forced melt flows significantly affect the alloys' microstructure. Within the framework of the MICAST project, as the ISS mirror experiments, Al12.6Si and Al18Si samples were solidified unidirectional. In some of the experiments, a 10 mT rotating magnetic field (RMF) was used during the solidification process, and the other solidification parameters were the same. The eutectic microstructure and the primary phase were investigated by light microscope. We investigated the shape and the size of the primary Si, the length of the eutectic lamellas, the average distance of the eutectic lamellas and the angle of the lamellas relative to the solidification direction. As was expected, the magnetic stirring caused a finer eutectic and primary silicon. Still, we found that not only did the magnetic stirring have an effect on the eutectic structure but also the composition of the alloy. The presence of the primary silicon modified the structure of the eutectic.

Challenges in Ultrasonic Cavitation for deagglomeration of Carbon Nanotubes

Catherine Tonry, Zhuocheng Xu, Christopher Beckwith, Andrew Kao, Milo Shaffer and Qianqian Li

University of Greenwich (UK); Imperial College London (UK)

Carbon nanotube (CNT) reinforced metal matrix composites (MMCs) have been shown to exhibit exceptional properties, especially in the context of high strength lightweight materials. While this has been demonstrated under laboratory conditions, there are numerous challenges that need to be overcome to scale to an industrial process. There are multiple difficulties in this process during both melt processing and solidification. A key challenge is the deagglomeration of carbon nanotubes. requiring breaking up and dispersing clusters to form a well-mixed suspension of CNTs, which is a necessary step in forming CNT reinforced metal matrix composites. One promising method is ultrasonic treatment (UST) that has been shown to deagglomerate and disperse CNTs in liquids. However, how material properties and processing conditions effect this dispersal is not currently well understood. A programme of experimental and numerical work has been undertaken using water as an analogue for the alloy melt to explore the underlying mechanisms in more detail. Fluid flow and bubble dynamics are both intimately coupled into the break and dispersion of CNTs. With the addition of surfactants, the surface tension can also be altered, having a strong effect on the coupled system. Our numerical modelling predicts how both flow and bubble dynamics are effected by changes to surface tension and is validated by experimental data experimental data in the form of high-speed in situ optical imaging. By understanding and validating the dependence of varying material properties, the numerical model can be calibrated to liquid metal melts, where in situ experiments are more complex due to difficulties in imaging, especially with nano structures present. This talk gives details of our combined work programme, but there will be focus on the numerical.

Tue-C-III / Fluid flow III: Solid-liquid-gas mixtures

Hydrogen bubble formation and interaction in Al-alloys during melting and solidification

Florian Kargl, Thomas Werner, Maike Becker and Laszlo Sturz

German Aerospace Center, DLR (Germany); Access e.V. (Germany)

During metallurgical processing, gas bubbles nucleate and interact with the microstructure, which can result in severe defects. Pores, their agglomeration and networks formed by them are lowering e. g. fatigue strength in aluminium alloys [1,2]. Hence, research on nucleation, growth and interaction of bubbles with the microstructure forming during solidification is a topic of great interest both from a scientific point of view and for the metallurgical industry. Here, we focus on bubble formation and interaction with the surrounding dendrite network in the mushy zone of Al-Cu and Al-Ge alloys. Experiments were carried out in a X-ray transparent Bridgman-Stockbarger furnace and in-situ monitored by X-radiography. The samples were pre-conditioned with a well-defined amount of hydrogen using a gas loading and casting furnace [3]. From the cast blocks thin rectangular alloy samples (5x50x0.15mm) were prepared and subsequently processed in horizontal configuration thus minimizing buoyancy effects. Solidification experiments showed bulging of the solidification front in the vicinity of a bubble, bending of dendrites approaching a bubble, and coronal outgrowth [4]. Further, we focused on thermal and solutal capillary effects [5]. We show that an accurate knowledge of thermophysical properties, in particular, surface tension as a function of temperature and composition is required to understand the observed cryophile migration of bubbles, namely Marangoni-motion towards the cold side and not as commonly observed and expected to the hot side. This behaviour is explained by taking into account the behavior of surface tension as derived from EML experiments. [1] Y.X. Gao, et al. Fatigue Fract. Eng. Mater. Struct. 27 (2004), 559. [2] P. Osmond, et al. Procedia. Eng. 213 (2018), 630. [3] T. Werner, et al. Rev. Sci. Instrum. 91 (2020), 043901. [4] T. Werner, et al. J. of Materials Science 56 (2021), 8225. [5] T. Werner, et al. Acta Mater. 224 (2022), 117503.

Freezing of Gas Bubbles in a Liquid

Bastien Isabella, Sylvain Deville and Cécile Monteux

ILM, UCBL, CNRS (France); SIMM, ESPCI, CNRS (France)

In many different industrial or scientific fields, such as environmental science, food cryopreservation, metallurgy, or even sapphire crystal growth some gas bubbles can be trapped in materials during solidification processes, affecting their mechanical or optical properties. In this talk, I will present our work about the study of the behavior of gas bubbles during freezing and especially near the solidification front between water and ice. To achieve this, we use confocal fluorescence cryomicroscopy to observe in situ the behavior of air or gas bubbles during all stages of the unidirectional solidification process. This process is complex because of the occurrence of different phenomena such as nucleation, or coalescence of bubbles and diffusion of gases in the liquid. More particularly, we are studying the dynamics of bubble nucleation caused by the solidification, as well as the incorporation dynamics of these bubbles at the solidification front between ice and water. The impact of solidification parameters, fluids flows, and surfactant on these phenomena will also be discussed. These observations will help us to better understand the physical and chemical mechanisms involved during the solidification of liquids containing dissolved gas, or bubbles, to estimate the critical concentration of nucleation in our system, and to determine how to control or restrain the engulfment of these bubbles during solidification.

Solidification and melting of salt-water phase change material

Radhika Sarawagi and Virkeshwar Kumar

Indian institute of Technology Kanpur (India)

Water-salt systems as phase change materials (PCMs) utilize the freezing and melting transitions of aqueous salt solutions to store and release thermal energy (latent heat and specific heat). The addition of salts lowers the freezing point and can improve the thermal stability and energy density of the PCM. Common examples include sodium chloride-water (NaCl-H2O), potassium nitrate-water (KNO3-H2O), and potassium carbonate-water (K2CO3-H2O) systems, which are used in cold storage, desalination, and thermal regulation applications. To investigate the successive solidification and melting of a binary system (water-KNO3), we conducted in-situ experiments using a three-sided cooling configuration in a cuboidal cavity with inner dimensions of 65 × 65 × 80 mm^3. Three salt compositions were studied: water-5% KNO3 (ice forms as the primary solid, hypo-eutectic composition), water-9.5 % KNO3 (eutectic composition), and water-23% KNO3 (salt forms as the primary solid, hyper-eutectic composition). In the hypo-eutectic and hyper-eutectic compositions, both thermal and solutal convection occurred, whereas in the eutectic composition, only thermal convection was observed. Shadowgraph imaging was employed to capture density changes and DSLR imaging was used to track the phase change interface. Eight thermocouples were placed inside the cavity to record temperature data and liquid samples were extracted during the experiments to analyse transport phenomena. The thermal data revealed similar cooling and heating curve patterns across the three compositions during solidification and melting. During solidification, cooling curves exhibited three distinct regions, while melting curves displayed a zigzag pattern. In both hypo-eutectic and hypereutectic regimes, double-diffusive layers formed during meltinga phenomenon reported for the first time. During the solidification of hypoeutectic and hypereutectic solutions, the solute concentration increased until it reached the eutectic point. Conversely, during melting, the solute concentration decreased with minor fluctuations. These findings provide valuable insights into the transport phenomena in phase-change material (PCM)-based binary salt systems.

Parallel sessions

Day 2 / Wednesday June 11, 2025

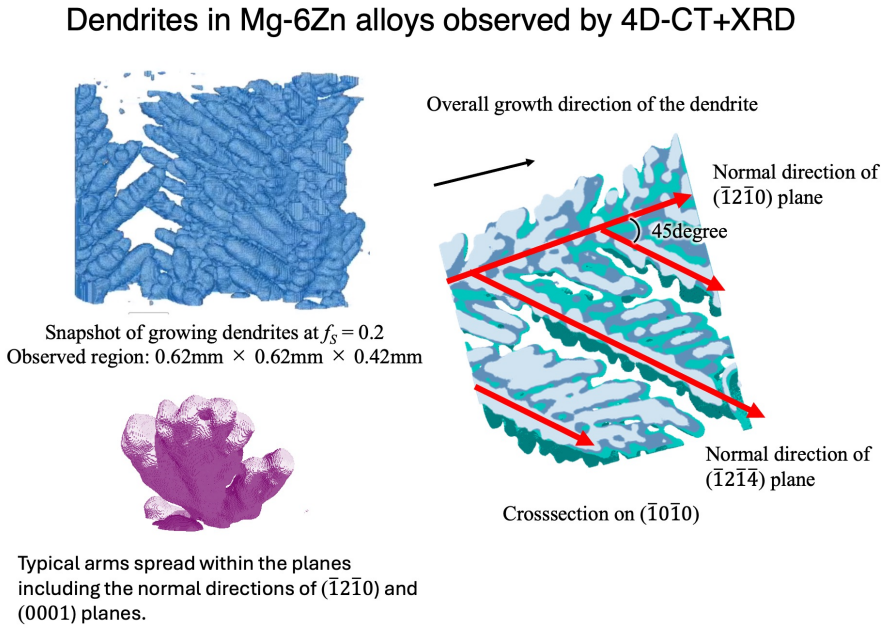
Wed-A-I / Dendritic growth & In-situ imaging

Direct observation of dendrite arm development in hexagonal Mg-Zn alloys

Hideyuki Yasuda, Arisa Nishiguchi, Ryoji Katsube and Taka Narumi

Kyoto University (Japan); Nagoya University (Japan)

Dendrite arms are known to frequently grow along <100> directions for various cubic alloy systems. On the other hand, the preferred growth directions for hexagonal alloy systems remain ambiguous. Hexagonal structures exhibit six-fold symmetry along the c-axis, representing relatively high symmetry, and two-fold symmetry including <0001> - <11-20> directions representing relatively low symmetry. It is of interest to determine the preferred growth directions for hexagonal alloy systems and to discuss the relationship between the growth directions and the lattice symmetry. Time-resolved and in-situ observation using X-ray tomography and diffractometry (4D-CT+XRD) has enabled to observe the dendrite arm development along specific crystallographic orientations. Thus, the 4D-CT+XRD is an effective technique for determining the preferred growth directions of dendrite arms, as it allows for the direct observation of dendrite arm development during solidification. 4D-CT+XRD observations/measurements for Mg-6mass%Zn alloys were performed at an imaging beam line BL47XU of SPring-8 (synchrotron radiation facility). Monochromatized X-ray with a energy of 37.7keV was used to capture the projections images with pixel size of 5.6μm × 5.6μm. Simultaneously, X-ray diffraction was measured. This measurement enables the observations of three-dimensional dendritic structures, including crystallographic orientations. The dendrite arms roughly grew along normal directions of {11-20} and {11-24} planes, although no growth was observed along the normal direction of {0001} plane. The growth directions clearly exhibited a six-fold symmetry along the c-axis. In contrast, the growth directions of the {11-20} and {11-24} normal directions were distributed within the planes including the normal directions of {11-20} and {11-24}. The weak constraints on the growth directions within these planes characterized the dendrite growth in the Mg-Zn alloys and consequently the solidification structure.

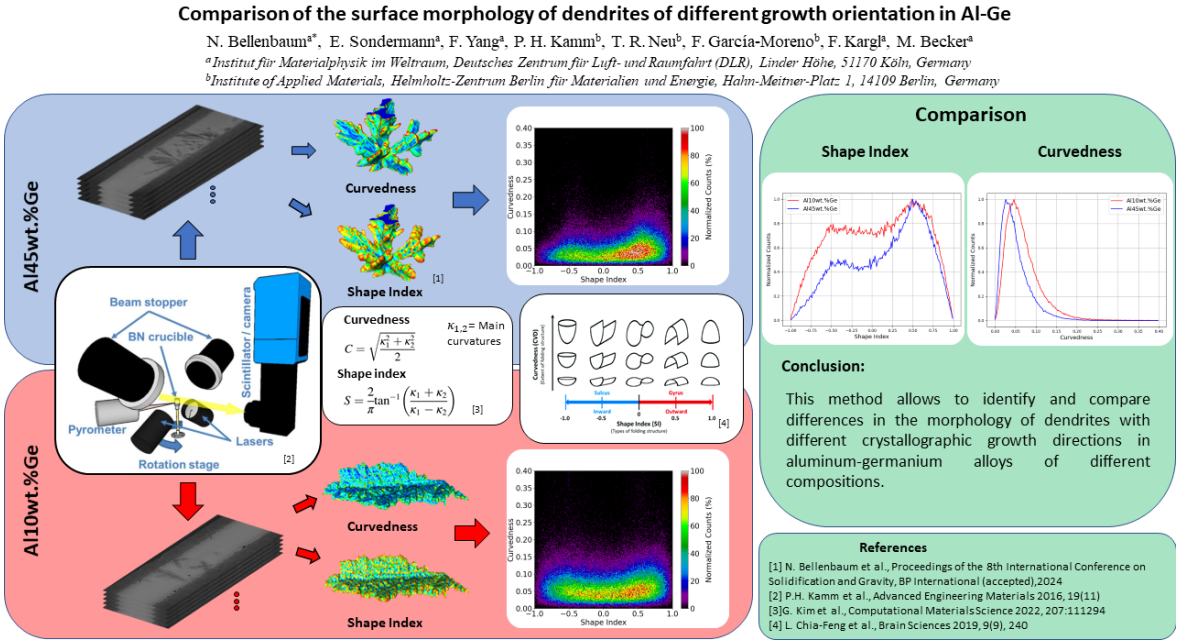


Comparison of the surface morphology of dendrites of different growth orientation in Al-Ge

Nlis Bellenbaum, Elke Sondermann, Fan Yang, Paul Hans Kamm, Tillmann Robert Neu, Francisco García-Moreno, Florian Kargl and Maike Becker

Deutsches Zentrum für Luft- und Raumfahrt, DLR (Germany); Helmholtz-Zentrum Berlin für Materialien und Energie (Germany)

Dendritic solidification is a common growth form in metallic alloys and has a significant influence on the mechanical properties. However, the anisotropy of the interfacial energy between solid and liquid, which influences the growth direction and shape of the dendrites, is not known for many alloys. In some alloys, such as aluminium-germanium, a dendrite orientation transition can be observed, which is caused by the change in anisotropy with composition. Three different growth forms of fcc-Al dendrites depending on the alloy composition were demonstrated by Becker et al. in X-radiography in-situ experiments, whereby the directions <100> at low germanium content, <110> at high and a mixture of both between the concentrations could be observed. To analyze the morphology of equiaxed dendrites in greater detail, a time resolved X-ray tomoscopy experiment was carried out with thin samples (300µm) at the TOMCAT beamline of the Paul Scherrer Institut in Switzerland. Alloy compositions between 5% and 50% Al-Ge were used. The thin square-like samples were contained in a slitted boron-nitrite (BN) cylinder held in place in a sandwich configuration by equally sized graphite-foil pieces. The BN-cylinder was heated by two infrared lasers from the side whilst continuously rotating around its vertical axis. Temperature was calibrated and measured by pyrometry on the BN-cylinder. Full tomograms with an effective voxel size of 2.75 µm were taken with a maximum speed of 20 tomograms per second. The dendrites were segmented and the interface properties were investigated with a focus on their growth shape. This shape can be described by the local curvatures of the dendritic surface. An interface shape distribution map was used to visualize the results. This method allows to identify and compare differences in the morphology of dendrites with different crystallographic growth directions in aluminum-germanium alloys of different compositions.

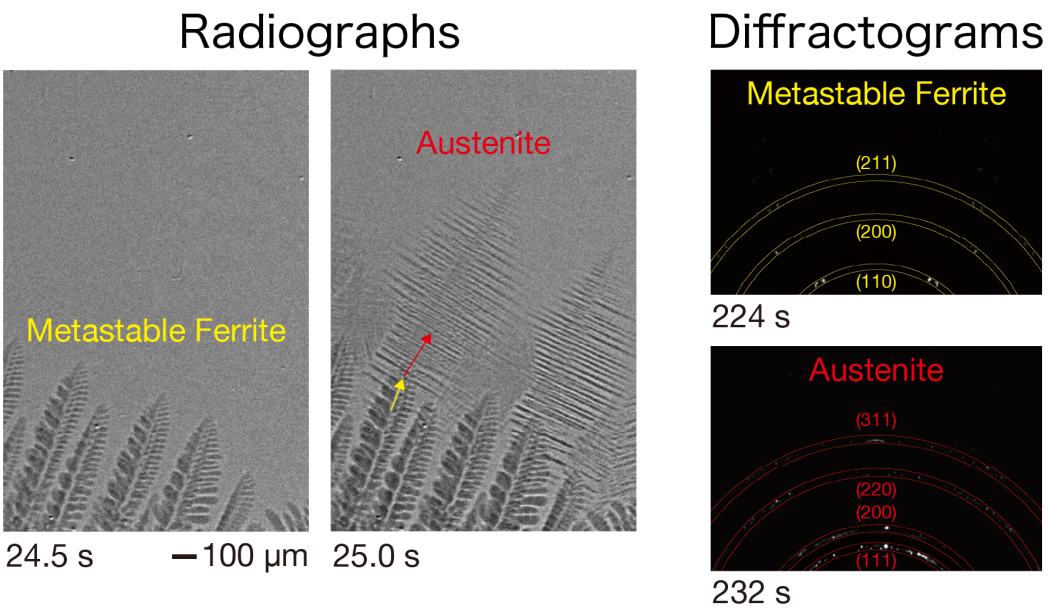


Characterization of austenite grain structure evolution through metastable ferrite nucleation and ferrite-austenite transformation in Fe-Mn-C austenitic steel using X-ray imaging techniques

Taka Narumi, Kengo Fujita, Makoto Ohta, Ryoji Katsube and Hideyuki Yasuda

Kyoto University (Japan); Nagoya University (Japan)

Undercooled melts of Fe-based alloys are subject to competition between the ferrite and austenite nucleation due to the polymorphism of Fe, resulting in various solidification sequences. Nucleation-controlled phase selection and subsequent microstructure evolution are issues of theoretical and practical interest in solidification of Fe-based alloys. This study demonstrates that solidification of the austenite was initiated by metastable ferrite nucleation followed by ferrite-austenite transformation even in Fe-22mass%Mn-0.7mass%C alloy, where the austenite is the primary phase in equilibrium. X-ray radiography was performed to observe the evolution of austenite grain structure through metastable ferrite nucleation and subsequent ferrite-austenite transformation. Time-resolved X-ray diffractometry was performed using a time-resolved X-ray tomography setup to characterize the crystallographic orientation relationship during the solidification sequence. X-ray radiography showed that the metastable ferrite nucleation was selected at various undercooling (10-60 K from the liquidus temperature for the austenite) when the specimen was cooled from a complete molten state. In the subsequent cooling process, the ferrite massively transformed to the austenite in the solid state, producing multiple austenite grains within a single ferrite grain through ferrite-austenite transformation. The grain size typically ranged from 100 to 500 μm. The X-ray diffractometry revealed a crystallographic relationship between the ferrite and austenite, and the twinning relationship was often confirmed in the austenite grain structure. Notably, the twinning relationship was observed even when the austenite solidified without the detection of the ferrite. Furthermore, a crystallographic feature that consistently shows the occurrence of ferrite-austenite transformation remained in the austenite grain structure. Consequently, this study proposes that the metastable ferrite nucleation will be preferably selected, and the subsequent ferrite-austenite transformation must have the potential to control the austenite grain size in the as-cast microstructure.



Time-resolved and in-situ observation of dendrite fragmentation during undercooled solidification in Cu-Fe-P alloys

Tomohiro Nishimura, Kohei Komori, Yutaka Urakawa, Taka Narumi and Hideyuki Yasuda

Kobe Steel, Ltd. (Japan); Kyoto University (Japan)

Copper alloys are used in electronic devices and other applications, and future demand growth and improved quality requirements are expected. Refining of the solidification structure is an effective technique for improving the mechanical properties of copper alloys. Time-resolved and in-situ observation using X-ray imaging is a research technique that enables direct observation of the solidification process. In this study, we report on the characteristics of dendrite fragmentation during undercooled solidification in Cu-0.1mass%Fe-0.03mass%P alloys. X-ray imaging was performed at SPring-8 (Japan). Sample with 10 mm x 10 mm x 0.1 mm was heated to melt (superheat 60 K) and then cooled at a constant rate to observe the solidification process. Monochromatic light of 28 keV was used for observation. The time resolution of the imaging was one image per second. The observation area was 5 mm x 5 mm, and the spatial resolution of the transmission image was 6.45 μm x 6.45 μm per pixel. As an example, the sample was cooled at 0.83 K/s. The solidification occurred when the sample was undercooled from the liquidus temperature by about 25 K. In the entire observation area, fragmentation of the dendrite arms occurred almost simultaneously (within 1 second) during the undercooled solidification. In addition, fine dendrites such as secondary dendrite arms fragmented instead of relatively thick primary dendrite arms. Almost simultaneously with the dendrite fragmentation, the solid fraction temporarily decreased. Therefore, it is considered that the dendrite fragmentation was caused by the remelting of the dendrite arms. This observation revealed that there are cases of simultaneous fragmentation of dendrite arms immediately during undercooled solidification. The scientific findings of this study are that it demonstrated that fragmentation simultaneously occur even in compositions that are close to pure alloys and in which the decrease in liquidus temperature due to solute composition is small.

Effect of hypergravity on microstructural development in Al-10wt.%Cu alloy during controlled directional solidification

Sonja Steinbach, Ali Jafarizadeh-Koohbanani, Florian Kargl, Thomas Isensee and Damien Tourret

DLR - Institute of Materials Physics in Space (Germany); IMDEA Materials (Spain)

Many studies have investigated the effect of external fields (electric currents, magnetic and ultrasonic fields) on the solidification structures in castings. In contrast, research on the effect of hypergravity fields as in centrifugal casting is lacking. Although some researchers have looked into the effect of super gravity fields or centrifugal fields on refining the solidification of cast structures, the effect of hypergravity on directional solidified microstructures is not fully understood. From previous experiments within the literature [1] we know that the primary dendrite arm spacing decreases as gravity increases. And at very low gravity levels we also know that the primary dendrite arm spacing becomes very large. But the question arises as to what happens to the microstructure when it is solidified at higher gravity levels. In this context, DLR built a new furnace [2], and first experiments were performed with Al-10wt.%Cu alloy samples directionally solidified at different gravity levels up to 6g on a centrifuge. The samples solidified in hypergravity are evaluated with regard to the processing parameters and to the primary dendrite spacing. The results are compared with the microstructure from lab in-situ experiments at 1g, with a microgravity experiment on the sounding rocket MAPHEUS, accepted steady-state growth models, and results from multiscale computational simulations resolving dendritic arrays and gravity-induced flow (namely using a dendritic needle network approach coupled with a Navier-Stokes solver [3]). This constitutes an important step towards a better theoretical understanding of the influence of hypergravity on the microstructure formation. This project was funded by DLR-DAAD Research Fellowships Programme. [1] C. C. Bataile, R. N. Grugel, A. B. Hmelo and T. G. Wang, Met. Mat. Trans. 25A (1994) [2] A. Jafarizadeh-Koohbanani, S. Steinbach, J. Drescher, J. Frenzel and F. Kargl, Rev. Sci. Instrum. 94, 083703 (2023) [3] T. Isensee, D. Tourret, Acta Mat. 234 (2022)

Segregation Channels and Crystal Multiplication During the Solidification of an Aqueous Ammonium Chloride Solution

Andreas Ludwig, Golshan Shayesteh, Menghuai Wu and Abdellah Kharicha

Montanuniversitaet Leoben (Austria)

An experimental investigation of the solidification dynamics of an aqueous ammonium chloride solution, conducted in a relatively large rectangular test cell subject to vertical side cooling, reveals several interesting phenomena. An increasing number of equiaxed crystals influences both the growth of the vertical mushy layer and the flow in the bulk melt. The rising melt flow within the solidifying mushy zone creates segregation channels and leads to the formation of indentations at the exits of these channels. Crystals descending along the forefront of the mushy layer may either adhere to protruding dendrite tips or sediment onto the lower edges of the indentations. These processes lead to crystal agglomerations, which collapse once they grow too large. The subsequent impact of the sliding crystals on the lower mushy zone regions causes further fragmentation, a phenomenon known as crystal multiplication. The entire process of crystal agglomeration and sliding can also be referred to as a crystal avalanche.

Wed-A-II / Eutectics & Peritectics

Lamellar eutectic grains with a crystallographic mosaicity

Silvere Akamatsu, Mehdi Medjkoune, Karthikeyan Saravanabavan, Ulrike Hecht and Sabine Bottin-Rousseau

Sorbonne University & CNRS (France); University of Lorraine (France); CEA Liten (France); Access e.V. (Germany)

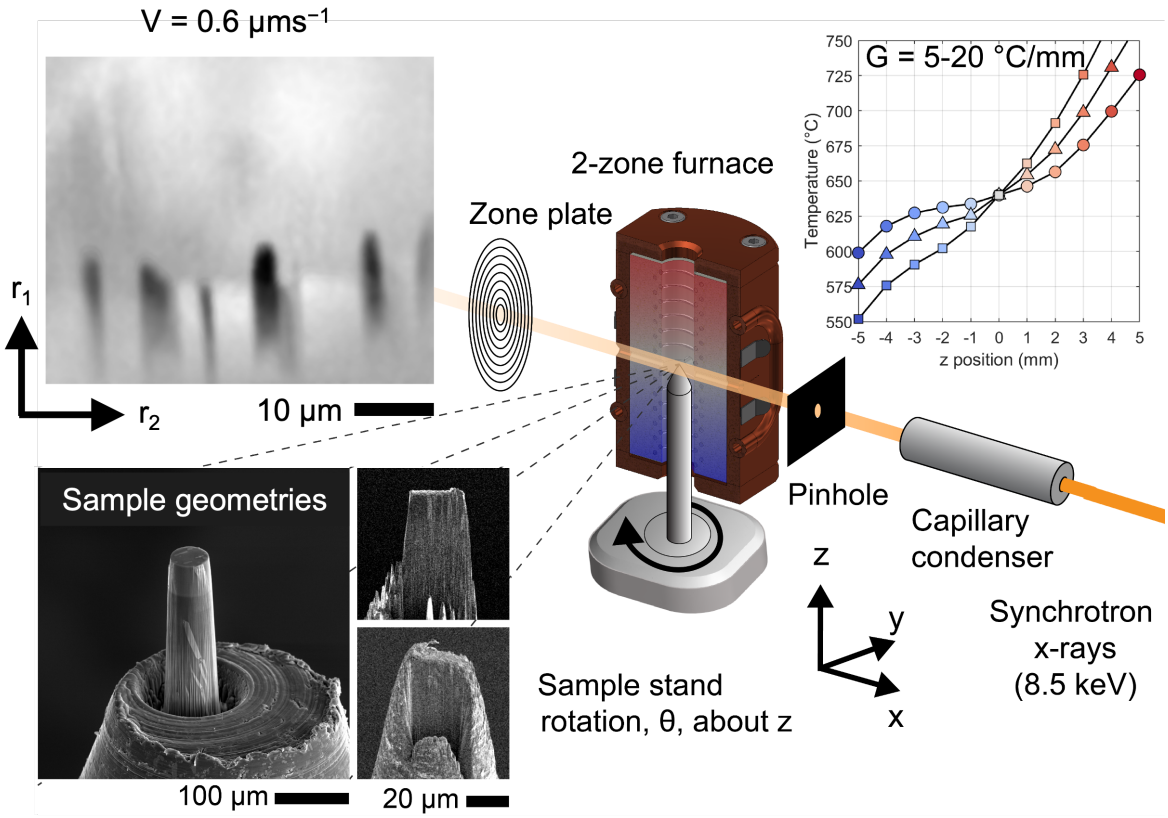
Upon directional solidification, many regular binary eutectic alloys form eutectic grains with remarkable crystal orientation relationships. In those systems, the dynamics of coupled-growth patterns and the shape of the frozen composite microstructures are sensitive to the interfacial anisotropy of the interphase boundaries in the solid. In practice, the problem is often further complexified by spatial variations of the orientation of the crystals on various length scales ranging down to the interphase spacing. Both the origin of this crystallographic mosaicity and its consequences on the eutectic-growth dynamics are largely ignored. We present an experimental exploration of the mosaicity in thin samples of the lamellar-eutectic Al-Al2Cu, combining in situ optical observations during directional solidification, and ex situ crystallographic analysis (EBSD). We also performed a numerical investigation (dynamic boundary-integral) of lamellar-eutectic arrays with an imposed spatial modulation of the interfacial anisotropy of the interphase boundaries in the solid. This allowed us to find out how a mosaic pattern can evolve toward a steady-state regime.

Capturing solidification in real-time at the nanoscale via full-field x-ray imaging

Paul Chao, Jonathan Goettsch, Soumyadeep Dasgupta, Emile Hazemann, Xianghui Xiao, Alan Taub and Ashwin J. Shahani

Sandia National Laboratories (USA); University of Michigan (USA); Brookhaven National Laboratory (USA)

The ability to directly observe the evolution of microstructure represents a milestone in non-destructive characterization. In particular, x-ray tomographic imaging has found success in uncovering the underlying mechanisms of phase transformations in partially and fully solidified metals. While synchrotron-based x-ray microtomography has provided valuable information on the solidification of large-scale features (such as dendrites), smaller-scale features (such as eutectic lamellae) have remained out of reach, until now. Here, we showcase the new capabilities in full-field x-ray nano-imaging via transmission x-ray microscopy at Brookhaven National Laboratory's National Synchrotron Light Source II (NSLS-II). This enables us to obtain unprecedented insights on the evolution of eutectics during solidification, melting, and under external perturbations like an imposed electric field. Our efforts are made possible by a new, two-zone furnace that permits real-time studies of directional solidification with precise monitoring of the thermal field. As a result, we can correlate the morphology of the solid-liquid interfaces with the 3D shapes of the eutectic solids frozen behind the growth front. We discuss the broader impacts of these findings on the fundamental science of eutectic solidification and outline some opportunities for future investigations using our new experimental platform at NSLS-II.

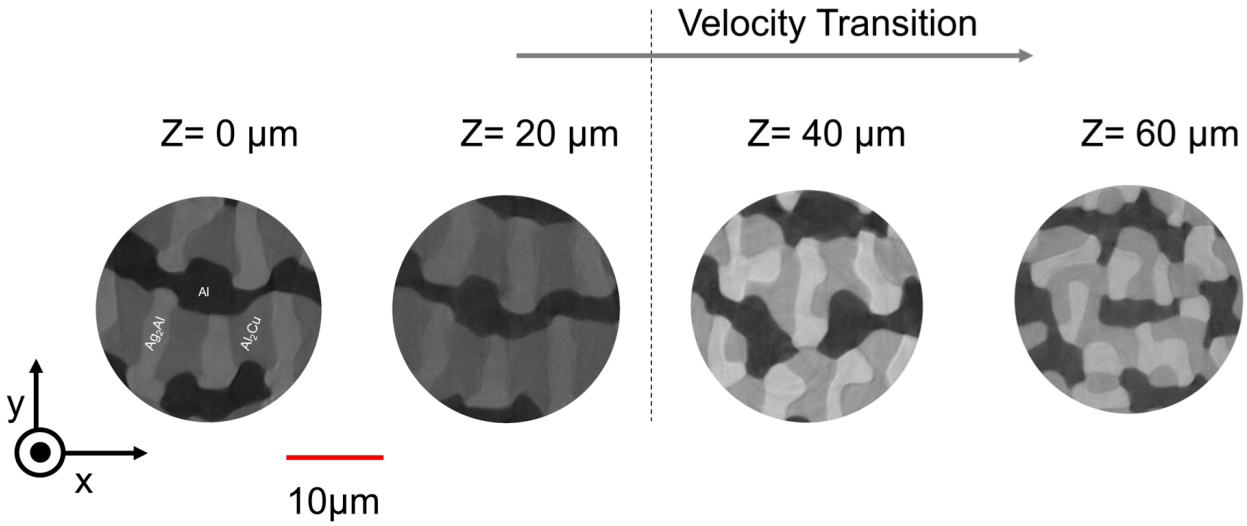


Synchrotron x-ray nanotomography uncovers microstructure of a three-phase eutectic solidified in microgravity

Soumyadeep Dasgupta, Xianghui Xiao, Melis Şerefoğlu, Ulrike Hecht and Ashwin J. Shahani

University of Michigan (USA); Brookhaven National Laboratory (USA); Marmara University (Turkey); Access e.V. (Germany)

Microstructure selection of two-phase eutectics is reasonably well understood, but the same cannot be said about three-phase eutectics. Our study aims to advance fundamental understanding of pattern formation in the Al-Ag-Cu system during (near-) invariant eutectic solidification. To examine the microstructure selection under diffusive conditions, the material was directionally solidified in a microgravity environment aboard the International Space Station. We imposed a velocity jump during the solidification process to determine the spacing adjustment and pattern recovery mechanisms. Following solidification, we investigated the three-phase microstructure at high spatial resolution (~50 nm) via synchrotron based x-ray nanotomography. With the wealth of detailed 3D data, we quantified various attributes of the three-phase pattern before, during, and after the velocity jump: the phase fractions, eutectic length scales, phase connectivities, and interfacial shapes. We find that the arrangement of solid phases is markedly different before and after the transition, which has important implications on the redistribution of solute ahead of the eutectic-liquid interface. Broadly, our research offers new insights into the selection of eutectic morphology and topology under directional solidification conditions, with implications to a wide array of multi-phase systems.

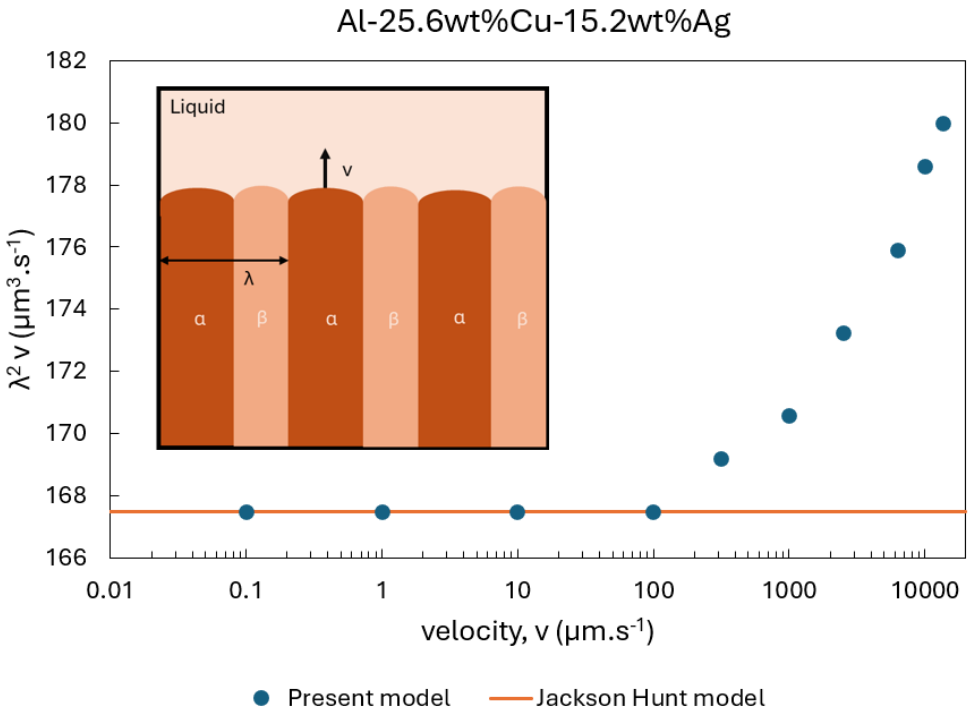


Numerical Modeling of Eutectic Growth in Multicomponent Alloys

Racha Hammoud, Oriane Senninger and Gildas Guillemot

Mines Paris - PSL University, CEMEF (France)

Given the temperature gradient, cooling rate and composition of a metal alloy, what microstructure will form during the solidification process? This is a crucial question, as recent advances in material forming techniques have led to significant variations in cooling conditions between processes. For example, solidification velocity and temperature gradient differ largely between additive manufacturing and ingot casting, resulting in the formation of distinct structures, such as eutectic or dendritic. It is therefore crucial to predict these microstructures with respect to the cooling conditions, as they ultimately influence end-use material properties. Nevertheless, experimental prediction of these microstructure formed regarding local solidification conditions and alloy properties is a costly and time-consuming process. The need to develop appropriate modelling tools is consequently of large importance in this aim. Solidification microstructure selection maps (SMSM) can predict the primary microstructure based on the aforementioned parameters. However, current models describing the growth of these structures are limited, particularly in the case of eutectic on multicomponent alloys. Regarding this limitation, we aim to develop a numerical model for generating SMSM. This presentation focuses on the step dedicated to the development of a eutectic growth model, extending past activity dedicated to binary alloys in [Senninger, O. et al. (2018). Acta Materialia, 161, 110-126]. The model's key strength is the consideration of non-linear properties, using thermodynamic coupling, on the multicomponent alloys of interest. In addition, shrinkage flow induced by the difference between liquid and solid densities is assumed. Currently, the implementation of Newton-Raphson method provides clear enhancement in the tool and enables model application to a large range of velocities. Moreover, the model is evaluated on diverse alloys compositions under varying cooling conditions, giving promising results favorably compared with theoretical and experimental data reported in literature.



Time-resolved and in-situ observation of solidification in Cu-Sn alloys

Yutaka Urakawa, Tomohiro Nishimura, Kohei Komori, Taka Narumi and Hideyuki Yasuda

Kobe Steel, Ltd. (Japan); Kyoto University (Japan)

Time-resolved and in-situ observation using X-ray imaging is a powerful method that enables direct observation of the solidification process. Observations of carbon steel using this method have revealed that a massive-like transformation may be selected instead of the peritectic reaction. Therefore, the phase transformation mechanisms in peritectic system alloys are of interest. In this study, we report the characteristics of the solidification process in Cu-Sn alloys, which are a type of peritectic system alloys. Time-resolved and in-situ observation was performed at SPring-8 (Hyogo, Japan). Sample with 8 mm x 8 mm x 0.1 mm was heated until melted (superheat 0 K) and then cooled at a constant rate to observe the solidification process. Monochromatic light of 28 keV was used for observation. The time resolution and spatial resolution of the transmission image were 8.33 frames per second and 2.74 μm x 2.74 μm per pixel, respectively. In addition, the phase transformation during the solidification process were determined by DTA. During the cooling process of the Cu-20mass%Sn alloy with a cooling rate of 0.83 K/s, a phase transformation from the α phase to the β phase was observed following solidification was complete. This phase transformation occurred when the temperature was undercooled from the peritectic temperature by 68.5 K. In addition, the number of diffraction points increased during the phase transformation. Therefore, a solid-state transformation with characteristics distinctly different from the peritectic reaction occurred in the Cu-Sn alloy. DTA analysis also indicated that a solid-state transformation, rather than a peritectic reaction, was selected. In this study, we employed time-resolved and in-situ observation using X-ray imaging to observe the solidification process in Cu-Sn alloys for the first time, and identified the solid-state transformation. This results suggest that this solid-state phase transformation is a phenomenon common to peritectic system alloys in general.

Phase-field simulations and theoretical description of peritectic coupled growth

Mathis Plapp

CNRS & Ecole Polytechnique, PMC (France)

Contrary to eutectic coupled growth, which is the most common growth mode for the solidification of eutectic alloys close to the eutectic composition, coupled growth occurs during the directional solidification of peritectic alloys only for specific ranges in composition, growth velocity, and applied temperature gradient. Only a few specific alloy systems have been studied in detail so far, among which Fe-Ni and Cu-Sn. An amended Jackson-Hunt-like theory that includes an approximation for the non-planar geometry of the solidification front is developed. The results are compared to phase-field simulations of the Cu-Sn system. The convergence behavior of phase-field models of peritectics with decreasing interface thickness is analyzed. Differences with the sharp-interface treatment by boundary-integral methods can be linked to the phenomenon of trijunction rotation, which is much stronger in peritectic than in eutectic two-phase growth. If this rotation is taken into account, a good agreement between simulations and theory is obtained.

Peritectic Layered Structures during Initial Transient

László Rátkai, Andreas Ludwig, Johann Mogeritsch and Tamás Pusztai

Wigner Research Centre for Physics (Hungary); Montanuniversitaet Leoben (Austria)

A peritectic alloy can form a layered structure with alternative alpha and beta lamellae, either perpendicular or parallel to the sample axis. The latter, known as Peritectic Coupled Growth (PCG), resembles the couple growth mode observed in eutectic alloys. Models for steady-state growth conditions exist for both growth forms. However, recent experiments conducted under microgravity conditions aboard the International Space Station, using the TRIS-NPG model system, revealed that PCG occurred before a steady-state was reached, during the so-called initial transient stage. This observation prompted the development of an extended phase-field model for peritectic solidification that accounts for the initial transient. The model was applied to two different scenarios: (i) a temperature gradient aligned with the sample axis, and (ii) a slight inclination between the temperature gradient and the sample axis. For both scenarios, we will demonstrate how the morphology evolves during the initial transient. In particular, we will discuss how both growth forms, perpendicular and parallel to the sample axis, represent the extreme ends of a more general case.

Wed-B-I / Modeling across scales I

Recent advances in atomistic modelling of alloy melt structures as input for solidification modelling

Philippe Jarry, Johannes Sandberg, Emilie Devijver, Thomas Voigtmann and Noel Jakse

Constellium C-TEC (France); University Grenoble Alpes & CNRS, SIMaP (France); German Aerospace Center, DLR (Germany)

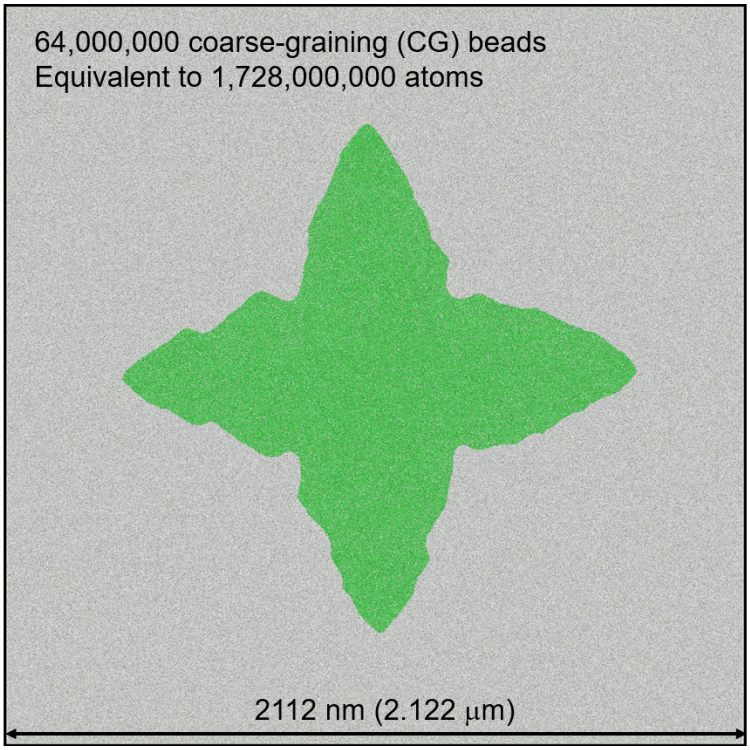
Solidification patterns result from a trade-off between diffusion of species and capillarity which solidification modelling usually takes as phenomenological inputs. It is now a well-established fact that solutes do not diffuse alone, rather solvated by atoms in motifs resulting from the interplay between topological and chemical Short-Range Order. Although not treated here, there are indications that the melt structure not only governs solute diffusivity but also the attachment kinetics contribution to the growth anisotropy. Understanding what governs alloy melt structuration at the atom scale is therefore strategic: can we tune the melt to obtain desirable solidification structures through a Diffusion / Anisotropy by Design approach? We will give an overview of recent advances in Ab Initio Molecular Dynamics studies of model binary, ternary and quaternary Al alloy melts that provide thorough understanding of the link between Short-Range Order and atom diffusivity, as well as an update on the upscaling of atomistic modelling of alloy melts by use of Machine-Learning potentials trained on ab initio calculations recently developed in the case of Al-Ni melts

Direct Observation of Dendritic Growth from Atomistic Simulation

Yasushi Shibuta

University of Tokyo (Japan)

Recent advancements in computational environments have significantly expanded the spatial scales accessible to molecular dynamics (MD) simulations. For instance, large-scale MD simulations of nucleation, solidification, and grain growth in metallic materials have achieved scales of up to 10 billion atoms and several micrometers [1]. By incorporating coarse-graining (CG) methods [2], it has become possible to directly simulate the formation of the characteristic four-fold symmetric dendritic structures during solidification, starting from the initial nucleus [3]. In this study, we performed large-scale CG-MD simulations to investigate crystal growth from a seed crystal in undercooled nickel melt within a quasi-two-dimensional system. During solidification, the release of latent heat raises the temperature of the solid phase, while the liquid phase experiences enhanced cooling to maintain the system's average temperature at the predefined undercooling level. The resulting negative temperature gradient at the solid-liquid interface, where the liquid side is cooler, destabilizes the interface and promotes dendritic growth. Conversely, when a Langevin thermostat was employed to instantly remove latent heat, a uniform temperature distribution was observed, and dendritic growth was suppressed. These findings demonstrate that even under identical average temperatures and statistical conditions, simulation outcomes can vary significantly depending on factors such as the type of heat bath and the rate of heat removal. Therefore, it is crucial to establish simulation conditions that accurately reflect the assumed temperature field, particularly in MD studies involving phase transitions. In this presentation, we will discuss the definition of temperature in MD simulations and the critical influence of the temperature field on simulation outcomes. [1] Y. Shibuta et al., Nature Comm. 8 (2017) 10. [2] L. Chalamet, D. Rodney, Y. Shibuta, Comp. Mater. Sci., 228 (2023) 112306. [3] Y. Shibuta, ISIJ Int., 64 (2024) 1107.

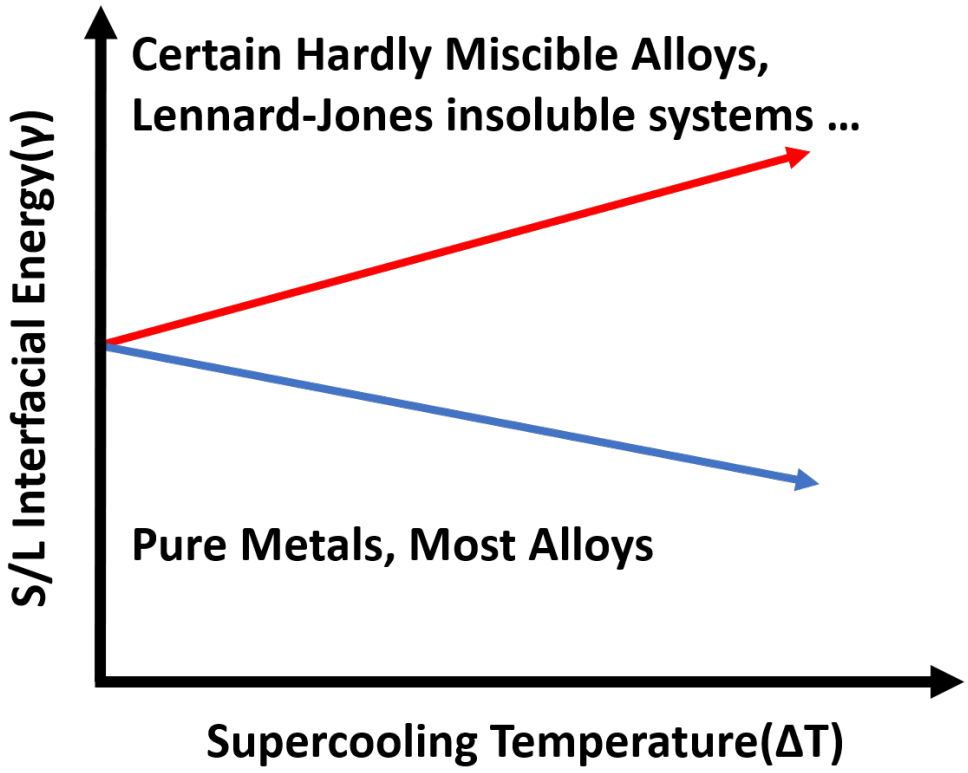


Unusual Temperature Dependence of the Solid-Liquid Interfacial Energy in the Binary Lennard-Jones System

Qing-Xi Chen, Lei Wang, Jin-Cheng Wang and Jeffrey Hoyt

Northwestern Polytechnical University (China); McMaster University (Canada)

It is well-known that the solid-liquid interfacial energy varies with temperature and composition. In most material systems, this energy decreases as temperature decreases. However, in Cu-Zr and Al-Sm systems, an abnormal behavior is observed: the solid-liquid interfacial energy increases with decreasing temperature. This unusual phenomenon could compete with the driving force of nucleation, thereby influencing the nucleation behavior in these systems. Both Cu-Zr and Al-Sm systems exhibit extremely low solubility of solute elements, which can significantly alter the thermodynamic properties and microstructure of the interface. However, how poorly soluble elements affect the relationship between solid-liquid interfacial energy and temperature, and whether this relationship is a common feature of systems with low solubility, remains an open question. To address these questions, we employ atomic simulation methods to investigate binary Lennard-Jones systems with varying atomic size ratios. In systems with a significantly large atomic size ratio (>15%), an anomalous increase in solid-liquid interfacial energy with decreasing temperature is observed. This behavior is investigated through thermodynamic analysis, specifically using the Gibbs adsorption equation, and through examination of microstructural features. These findings deepen our understanding of the thermodynamic and microscopic properties of solid-liquid interfacial energy and could guide the development of techniques for regulating interfacial energy through doping with poorly soluble elements.



Assessment of the meshless RBF-FD method for the 3-D phase-field modelling of dendrite growth

Tadej Dobravec, Boštjan Mavrič and Božidar Šarler

University of Ljubljana (Slovenia)

This work aims to analyse the performance of the radial basis function generated finite difference (RBF-FD) method for solving the standard 3-D test case for dendrite growth from a supercooled pure melt. The RBF-FD method is a finite-difference-like meshless method based on collocation in overlapping local support domains. In the method, we apply fifth-degree polyharmonic splines as radial basis functions and second-order monomial augmentation. We accelerate the calculation by a 3-D space-time adaptive algorithm based on the octree data structure. The test case considers cubic dendrite growth at fixed supercooling for different strengths of surface energy anisotropy. We analyse the accuracy when simulating growth in three different preferential directions (100, 110, 111). This test case was initially solved using the finite-difference method, and the authors reported on the strong influence of mesh-induced anisotropy. They proposed modification of the parameters of the phase-field model, effectively cancelling the problematic mesh-induced anisotropy and allowing the utilisation of larger node spacings. Mesh-induced anisotropy was later also observed when using the finite-element method. In the current study, we aim to solve the phase-field model in its original form, i.e., without modifying the parameters of the phase-field model. We discretise the equations using the same regular node distribution as in the finite-difference method. For comparison, we also solve the test case using the non-linear preconditioned phase-field model. We analyse how the size of the local support domains in the RBF-FD method affects the accuracy and mesh-induced anisotropy. We show that the phase-field model can be solved with reasonable accuracy without modifying its parameters if the sizes of local support domains are large enough. As expected, we accurately solved the test case with larger node spacings when utilising the non-linear preconditioning.

Bridging length scales in additive manufacturing conditions with in-situ rapid solidification experiments and simulation

Tatu Pinomaa, Adriana Eres-Castellanos, Pascal Thome, Joni Kaipainen, Abhishek Biswas, Nikolas Provatas, Amy J. Clarke, Anssi Laukkanen, Joseph T. McKeown and Thomas Voisin

VTT (Finland); Los Alamos National Laboratory (USA); University of Arizona (USA); McGill University (Canada); Lawrence Livermore National Laboratory (USA)

Simulating AM microstructures remains a formidable challenge. Focusing on pure aluminum and aluminum-copper alloys, we consider thin-film conditions via dynamic transmission electron microscopy (DTEM), followed by AM single scan tracks; for both cases, we acquire in-situ data about the melt pool geometry evolution, allowing for quantitative calibration of the thermal distributions in the simulations. We perform quantitative phase field simulations describing DTEM experiments, including heat diffusion and latent heat release via multi-grid method. The AM single scan tracks are paired with melt pool flow simulations, followed by phase field simulations in selected G-V conditions. Our model predictions agree well with characterized microstructures in terms of microsegregation patterning and grain boundary trajectories. We discuss the general role of alloying in competitive grain growth in rapid solidification, and how growth morphologies affect grain boundary trajectories. We also examine precipitation, (mis)alignment of crystal 100-direction and thermal gradients, and crystal orientation gradients.

Modelling of microstructure evolution during polymer solidification using the phase-field method

Ahmed Elmoghazy, Andreas Prahs, Daniel Schneider and Britta Nestler

Karlsruhe Institute of Technology (Germany)

The crystallization of polymers plays a crucial role in shaping the mechanical and thermal characteristics of materials produced via processes like extrusion and injection molding. The microstructure, morphology and degree of crystallinity achieved during these processes are essential factors that influence the final properties of semi-crystalline polymer parts. This study presents a thermodynamically consistent multiphase-field model for polymer crystallization, coupling the Nakamura equation [1] with a multiphase-field formulation along with the heat conduction equation using a latent heat contribution. The latent heat term incorporates both the effects of crystallinity as well as phase evolution. The Helmholtz free energy density of the system is represented as the sum of contributions from crystallinity and thermal energy, ensuring thermodynamic consistency. Different types of driving forces were tested (e.g. from [1] and compared against experimental data. The model also incorporates material parameter dependencies on local crystallinity, such as density, interfacial energy, thermal conductivity, and specific heat capacity. The developed model is implemented in an in-house simulation framework, PACE3D, and applied to study the solidification and microstructure evolution of PA6 under varying cooling rates. Different domain sizes were simulated and compared to study the effect of the exothermic heat contribution. This contribution highlights the importance of thermodynamic consistency and parameter coupling in predictive modeling of polymer crystallization and microstructure morphology during the solidification process. The results offer a route for advancing material design and optimization in polymer-based applications, e.g. additive manufacturing [2]. [1] N. Afrasiabian, A. Elmoghazy, J. Blarr, et al., Crystallization and crystal morphology of polymers: A multiphase-field study, Journal of Thermoplastic Composite Materials, Nov. 2024 [2] A. Elmoghazy, A. Heuer, A. Kneer, et al., Phase-field modeling of the morphological and thermal evolution of additively manufactured polylactic acid layers and their influence on the effective elastic mechanical properties, Progress in Additive Manufacturing, Dec. 2024

Wed-B-II / Modeling across scales II

High-performance phase-field lattice Boltzmann simulations for semi-solid deformation

Tomohiro Takaki

Kyoto Institute of Technology (Japan)

Semi-solid deformation is a critical phenomenon in both casting and semi-solid metal processing, involving a complex interplay of multi-physics phenomena such as solidification and melting, grain motion, graingrain interactions, deformation of solid grains, thermal and solutal transport, and liquid flow. Because semi-solid deformation causes solidification defects such as macrosegregation and porosity, it is essential to clarify the detailed deformation behavior. Numerical simulation plays a vital role in elucidating the underlying mechanisms. In this study, we developed a multi-phase-field lattice Boltzmann (MPF-LB) model capable of capturing key aspects of semi-solid deformation in binary alloys, including phase transformation, grain motion, graingrain interactions, and liquid flow. Using the developed model, we systematically conducted two-dimensional simple shear deformation simulations by varying the solid fraction, deformation rate, and grain morphology. Special attention was given to the formation and evolution of shear bands. Preliminary three-dimensional simulations, which represent a challenging task requiring high-performance computing, are also presented. Furthermore, we demonstrate semi-solid deformation simulations under more complex conditions, including rotating vane flow and compression of a cylindrical sample.

Large scale simulations of bi-crystal competition with buoyancy driven fluid flow

Peter Soar, Ivars Krastins, Paul Brown, Owen Draper, Nick Green and Andrew Kao

University of Greenwich (UK); Rolls-Royce plc., Derby (UK); University of Birmingham (UK)

During the solidification process, competition between differently oriented dendrites plays a key role in the formation of the microstructure which ultimately dictates the material properties of the parts. Many of the numerical studies exploring this phenomenon have used a 2D representation of the system, however this idealised assumption can lead to some mismatches with the behaviour observed in experiments. The geometric complexities of the interactions of grains across of the full range of 3D orientations becomes largely overlooked and any fluid flow behaviour becomes dubious as liquid cannot flow around the dendrites as it would in reality. While there have been 3D studies of this dendritic competition, many of these have been done using the phase field method which limits the physical size of the domain that can be reasonably simulated due to the fine cell sizes required by the method. In this study we have applied a Cellular Automata dendritic solidification code deployed in parallel on the University of Greenwich High Performance Computer system, which allows the simulation of microstructure at an industrially relevant scale. This has been coupled to a Lattice Boltzmann solver for the simulation of buoyancy driven fluid flow which can operate on a macroscopic scale and cause large scale solute redistribution that impacts the dendritic competition in ways that could not be observed in a simulation of a smaller physical domain size. To help elucidate this phenomenon, we present a numerical study of a converging bi-crystal dendritic system that varies the 3D orientations of the bi-crystals and examines the impact of different thermal conditions on the development of the microstructure. Where possible these simulations are related to published experimental results to support the modelling results and provide a deeper understanding of the mechanisms.

Multiscale modeling of diffusive grain interactions during equiaxed dendritic solidification

Abdelhalim Chirouf, Benoît Appolaire, Yann Le Bouar, Alphonse Finel and Miha Založnik

Université de Lorraine, CNRS, IJL (France)

Dendritic crystal grains are the most common growth form in solidification of metal alloys. The growth of equiaxed dendritic grains during the solidification of an alloy is accompanied by the ejection of chemical species (solutes) into their environment. Nearby grains interact via the solute diffusion field in the liquid phase. These interactions depend to a large degree on the spatial arrangement of the grains. We show that the spatial arrangement does not only affect the shape and the size of grains but also governs the overall kinetics of the phase transformation in the mushy zone. In current macroscopic averaged (mean-field) models the description of the spatial arrangement is entirely neglected. The diffusive interactions are thus overly simplified and the power of these models to predict of the solidification kinetics is impaired. In this study we investigate diffusive grain interactions during equiaxed solidification by full-field simulations of a representative elementary volume (REV) containing an ensemble of grains. The simulations are done with the Grain Envelope Model (GEM) for different periodic and random arrangements of grains. We compare the full-field results to state-of-the-art mean-field models and we point out the limitations of the latter. We propose an analysis of the interactions of individual grains with their local neighborhood, defined by a Voronoi tessellation. Based on this analysis we propose an improved macroscopic model that includes a description of the spatial arrangement of grains.

Phase-Field Investigation of Solidification Cracking Probability During Laser Beam Welding

Muhammad Umar, Nishant Prajapati, Daniel Schneider and Britta Nestler

Institute for Applied Materials - Microstructure Modelling and Simulation (IAM-MMS), KIT, Karlsruhe (Germany)

Austenitic stainless steels, renowned for their exceptional corrosion resistance and mechanical properties, find extensive applications in consumer goods, medical diagnostic machinery, and chemical processing industry. However, their applications involving high-speed welding processes, such as laser beam welding, are constrained due to occurrence of solidification cracking. This phenomenon is attributed to extreme cooling rates which affect solute redistribution and concentration gradients during early solidification stages. This study investigates the thermochemical factors contributing to solidification cracking probability during dendritic solidification of austenitic stainless steels, focusing on a quaternary (Fe-C-Cr-Ni) alloy configuration. For this purpose CALPHAD-fitted Gibbs energy functions are integrated into a grand potential-based multicomponent and multiphase-field approach to simulate thermally undercooled liquid solidification. Additionally, the model investigates the influence of local morphology, temperature distribution, dendrite orientation and micro-segregation on stress and strain localization. Mechanical parameters i.e., elastic modulus, Poisson ratio and thermal expansion coefficient are considered at near solidification temperature to reach a better prediction of local mechanical behaviour. By analysing the impact of these local variables on crack formation susceptibility in the inter-dendritic region, this research aims to enhance the understanding of the process-structure-property relationship during austenitic stainless steel solidification. The simulation results can be qualitatively well compared with experimental observations and quantitatively validated against the theory. The findings reveal that the dendritic structure under variable local thermochemical and orientation conditions has a notable effect on the local mechanical behaviour. It is observed that the local stress-strain peaks increase when highly misoriented dendrites with a substantial difference in local concentrations coalesce in the centre of the weld seam. Thermal contractions play a vital role and produce maximum eigenstrain in the center of the seam, which adds up to enhance the probability of solidification cracking.

Finite Element Modelling of Multi-Pass Welding in 304L Stainless Steel Cladded with Low Alloy Low Carbon Steel

Ali Fahem, Hong Dong and Elsiddig Elmukashfi

University of Leicester (UK)

This study investigates the thermal history and residual stress evolution in multi-pass welding of 304L stainless steel cladded with low alloy low carbon steel using finite element (FE) modelling. A six-pass welding process was simulated to replicate thermal and mechanical effects, with material properties derived from JMatPro software to ensure accurate representation of temperature-dependent behaviour. Thermal simulations captured the temperature distribution and cooling rates across the weld and heat-affected zones (HAZ), reflecting the cumulative effects of multi-pass heat input. Residual stresses were predominantly tensile in the cladding layer, transitioning to compressive in the substrate. Microhardness measurements showed an average of approximately 200 HV for Q345R steel and 250 HV for 304L stainless steel, with a peak of 275 HV at the interface. Tensile and compression tests revealed enhanced tensile strength and ductility, while toughness increased in both normal and rolling directions. Microstructural analysis identified distinct zones at the interface caused by carbon and chromium diffusion, leading to decarbonisation in Q345R steel and carbonisation in stainless steel. These experimental results validate the predictions of thermal history and mechanical properties obtained from the JMatPro-supported FE model. This study demonstrates the robust predictive capability of FE modelling for multi-pass welding, offering insights into optimising welding procedures and improving the structural performance of cladded systems for industrial applications.

Stress generation in the container during solidification of water

Radhika Sarawagi and Virkeshwar Kumar

Indian institute of Technology Kanpur (India)

During freezing, most materials shrink as their density increases, with significant shrinkage occurring at the melting point. At the phase change, the shrinkage volume is typically given by (~((ρ_s-ρ_l)/ρ_s) V_0). However, materials like water, bismuth, and antimony expand during solidification due to a lower solid phase density. Water, in particular, is widely used in anti-freezing liquids for cooling engines, turbines, and power plants. If the temperature of the anti-freeze liquid container drops below its freezing point, the liquid can expand and deform the container. To investigate this phenomenon, we conducted both numerical simulations (Ansys) and experimental studies to understand the stresses exerted on the container during water freezing. In our experiments, we used a three-sided cooling configuration to track the ice expansion front and validate the numerical simulations. Subsequently, we employed coupled simulations (FSI:fluid-structure interaction simulation), where solidification was modeled in Fluent, and container deformation was analyzed using the transient structural capabilities of Ansys. We simulated the solidification process in a rectangular aluminium container (inner dimensions of 10×10×5 cm^3, 2 mm wall thickness) with its outer walls maintained at -25°C. The container was filled with water to 90% of its height, leaving 10% of the volume for air to accommodate expansion (theoretical shrinkage volume~-8.5%). In the FSI simulation, the inner wall of the container was treated as the interface between the fluid and solid regions. For stress measurement, a two-way coupling approach was used, resulting in a lower pressure generation (~6MPa). In contrast, with one-way coupling, the pressure reached up to 30MPa. The continuous deformation of the container in the two-way coupling approach reduces the pressure. The maximum deformation observed was approximately 1.3mm, which represents 65% of the initial thickness of the container. To the best of the author's knowledge, this is the first study to demonstrate FSI during freezing.

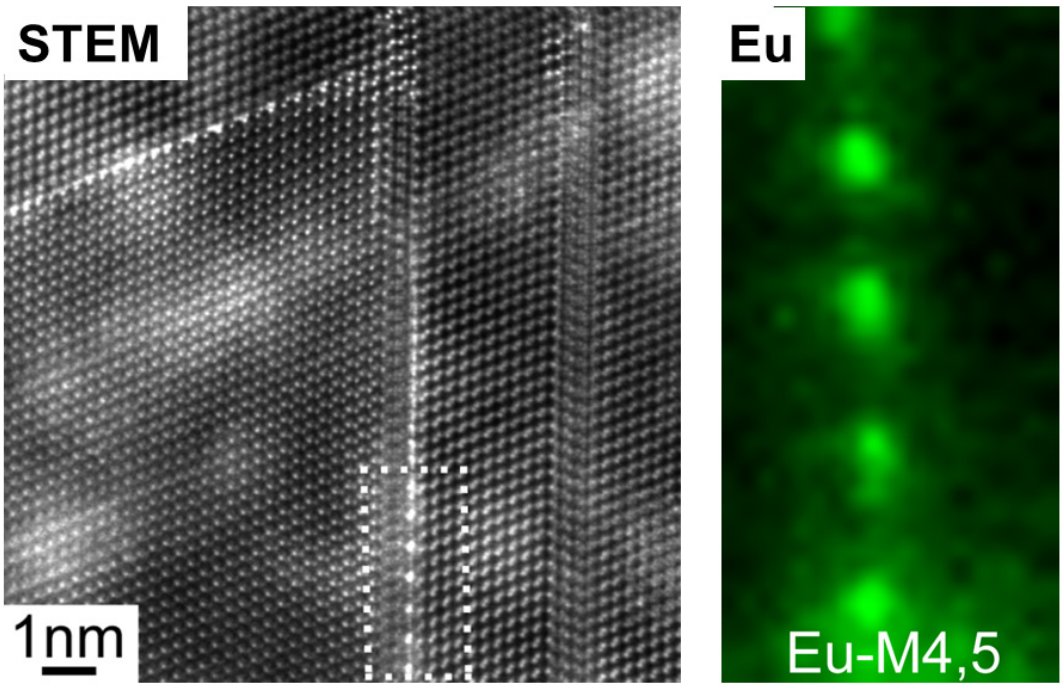
Wed-C-I / Aluminum alloys I

Atomic DFT simulation and experimental TEM APT observations on the distribution of modifying solutes within eutectic Si in Al-Si based alloys

Jiehua Li

Montanuniversitaet of Leoben (Austria)

Modifying the eutectic Si from flake-like to fibrous in Al-Si based alloys (i.e. A356, A357) is of great necessity to improve the performance of Al-Si alloys. Three well-known modification mechanisms (the impurity-induced twinning (IIT) mechanism and the twin plane re-entrant edge (TPRE) mechanism as well as the poisoning of the TPRE mechanism) are generally accepted to be valid under certain conditions. However, IIT, TPRE or poisoning of TPRE mechanism cannot be used to interpret all observations accompanying modification, indicating that other factors may be also valid. Solute entrainment was therefore proposed [1]. In this talk, I will report atomic density functional theory (DFT) simulation and experimental transmission electron microscopy (TEM, including high angle annular dark field imaging (HAADF) and electron energy loss spectroscopy (EELS) in scanning transmission electron microscopy (STEM)) together with atom probe tomography (APT) on the distribution of modifying elements (Sr, Na and Eu) within eutectic Si. Both atomic DFT simulation and experimental TEM APT observation reveals that modifying elements have three different roles: (i) the adsorption at the intersection of Si facets, inducing IIT growth mechanism, (ii) the adsorption at the twin plane re-entrant edge, inducing TPRE growth mechanism, and (iii) the adsorption ahead of the growing Si twins, inducing a solute entrainment within eutectic Si. This talk not only demonstrates a direct experimental support to the well-accepted poisoning of the TPRE and IIT growth mechanisms, but also provides a full picture about the behavior of modifying solutes, including the solute entrainment within eutectic Si.

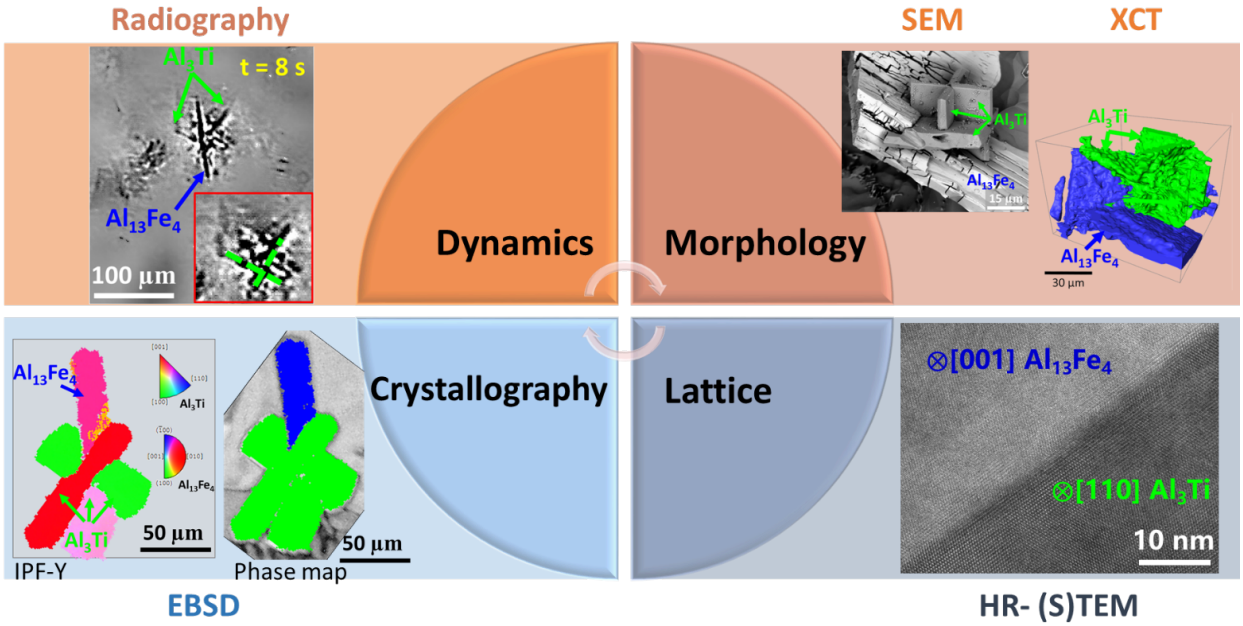


Revealing and controlling the formation dynamics of Fe-rich intermetallic compounds for impurity-tolerant alloy recirculation

Shikang Feng, Patrick Grant and Enzo Liotti

University of Oxford (UK)

In engineering Al alloys, second-phase intermetallic compounds (IMCs) that form during casting control critically alloy mechanical properties, corrosion performance and recyclability, despite their relatively low volume fraction (typically <5 vol.%). Due to the ubiquity of Fe in alloy feedstock, especially as the recycled fraction increases, Fe-rich IMCs form during solidification, generally in coarse (typically 50 μm to several millimetres), anisotropic morphologies. These IMCs, such as θ-Al13Fe4, α- and β-AlFeSi cannot be fully re-dissolved during downstream heat treatment, and can cause severe stress localisation and undermine alloy tensile ductility and toughness. These aspects hinder high-value upcycling of increasingly abundant post-consumer Al resources. Therefore, understanding Fe-rich IMCs has remained an active area of research, with a particular interest in refining their size as a means to render them more mechanically benign. Nonetheless, there remains opportunity for deepening the understanding of how to manipulate IMC formation through composition and solidification changes. We use in situ X-ray radiography, complemented with post-solidification electron backscattered diffraction (EBSD) and X-ray computed tomography (XCT), to investigate systematically the formation of Al13Fe4 that is found in a wide range of commercial Al alloys, using a model hypereutectic Al-Fe alloy. First, we show with a large real-time imaging dataset how IMC number density and formation rate can be effectively enhanced by inoculant additions and control of solidification conditions. Then, using a large post-solidification crystallographic dataset, we reveal reproducible IMC-inoculant orientation relationships, despite low crystal symmetry, and unveil a strong link between IMC formation and a twinning-induced IMC pseudo-symmetry. Finally, we show how we fuse the multi-technique insights to control the size and morphology of otherwise coarse, plate-like IMCs in recycled engineering alloys with high Fe contents. This work paves a potential pathway to designing next-generation, impurity-tolerant Al alloys and processes for greater alloy recirculation.

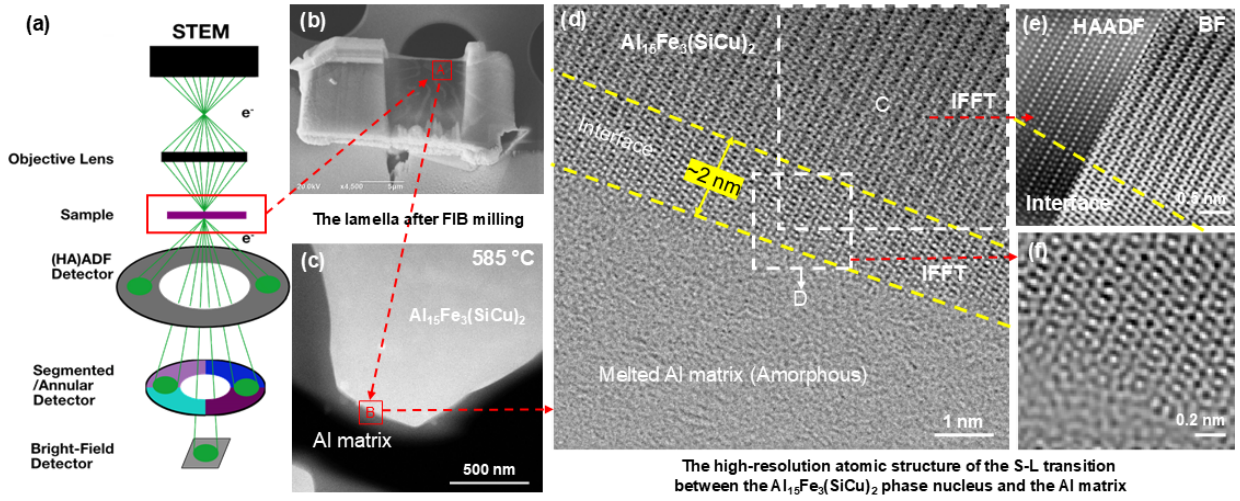


In situ STEM studies of the atomic structure transition across phase boundaries of a recycled Al alloy in melting and solidification

Yueyuan Wang, Kang Xiang, Mohsen Danaie, Chris Allen, Matthew Spink and Jiawei Mi

University of Hull (UK); Diamond Light Souce (UK)

Research into the dynamics of atomic structure transition in the liquid-to-solid solidification and/or the solid-to-solid phase transformation processes have been always a central topic in the matter physics and materials science field. An understanding of the atomic level structure changes is vital for providing scientific principles on how to control and manipulate the atoms to form the desired nano/microstructures. However, so far, real-time studies of the atomic structure evolution in metal alloys that are subject to high-temperature environment have been very challenging and sometimes extremely difficult. Recently, we have made an attempt to study the nucleation and growth dynamics of the intermetallic phases in an Al-recycled alloy with the composition of Al5Cu1.5Fe1.0Si. We used the JEOL STEM equipped with a wildfire nano-chip high temperature in-situ heater (up to 1000°C) available at the ePISC of the Diamond Light Source to image in real-time the atomic structure transition across the interfaces between the Al matrix and the Al2Cu and Al3Fe intermetallic phases respectively in the melting and cooling processes. We have found that the atomic structure transition occurred within approximately ten atomic layers across the interface with a transition from an amorphous to a crystalline state. While the different solute atoms diffused to the preferred location and formed the intermediate structure. We also studied the Al2Cu phase melting and solidification dynamics in the range of 20~585°C. The results show that the Al2Cu phase has a well-defined orientation relationship with the α-Al matrix, i.e., ((001)Al2Cu || {001} α-Al). This may contribute to the decrease of the nucleation energy barrier at onset of nucleation, indicating that, by adding different solute elements in recycled Al alloys, it is possible to control the nucleation dynamics and to achieve the optimal structure, size and morphology of the Fe containing intermetallic phases in the recycled Al alloys.



The high-resolution atomic structure of the S-L transition between the $Al_{15}Fe_3(SiCu)_2$ phase nucleus and the Al matrix

The effects of scrap addition on the structure and mechanical properties of hypereutectic Al-Fe alloys

Suwaree Chankitmunkong, Tawatchai Tangsuksan and Dmitry Eskin

King Mongkut's Institute of Technology Ladkrabang (Thailand); Brunel University of London (UK)

Hypereutectic Al-Fe alloys represent a new group of alloys with promising properties, offering moderate strength, high thermal stability, precipitation hardening capability and recyclability. In this study we used recycled beverage can scrap to produce Al-Fe alloys in order to demonstrate the suitability of these alloys for circular economy. Ultrasonic melt processing was applied to refine the structure. The scrap introduced impurities in the otherwise binary alloys, which modified the structure, improved strength and enabled precipitation hardening due to AlMnFeSi dispersoids and Mg-Si precipitates. The effects of scrap fraction in the alloy properties were quantified. This study highlights the potential of using recycled materials and advanced processing techniques to develop sustainable, high-performance aluminum alloys for a range of industrial applications.

Calphad-based multi-phase-field simulations of intermetallic compounds in secondary aluminum alloys with high impurity levels

Janin Eiken, Bernd Böttger and Markus Apel

Access e.V. (Germany)

The recycling of aluminum reduces production costs, energy consumption, and CO emissions. However, the inevitable accumulation of impurities promotes the formation of potentially harmful intermetallic compounds. Understanding and controlling intermetallic precipitation is crucial for improving the usability of secondary aluminum alloys. Calphad-based phase-field simulations provide valuable insights into the effects of alloy composition and processing conditions on precipitation sequences and phase fractions. In this study, we apply the multi-phase-field software Micress® to investigate the formation of Fe-rich intermetallics during the solidification of a secondary AlSi7Mg alloy with additions of Mg, Cu, Fe, and Mn. The modeling of the intermetallic compounds accounts for stoichiometric constraints and the interdependent solubility of Fe and Mn on shared sub-lattices. The Fe/Mn ratio strongly influences the formation sequence of the different intermetallic phases. High Fe levels favor the growth of brittle, plate-shaped β-Al9FeSi2 precipitates, which reduce ductility and toughness. Mn can counteract the negative effects by promoting the formation of α-Al15(Fe,Mn)3Si2 and α-Al8Fe2Si precipitates with less detrimental, polyhedral or script-type morphology. A key objective of the phase-field simulations is to determine the interplay between the Fe/Mn ratio and the processing conditions in terms of phase fraction and precipitate distribution.

An autonomous high throughput microstructure-property modelling approach toward design of recycling friendly Al-Si foundry alloys

Qiang Du, Astrid Marthinsen and Kjerstin Ellensen

SINTEF Industry (Norway)

We report our recent research activities on an autonomous high throughput microstructure-property modelling framework towards the whole fabrication route of Al-Mg-Si foundry alloys, i.e. casting, solid solution and ageing heat treatment. The framework is established with a high throughput simulation scheduling software, PyMat, which could drive various microstructure and property modelling software to perform sequential high throughput autonomous simulations. The microstructure models, consists of CALPHAD-coupled classical Scheil model, Pseudo Front Tracking Model, Kampmann Wagner Numerical models. They can predict the fractions of eutectic phase/Intermetallic phase after solidification, the solute levels after solution heat treatments and the size distributions of hardening particles after aging heat treatment for industrial aluminum alloys. The predicted microstructural features are then used to inform the materials constituent behaviour, castability, quench-ability, and to the final mechanical properties and electrical conductivities. Especially to predict the final yield strength of the foundry alloy, an eutectic phase strength model is proposed based on the mixture law and experimental data. All these chain models and the relevant aluminum thermodynamic database are validated by comparing the models predictions with experimental results. We demonstrate that the CALPHAD-coupled microstructure and properties models can be used in an efficient and high-throughput manner to predict the microstructural evolution from initial melt to the final product for a wide range of compositional window Al-Cr-Fe-Mg-Mn-Si alloys and processing conditions. It is anticipated that the proposed modelling framework is valuable in in aluminium alloys design and high pressure die casting processing parameter optimization, especially within in the context of green alloys.

Wed-C-II / Aluminum alloys II

Design of crack-resistant and high-temperature aluminium alloys for a range of casting technologies

Chengbo Zhu, Dmitry Eskin, Iakovos Tzanakis and Peter Lee

Brunel University of London, BCAST (UK); Oxford Brookes University (UK); University College London (UK)

Aluminium alloys are cost-effective and lightweight materials that are widely used in the transportation industry, where cost and weight are the main considerations for material selection. Operating at elevated temperatures (T>~0.5T_m, where T_m is the absolute melting temperature of Al) is known to be a weakness of these alloys. We propose a new methodology to design Al alloys with thermal stability and low cracking susceptibility using various theoretical and experimental techniques. Following the methodology, two new alloys based on Al-Fe-Mn-Ni-Ce system were cast in a range of cooling rates and investigated. To find alloys with low cracking tendency, only compositions with a small freezing range at the final stage of solidification were selected. Then, the solidification contraction of those alloys was experimentally measured to further screen the compositions with a lower thermal strain accumulated upon solidification. After the screening, the microstructural morphologies obtained under different cooling rates were characterised. In the experiments, no hot tearing was observed. The results showed that the microstructures in the alloys were stable after 24 hours of heat treatment at 450°C with no structure coarsening, and a high proportion of the strength was retained after the tensile test at 300°C. The methodology can be applied to designing Al alloys for both conventional casting and additive manufacturing.

Investigating solidification path of Al-Mg alloy for welding and casting conditions

Nicolas Coniglio, Fabrice Guittonneau, Laurent Barrallier and Marie Bedel

ENSAM (France)

Solidification cracking is a commonly encountered defect in aluminum welds rendering some of them unwedable. As the metal solidifies, the remaining liquid in the mushy zone is subjected to tensile stresses due to shrinkage and thermal contraction, which can lead to cracking. This crack initiates and grows behind a weld pool within the two-phase mushy zone. The susceptibility of a metal to this defect has been correlated to its solidification path, where a wide solidification range allows greater stresses to build up. Nevertheless, despite decades long efforts of investigation, there remains a lack of understanding about why the long-freezing range Al-Mg alloys demonstrate good weldability. The present work addresses this knowledge gap by investigating the solidification path of a commercial Al-Mg alloy in two distinct conditions corresponding to sand gravity casting and arc welding processes. Each of these thermal conditions affects in different manners the solidification path and the Mg distribution in the solidified material. The evolution during solidification of the solid fraction and the alloying content deviate experimentally from the theoretical predictions established by the Scheil and Lever models. These differences may arise from deviations between the idealized theoretical conditions and the actual welding or casting processes. Microstructural analyses indicate a heterogeneous distribution of Mg alloying element in the solidified matrix with localized enrichment or depletion of magnesium. Mass-balance analysis applied on EDS maps estimated partition coefficient values of Mg in Al deviating from the equilibrium value and varying during solidification progress. This influences in particular the formation of low-melting constituents that affects the resistance to solidification cracking. The findings of this study have significant implications for better understanding the weldability of Al-Mg alloys. These insights are essential for advancing mechanistic models of solidification cracking, potentially leading to improved welding practices and alloy formulations.

Influence of composition on microstructure formation in undercooled directionally solidified aluminium alloys

Thomas Schenk, Svetlana Tsareva, Jean-Philippe Tinnes, Ahmed Kaci Boukellal and Julien Zollinger

Université de Lorraine & CNRS, IJL (France)

Aluminum alloys can have particular microstructures, some of which are not yet fully explained: twinned dendrites, ISRO-mediated equiaxed grains... The composition of the alloy plays a key role in these phenomena. In this work, a first systematic study of the effect of alloying element is made. A wide range of Al alloys was investigated. From pure aluminum, additions of Fe, Si, Mn, Zr, and combination of the latter were tested. Using the free-falling droplet experiments instrumented with pyrometers and photodiode, samples were processed for further microstructural analysis, including electron backscattered diffraction (EBSD). Different solidification patterns were obtained depending on the chemical composition of the alloy, including fully columnar; columnar and equiaxed microstructures; with in some case, feathery grains of twinned dendrites. The experimental thermal data is used to model the solidification microstructure selection and relate phase formation to the local thermal field. The results are discussed based on the nature of the alloying element and related phase formation, and on previous results from the literature.

Evaluation of the cooling rate during solidification process of DC casting aluminum alloy industrial ingots

Kangcai Yu, Jun Li, Yongfu Wu and Xiang Li

Chinalco Materials Application Research Institute Co. Ltd (China); Shanghai Jiao Tong University (China); Chinalco Advanced Manufacturing Co., Ltd (China)

The cooling rate is one of the most critical parameters in the casting process, having a profound impact on the solidification behavior and subsequent microstructure of the ingots, which is difficult to measure in industrial-scale ingots. Although there are several methods for calculating the cooling rate, including the average cooling rate and the instantaneous cooling rate, how to accurately calculate the cooling rate is still a difficulty in the industry. In this study, the cooling rates through different calculate methods in the DC casting process of aluminum alloy is evaluated by experimental microstructure. A new cooling rate calculation method based on the streamline of the liquid phase is proposed, which considers the effect of flow field inside the liquid sump. This cooling rate method has a higher accuracy in predicting the primary coarse phases distribution in the ingot. It was found that the lowest cooling rate in the ingot is not at the center of the ingot, but at the position approximately 3/8 of the ingot thickness, which is consistent with the grain size distribution. The influence of ingot size, casting speed, casting temperature, secondary water flow rate, and other parameters on the distribution of cooling rates is systematically studied, which provides a reference for the control of the solidification microstructure of DC casting industrial aluminum alloy ingots.

Simulation of Fluid Flow for a Dual-Alloy Injector Casting Process

Maximilian Erber, Georg Fuchs, Benedikt Kirchebner and Wolfram Volk

Technical University Munich (Germany)

As the demand for lightweight construction increases, so do the requirements for castings. Those can be contradictory and difficult to be met by using a single alloy composition. Therefore, a casting process was developed that allows the casting of two aluminum alloys in a single process. In this procedure, two aluminum melts are filled into the mold through one or more ceramic injectors. The outlet of the injector is located below the surface of the melt during the filling process and is pulled out of the mold as the melt height increases. Consequently, the necessity for an ingate system is negated, thereby reducing the amount of circular material. In this work this process is simulated. The validation strategy for these simulations involves the use of temperature measurements, as well as spark spectroscopy and microscopy. The objective of this study is to identify potential enhancements to the process, determine viable process windows, and predict the local alloy composition of the cast component.

Modification of the regulation model for continuous casting of aluminium alloys to account for the melt convection

Igor Vusanovic and Bozidar Šarler

University of Montenegro (Montenegro); University of Ljubljana (Slovenia)

In the online regulation of continuous casting of aluminium alloys, a simplified model must be used that does not involve thermo-solutal convection in the melt due to the computational time restriction. This regulation model involves only heat conduction with a predefined velocity. We compare this model with a second, physically more involved model, that additionally copes with thermal convection in the melt. This model is computationally much more involved and unsuitable for online regulation. Both models are compared regarding the amount of melt volume, sump depth, and position of the solidus and liquidus isotherms in the mould. A correction to the regulation model is proposed that matches the important output parameters of the second model. Both transient models and the corrections are constructed in a non-dimensional setting to systematically assess the differences.

Parallel sessions

Day 3 / Thursday June 12, 2025

Session Thu-A-I / Microgravity II

Dendritic Array Stability in a 3D Diffusion Controlled Directionally Solidified Alloy System: Benchmark Experiments and Computation

Mehdi Medjkoune, Trevor Lyons, Fatima Mota, Jiefu Tian, Kaihua Ji, Louise Littles, Alain Karma and Nathalie Bergeon

Aix Marseille University & CNRS, IM2NP (France); Northeastern University (USA); Lawrence Livermore National Laboratory (USA); NASA Marshall Space Flight Center (USA)

The exploration of solidification microstructures is of industrial interest to monitor microstructures, which directly influence the macroscopic properties of materials, but it also contributes to the understanding of non-linear self-organizing dynamics in non-equilibrium systems. The dynamics and nonlinear nature of microstructure formation renders in situ observation of the interface a precious tool to gain knowledge on the time-evolution of the interface pattern. In addition, it has long been established that significant convection during solidification processes alters the formation of interfacial microstructures and complicates its analysis. The experiments presented were realized in the Directional Solidification Insert (DSI) of the DECLIC instrument onboard the International Space Station (ISS), on the framework of a collaborative project between the French and American space agencies, CNES and NASA. It is dedicated to the real-time in-situ observation of the interfacial microstructure during directional solidification of 3D bulk samples of transparent organic alloys. We present a comprehensive quantitative analysis of stability bands for dendritic arrays during directional solidification of a succinonitrile-0.46 wt% camphor alloy. We quantify the stable primary spacing range of spatially extended three-dimensional dendritic array structures under purely diffusive growth conditions. Through velocity jump experiments and detailed examination of sub-grain boundary dynamics, we characterize the key instabilities that limit the stability range. Phase field simulations are performed to characterize the stability limits of dendritic array structures for quantitative comparison with the flight experiments. Although the simulations qualitatively reproduce general trends, significant quantitative deviations are noted, indicating the influence of additional factors. These deviations are explored through phase field simulations of a ternary alloy that highlight the important effects of an additional fast-diffusing impurity. These findings contribute to a deeper understanding of dendritic growth dynamics and offer valuable benchmark data that could aid in refining predictive models and improving control of dendritic microstructures in metallurgical applications.

The X-Ray Facility (XRF): A new research capability for the International Space Station

Antonella Sgambati, Ana Frutos Pastor, Wim Sillekens, Till Eisenberg, Nicola Picchi, Emanuele Monchieri, Johan Olsson, Alessandro Mariani and Andrea Malagoni

European Space Agency, ESTEC (Netherlands); Airbus Defence and Space (Germany); Swedish Space Corporation (Sweden); Kayser (Italia); DTM Technologies (Italia)

Microgravity research is a niche within the materials science and engineering domain. Yet, scientists have been pursuing such research for decades now using platforms like parabolic flights, sounding rockets, and the International Space Station (ISS). The absence of gravity suppresses thermo-solutal convection in solidification processes amongst others, which in equivalent experiments on Earth conceals the underlying solidification mechanisms. The European Space Agency (ESA) is currently developing a research capability for the ISS to enable in-situ observation of metal-alloy solidification using X-ray radiography. This X-Ray Facility will consist of a core unit (with a microfocus X-ray source) and an experiment unit including diagnostics (i.e., a furnace with crucible/sample and scintillator/camera), allowing real-time imaging of the process for typically aluminium alloys. This paper will discuss the development project for this facility as it is currently carried out by a consortium of European industries and ESA with the support of a team of scientists. Following the common stages of a space payload development, the project is now about halfway and headed for the Critical Design Review. Focus of the presentation will be on those aspects that are of particular relevance from the scientific perspective, notably regarding the opportunities it will offer for solidification research and the constraints that have to be taken into account in designing and performing the experiments. This includes the main hardware and software technical features, communication (telemetry and data handling), as well as the preparation and implementation of experiment runs.

Analysis of preparatory directional solidification experiments using XRF (X-Ray Facility) for ISS

Guillaume Reinhart, Florian Kargl, Maike Becker, David Browne, Laszlo Sturz, Henri Nguyen-Thi, Ana Frutos Pastor, Antonella Sgambatti and Wilhelmus Sillekens

Aix Marseille University & CNRS, IM2NP (France); Deutsches Zentrum für Luft- und Raumfahrt, DLR (Germany); Access e.V. (Germany); European Space Agency, ESTEC (Netherlands)

The control of solidification processes requires a clear understanding of complex mechanisms acting at different scales in time and space. Grain nucleation, chemical diffusion, dendritic growth, fluid flow, and development of gas bubbles are typical examples of such phenomena. The study of solidification is made even more difficult on Earth where these mechanisms are disturbed by gravity-related effects, such as sedimentation and buoyancy-driven convection. However, experiments can be carried out in purely diffusive conditions by using microgravity platforms, allowing benchmark data to be collected. By this means, the impact of gravity can be highlighted, and models validated by comparison with ground experiments. X-radiography enables the in-situ monitoring of metal solidification processes and gives access to additional information on the dynamics of the underlying mechanisms. In the last decade, the use of this imaging technique has been adapted to the study of solidification aboard microgravity platforms such as sounding rockets and parabolic flights. However, the limited microgravity duration accessible via these platforms is not sufficient to reach steady-state conditions. The European Space Agency is currently developing a facility for the International Space Station (ISS) to overcome this limitation. Unlike the other microgravity platforms, XRF (X-Ray Facility) will enable multiple experiments so that statistical variations can be studied, and the principal parameters varied by design. The present contribution will bring forward experimental investigations carried out on Earth using the Experiment Unit 1 (EU-1), which is dedicated to the study of the directional solidification of aluminum alloys. While the objective of these activities was to validate the technical performance of the set-up, preliminary scientific insights were also gained. The grain structure formation and temperature field features during the directional solidification of Al-based alloys are derived from analyses of image sequences. The possibilities offered by this new device will be presented and discussed.

Examining equiaxed solidification under microgravity through multi-scale characterization

Fan Wu, Geetanjali Srivastava, Jonathan Mullen, Mert Celikin, Andrew Murphy, Wim Sillekens, David Browne and Wajira Mirihanage

University of Manchester (UK); University College Dublin (Ireland); South East Technological University (Ireland); ESA-ESTEC (Netherlands)

Metal solidification, the transformation from liquid to solid, is fundamental to manufacturing metallic components through casting, welding, and additive manufacturing. During solidification, complex phenomena such as fluid flow, solute segregation, and microstructural evolution are influenced by gravity. While in-situ X-ray radiography enables real-time observation of dynamic solidification phenomena, the effects of gravity cannot be eliminated in ground-based experiments. Therefore, experiments under microgravity environments enable the study of solidification fundamentals avoiding the gravity driven complexities as well as to test diffusion controlled solidification models. In this contribution, we present detailed analysis of equiaxed dendrite solidification of aluminium - 20 wt.% copper binary alloy. The experiments were conducted onboard MASER 13 sounding rocket. The solidification process conducted using an isothermal furnace was observed through in situ X-ray imaging. Advanced characterization using synchrotron X-ray computed tomography, electron backscattered X-ray diffraction and Energy-dispersive X-ray spectroscopy facilitated extract multiscale details of the as-solidified samples. By combining these details with extended in situ image analysis allowed us to unveil topological, crystallographic and chemical transitions associated with the equiaxed solidification occurred under microgravity.

Accelerating Analysis of In-Situ X-Ray Videos of Alloy Solidification using Machine Learning

Jonathan Mullen, Wim Sillekens, Mert Celikin and David Browne

University College Dublin (Ireland); ESA-ESTEC (Netherlands)

The role that gravity plays on the solidification behaviour of equiaxed dendrites in metallic alloys has long been an area of research interest. Experimental data has previously been successfully obtained in pursuit of an answer to this question, most notably via the acquisition of in-situ X-ray solidification videos under different gravitational conditions, including in microgravity through the use of sounding rockets. However, analysis of these videos has, until now, proven to be a manually-intensive, time-consuming and costly exercise, with the image characteristics of these videos demanding pixel-by-pixel and frame-by-frame measurement. This has made attempting to gain insights from already completed experiments very expensive. To rectify this situation, an automated analysis system has been developed, using the result of the MASER-13 sounding rocket flight for primary experimental inputs. Through the use of machine learning and a number of bespoke image analysis and dendritic behavioural estimation techniques, two in-situ, X-ray videos of Al-Cu were successfully analysed: one under terrestrial gravitational conditions and the other under microgravity. The obtained and discussed analysis demonstrates both the effectiveness of the developed solution as well as the significant reduction in time and resources required by the system in order to obtain said analysis, when compared to the manual alternative. Additionally, the resultant MASER-13 dendritic characterisation measurements provide an and an initial set of comparative results between the same material composition solidifying under different gravitational conditions.

Atmospheric suppression of dynamic nucleation during electromagnetic levitation experiments

Gwendolyn P. Bracker, Stephan Schneider, Mitja Beckers, Sarah Nell and Robert W. Hyers

Worcester Polytechnic Institute (USA); Deutsches Zentrum für Luft- und Raumfahrt, DLR (Germany)

Microgravity electromagnetic levitation provides a unique processing environment in which fundamentals of solidification may be studied. The electromagnetic levitation environment provides stable access to the undercooled region of the melt while also enabling a range of stirring conditions to be induced in the liquid. In the presence of high stirring conditions, dynamic nucleation can trigger solidification in sub-critically undercooled melts. This nucleation mechanism occurs as a result of the a very high pressure shock in the melt arising from the collapse of voids within the liquid. Within this local region of high pressure, the melting temperature shifts, as described by the Clausius-Clapeyron equation, and gives much deeper local undercoolings. Dynamic nucleation has been repeatably demonstrated during electromagnetic levitation experiments in vacuum in the International Space Station Electromagnetic Levitation Facility (ISS-EML) using zirconium and zirconium alloy samples. In experiments on the ISS-EML, a zirconium melt with 2.5 at% niobium was observed to solidify by dynamic nucleation 20 times out of 20 attempts in conditions in which classical nucleation theory predicts the sample be a stable liquid. Since dynamic nucleation relies on the excitation and collapse of voids within the melt, it is expected that the external pressure applied to the molten sample by a protective gas environment would suppress dynamic nucleation by restricting the void excitation. This hypothesis was explored in recent experiments in the ISS-EML using the same zirconium 2.5 at% niobium sample that solidified by dynamic nucleation in every attempt when processed in gas. During these experiments the sample was not observed to solidify by dynamic nucleation.

Sessions Thu-A-II & Thu-A-III / Special Symposium in memory of Dieter Herlach

From theory of dendrite tip kinetics to additive manufacturing of multicomponent alloys

Charles-Andre Gandin

Mines Paris - PSL University, CEMEF (France)

Dieter Herlach's contribution on non-equilibrium solidification using levitation of metallic alloys is seminal [1]. At the same time, Markus Rettenmayr started using the CALPHAD methodology to model dendrite tip kinetics and microsegregation [4], hence benefiting from a phenomenological description of thermodynamic equilibrium at phase interfaces. A combination of these efforts is found when using a levitated Ni 75 at% Al sample to validate a microsegregation model [2], leading to better understanding of phase competition taking place during atomization of Ni {75-80} at% Al alloys as a function of cooling rate [3]. However, insufficient coupling with non-equilibrium interface phenomena, such as solute drag, remained to be deplored. This was because non-equilibrium phase diagram was not directly computed through the CALPHAD methodology. The presentation will focus on a dendrite tip kinetics model, including non-equilibrium effects at the solid-liquid interface, and applying it to multicomponent industrial alloys [5]. For additive manufacturing of 316L stainless steels, the simulation results show potential to predict the morphology of the microstructure as well as phase competition between ferritic and austenitic phases formed from the melt. Comparisons with observations made available in the literature for laser powder-bed fusion are reported. Possible extensions of the model and its application to other systems and processes will be discussed. [1] D. M. Herlach, Materials Science and Engineering R 12 (1994) 177-272. [2] D. Tourret, Ch.-A. Gandin, T. Volkmann, D.M. Herlach, Acta Materialia 59 (2011) 46654677. [3] D. Tourret, G. Reinhart, Ch.-A. Gandin, G.N. Iles, U. Dahlborg, M. Calvo-Dahlborg , C.M. Bao, Acta Materialia 59 (2011) 66586669. [4] T. Kraft, M. Rettenmayr, H. E. Exner, Modelling Simul. Mater. Sci. Eng. 4 (1996) 161177. [5] P. Martin, G. Guillemot, C. A. Hareland, P. W. Voorhees, Ch. A. Gandin, Acta Materialia 263 (2024) 119473.

Grain texture development during rapid solidification of thin metallic films

Adriana Eres-Castellanos, Mingwang Zhong, Kaihua Ji, Alec Saville, Dan Coughlin, John Roehling, Joseph T. McKeown, Amy J. Clarke and Alain Karma

Colorado School of Mines (USA); Los Alamos National Laboratory (USA); Northeastern University (USA); Lawrence Livermore National Laboratory (USA)

Dieter Herlach's pioneering studies of rapid solidification in deeply undercooled melts have yielded lasting insights into microstructure development and provided critical tests of theoretical models. For most rapid solidification processes, however, quantitative comparison between theory and experiment has remained challenging due to the incomplete knowledge of anisotropic energetic and kinetic properties of the solid-liquid interface. These anisotropic properties, such as the interface free-energy and kinetic coefficient, are notoriously difficult to measure or to predict from atomistic simulations due to the lack of reliable interatomic potentials for many metallic alloys. This talk explores a new combined experimental and computational approach to infer these properties by exploiting a statistical analysis of grain texture evolution (SATE) during rapid re-solidification of thin metallic films following laser spot melting. Results are presented for dendritic AlSi alloys that demonstrate how SATE makes it possible to compare quantitatively computationally predicted with experimentally measured textures at different stages of solidification in an elliptical melt pool geometry despite the inherent stochasticity of the grain competition process. The results also shed light on the mechanisms governing grain competition at high growth rate.

Non-equilibrium effects in rapid solidification

Peter Galenko

University of Jena (Germany)

Experimental studies and theoretical modeling on rapid solidification are critically discussed. The discussion focuses on dendritic, eutectic and intermetallic crystal growth. The kinetic peculiarities and formation of microstructures during and after non-equilibrium effects resulting in impurity dopant, disorder trapping, solute drag and diffusionless crystal growth is considered. Outcomes and predictions of developed theories are tested against results obtained in terrestrial and microgravity experiments on solidification kinetics of elemental substances and alloys.

Phase selection during non-equilibrium solidification of undercooled Zr-Co melts studied by in situ X-ray diffraction

Dirk Holland-Moritz, Fan Yang, Chenchen Yuan, Uta Rütt, Olof Gutowski and Jozef Bednarcík

Deutsches Zentrum für Luft- und Raumfahrt, DLR (Germany); DESY Photon Science (Germany)

Zr-based alloys have attracted broad attention because of their ability to form metallic glasses even when cooling down the melts at moderate cooling rates. During cooling of the melts, glass formation competes with the solidification of crystalline phases from the undercooled liquid. From the metastable state of the undercooled liquid, apart from the stable solid phases, also metastable solid structures may form. Often these subsequently transform into more stable counterparts such that they cannot be found in the as-solidified material. Understanding of the solidification behavior of the competing crystalline phases is of fundamental importance to understand the glass forming ability of alloy melts. In this work we present in situ X-ray diffraction experiments on the phase selection during non-equilibrium solidification of undercooled glass-forming Zr-Co melts. In order to achieve large undercoolings, the melts were containerlessly processed under high vacuum conditions by application of the electrostatic levitation technique. This technique has been combined with the diffraction of synchrotron radiation at beamline P07 of DESY in order to determine in situ the structures of the solid phases formed during solidification. Different solidification pathways have been identified to occur during non-equilibrium solidification of Zr-Co melts.

Formation and transformation of the metastable bcc phase in undercooled Fe-Co and Fe-Ni alloy melts

Thomas Volkmann, Ivan Kaban, Douglas M. Matson, Jannatun Nawer, Robert W. Hyers and Gwendolyn P. Bracker

German Aerospace Center, DLR (Germany); Leibniz Institute for Solid State and Materials Research Dresden (Germany); Tufts University (USA); Worcester Polytechnic Institute (USA)

Solidification of metastable δ-phase (bcc) and subsequent transformation into the stable γ-phase (fcc) in undercooled Fe-Co and Fe-Ni alloy melts have been investigated on electromagnetically levitated samples. The effect of fluid flow on growth kinetics and transformation behavior has been analyzed by comparative experiments on ground and under microgravity utilizing the electromagnetic levitator ISS-EML onboard the International Space Station. Rapid solidification is monitored by a high-speed video camera, which enables the direct observation of propagation of the solidification front. While electromagnetic levitation on earth is accompanied with strong, turbulent melt convection the tests using ISS-EML allow the control of fluid flow by applying different levels of electromagnetic stirring during solidification. Metastable phase formation is revealed by a two-step recalescence event showing primary solidification of metastable bcc phase and subsequent formation of stable fcc phase within the mushy-zone of primary bcc phase. Besides the growth velocities of competing δ- and γ-phase a decisive parameter describing the kinetics of phase transformation is the delay time between nucleation of the metastable and the stable phase. The delay obtained from high-speed video recordings strongly decreases with rising undercooling prior to metastable bcc phase solidification and is raised if electromagnetic stirring is increased. The experimental results on transformation kinetics are discussed in terms of current models for dendritic growth and nucleation of the stable phase in a metastable mushy-zone. This research work is supported by the European Space Agency (ESA) in the frame of the projects MAGNEPHAS and PARSEC.

The influence of convection on phase transformation kinetics on ground and in microgravity

Douglas Matson

Tufts University (USA)

In order to attain high undercoolings in reactive molten metal alloy systems, containerless processing is used in conjunction with high-speed digital videography and radiation pyrometry. On ground, electrostatic levitation provides access to a quiescent melt while electromagnetic levitation provides access to turbulent stirring. To investigate conditions between these extremes, electromagnetic levitation is conducted in Low Earth Orbit. This presentation highlights some of the groundbreaking results obtained through collaborations with Prof. Dr. Dieter Herlach in the decades spanning investigations which have flown on the Space Shuttle Columbia and in the Columbus module of the International Space Station. In particular, emphasis will be placed on new solidification theories developed to explain how phase transformation kinetics are influenced by melt convection.

Additive Manufacturing of Metallic Glass from Powder in Space and at Synchrotron Radiation Facilities

Andreas Meyer, Fan Yang and Christian Neumann

Institut Laue Langevin (France); Deutsches Zentrum für Luft- und Raumfahrt, DLR (Germany)

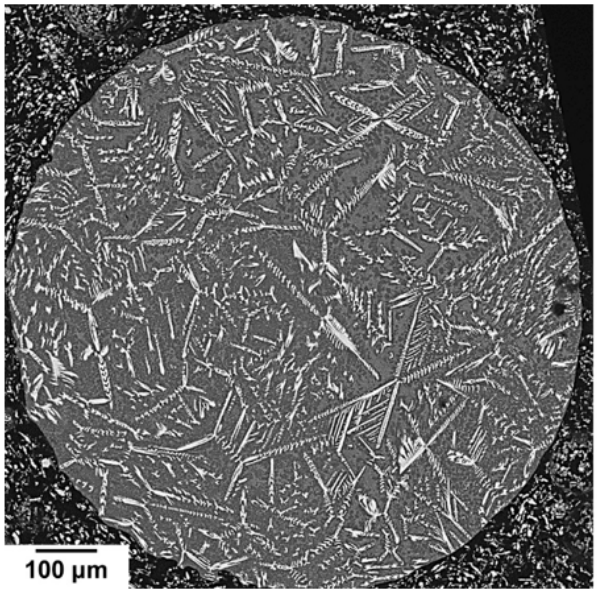
Additive manufacturing (AM) technologies appear to be a tremendous opportunity to meet spaceflight requirements, because they contribute to saving material, reducing mass to transport, and reducing production time. Laser-based Powder Bed Fusion (PBF-LB) is one of the most versatile AM processes in terms of possible geometries and scalable process parameters, and is adaptable to a wide range of materials. Metallic glasses possess attractive properties such as excellent corrosion resistance, good mechanical properties, and a low friction coefficient. Generally produced by casting, dimensions of bulk metallic glasses are usually limited to a few millimeters to centimeters. By builiding layer by layer in an AM process, it is possible to circumvent this size limitations. The largest challange to realize a PBF-LB process at low gravity is the powder handling. Here we present results from additive manufacturing of metallic glass on sounding rocket flights. An adaption of the sounding rocket payload to experiments at synchrotron radiation facilities allowed to study the phase selection during printing. Microstructure characterization of the build parts was performed using electron microscopy and X-ray diffraction computed tomography. For the fabrication of fully amorphous builds both on ground and in space, our findings point to higher scanning speeds, lower laser power, and lower oxygens contents, while particularly the later can be used to tune the amount of crystalline fractions in the sample.

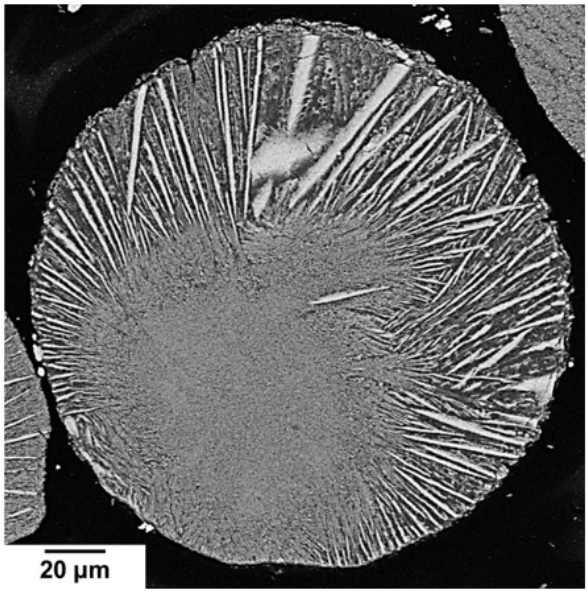
Non-equilibrium solidification of hypereutectic Al-20wt%Ce atomized particles

Jonas Valloton, José Marcelino da Silva Dias Filho, Alexandra Perez and Hani Henein

University of Alberta (Canada)

Containerless solidification of hypereutectic Al-20wt%Ce is investigated experimentally using the impulse atomization (IA) technique in a He atmosphere. The microstructure of larger IA powders consists of large primary Al11Ce3 dendrites surrounded by an α-AlAl11Ce3 eutectic, similar to what is observed in cast samples. Microstructure evaluation shows multiple nucleation events throughout the samples. Smaller atomized particles exhibit a strikingly different microstructure, with a very fine eutectic giving way to large intermetallic plates surrounded by a regular eutectic. This indicates that the undercooling was sufficient to bypass the nucleation of the primary intermetallic in favor of the eutectic. Particles of various sizes were further analyzed using 3D X-ray microscopy (XRM). The reconstructed particles were segmented based on microstructure (primary intermetallic, regular eutectic and fine eutectic) using a deep learning model built on a U-Net Architecture. Results show an increase in the volume fraction of the fine eutectic as the particle size decreases but never quite reaching 100%. Further segmentation of the fine eutectic using focused ion beam shows an increase in the fraction of Al11Ce3 with respect to equilibrium. This indicates a shift in the eutectic point towards a higher Ce concentration with higher undercooling.





Solidification and Crystallization of FeNiP microwires

Asuncion Garcia-Escorial, Jose Antonio Jimenez, Antonio Hernando, Irene Llorente, Rodolfo Miranda, Cristina Navio, Pilar Marin, Patricia de la Presa, Javier Calvo and Iban Llamas

CENIM-CSIC (Spain); IMDEA Nanociencia (Spain); Universidad Complutense de Madrid, Instituto de Magnetismo Aplicado (UCM-ADIF-CSIC) (Spain); Micromag 2000 (Spain); Universidad Antonio de Nebrija (Spain)

Ferromagnetic alloys with an ordered L10 structure could play an important role in the development of a sustainable society in the near future because of their strong magnetocrystalline anisotropy (MCA) and large coercivity. However, the presence of large amount of noble metals like Pt and Pd present in typical L10 structures (CoPt FePt and FePd) have limited their use as permanent magnets not only by their high cost, but also due to the high environmental consequences associated with a high energy consumption during their extraction processes. Although disordered FeNi alloys show small coercivity and weak magnetic anisotropy, an ordered L10 phase with ideal formula FeNi has been identify in meteorites. This phase has been called tetrataenite since it presents a tetragonal structure and it forms in iron meteorites during a billion-year cooling below 350°C in taenite grains. Tetrataenite has magnetic properties comparable to those of CoPt, with a high coercivity (5004000 Oe) and magnetic anisotropy (1.3 x 107 erg cm-3). Unfortunately, artificial production of a L10 phase with abundant and inexpensive elements like Ni and Fe from the disordered solid solution is extremely difficult because at the order-disorder transition temperature (about 320ºC) the atomic diffusivities of Fe and Ni become negligible (an atomic jump of Ni would occur in almost 10000 years). In this work, we have prepared amorphous and partially amorphous microwires of Fe-Ni-P to increase atomic diffusivity at a temperature close to order-disorder temperature for the L10 FeNi phase formation, in order to try to get tetrataenite or any other ferromagnetic phase in form of nanocrystals embedded in a paramagnetic matrix with high coercivity. We have characterized the solidification microstructure, as well as the crystallisation path, mainly by x ray diffraction measurement, to systematically clarify the contribution of different magnetic phases.

Thu-B-I / Additive manufacturing I

Metallurgy-driven thermomechanical analysis of solidification grain structures by coupling cellular automaton with crystal plasticity

Zixuan Li, Trung-Chien Vo, Charles-André Gandin, Michel Bellet, Yancheng Zhang and Manas Upadhyay

Mines Paris - PSL University, CEMEF (France); Ecole Polytechnique, LMS (France)

The role of solidification grain structures produced by additive manufacturing on the formation of residual stresses is investigated. This is made possible by combining a cellular automaton model to compute the solidification grain structure with a crystal viscoplasticity thermomechanical model. For calibration of the crystal viscoplasticity model, stress-strain curves from experiments on an isotropic polycrystal structure are considered, using small thermo-elasto-viscoplastic deformations with an isotropic hardening model. Calibration is validated by performing tensile tests on representative volume elements of grain structures produced for different laser scanning trajectories, demonstrating the role of the texture. The first application is presented at the scale of a few laser tracks on a polycrystalline 316L stainless steel. The resolution scheme successively involves heat transfer, melting and solidification [1] and thermomechanical analyses, hence predicting concomitant stress and strain evolution within the grain structure. The development of a solidification texture is simulated. The stress distribution among the grains reveals a higher probability for larger stress variations at high angle grain boundaries. Results are directly affected by the scanning strategy. A second application concerns the scale of an IN718 component. The grain structure is pre-calculated using the hybrid cellular automaton methodology [2]. For each new layer built, the grain structure is made available for the crystal plasticity model, together with the temperature field. A comparison of residual stresses and displacements for a reference monocrystalline propeller geometry with a polycrystalline grain structure is presented, demonstrating the effect of local grain textures. [1] Th. Camus, D. Maisonnette, O. Baulin, O. Senninger, G. Guillemot, Ch.-A. Gandin, Three-dimensional modeling of solidification grain structures generated by laser powder bed fusion, Materialia 30 (2023) 101804. [2] Y. Zhang, G. Guillemot, Th. Camus, O. Senninger, M. Bellet, Charles-André Gandin, Part-Scale Thermomechanical and Grain Structure Modeling for Additive Manufacturing: Status and Perspectives, Metals 14 (2024) 1173.

On the Compositional Criteria to Predict Columnar to Equiaxed Transitions in Metal Additive Manufacturing

Duyao Zhang, Ryan Brooke, Dong Qiu and Mark Easton

University of Bath (UK); RMIT University (Australia)

Predicting the columnar-to-equiaxed transition (CET) and grain refinement in additively manufactured (AM) alloys using thermodynamic databases remains a significant challenge and a topic of ongoing debate. Current efforts aim to design alloy compositions that promote fully equiaxed microstructures, thereby addressing the mechanical anisotropy often associated with the large columnar grains in AM alloys. This study evaluates three parameters proposed in the literature: non-equilibrium solidification range (ΔTs), growth restriction factor (Q) and constitutional supercooling parameter (P) across various AM Ti alloys. Experimental results confirm that P is the most reliable parameter for selecting alloying elements in AM alloys. Numerical CET models further demonstrate that P is closely linked to dendrite tip undercooling at the high growth velocities characteristic of AM. Additionally, process parameters play a crucial role in achieving CET and grain refinement in AM processes.

Thermal and Microstructure Simulations for LPBF processes with Different Laser Beam Profiles

Raveeshankar Sambathkumar, Rocio Avila Hernandez, Sayan Chatterjee, Juri Munk, Jan Haubrich and Jürgen Jakumeit

Access e.V. (Germany); Deutsches Zentrum für Luft- und Raumfahrt, DLR (Germany)

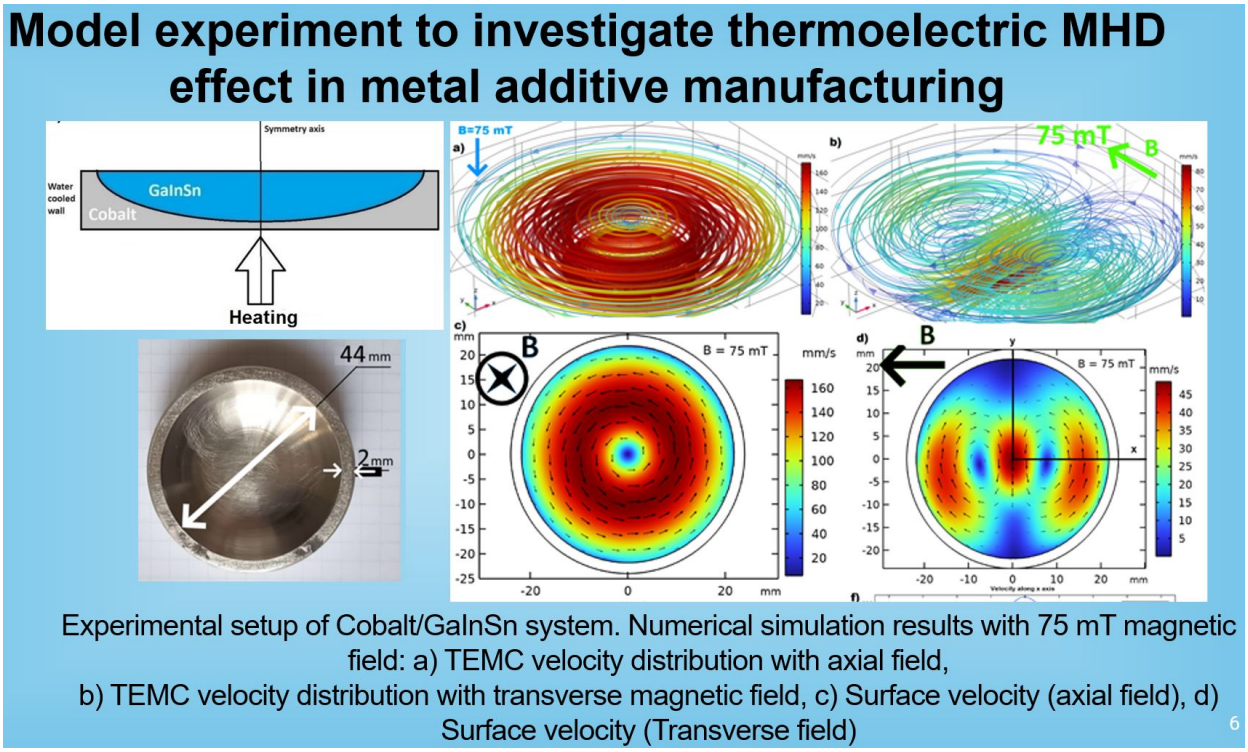
Laser Powder Bed Fusion (LPBF) is a critical additive manufacturing technique for producing complex metal parts by selectively melting metal powder with a laser beam. The melt pool geometry directly influences the quality, dimensional accuracy, and mechanical properties of the final component, making its control essential for optimal results. Traditionally, the Gaussian laser beam profile has been used in LPBF, but it often leads to localized overheating at the center of the melt pool, resulting in keyhole formation and other defects. To mitigate these issues, alternative laser beam profiles that combine Gaussian and ring-shaped profiles are explored. This combination helps to distribute the energy more evenly across the melt pool, reducing the risk of overheating and improving melt pool stability. In this study, different combinations of Gaussian and ring-shaped laser beam profiles are analyzed using an in-house developed finite volume (FV) code. The code simulates the thermal behavior of the melt pool in single-track LPBF and is validated against experimental data. Furthermore, a Cellular Automaton (CA) model based on the LGK dendrite growth theory is used to simulate microstructure evolution during solidification. The simulations provide insights into grain growth and the solidification microstructure, which directly influence the material's mechanical properties. The thermal and microstructure simulations demonstrate the potential of different laser beam profiles to enhance the LPBF process. Additionally, the developed FV code and CA model offer valuable tools for advancing LPBF technology, enabling more precise control over laser beam shaping and melt pool behavior, ultimately improving part quality and reproducibility in future applications.

Magnetohydrodynamics effects in metal additive manufacturing

Imants Kaldre, Valdemars Felcis, Ivars Krastins, Andrew Kao, Catherine Tonry and Peter Soar

University of Latvia (Latvia); University of Greenwich (UK)

Metal additive manufacturing is one of the new and rapidly emerging technologies. During additive manufacturing processes small quantity of metal is melted and solidified. In this melting and solidification phase additional control mechanisms are actively being sought to improve microstructures and ultimately built parts. Magnetohydrodynamics (MHD) control of the melt pool can be done by using external magnetic fields. There are numerous studies about metallic alloy solidification under magnetic fields showing that heat and mass transfer can be modified by this method and significant effects on solidified metal can be achieved. Magnetohydrodynamics control of the liquid metal is recently being considered to solve various problems, such as precisely timed and accurate droplet size ejection from the printhead, re-orientation of heat transfer in the melt pool, control of oxidation of molten metal, and convective transport of heat and mass. There are strong thermal gradients during metal AM processes, which lead to thermoelectric currents at the solid-liquid interface. An external magnetic field interacting with these currents generates a Lorentz force leading to fluid flow in the liquid melt pool, known as Thermoelectric Magnetohydrodynamics (TEMHD) convection. Static magnetic fields can also significantly damp the melt flow perpendicular to the field direction, while along the field lines flow is not affected. This leads to altered molten phase flow morphology depending on the orientation of the magnetic field. We present scale experiments to investigate the TEMHD flows caused by applied static magnetic fields in various directions. This model experiment is linked to wire-fed laser additive manufacturing and results are used to interpret the outcome of 3D printing under applied magnetic field of various aluminium alloys.



Experimental setup of Cobalt/GaInSn system. Numerical simulation results with 75 mT magnetic field: a) TEMC velocity distribution with axial field,
b) TEMC velocity distribution with transverse magnetic field, c) Surface velocity (axial field), d) Surface velocity (Transverse field)

Columnar dendritic growth in additive manufacturing

Guillaume Boussinot, Ivan Cazic and Markus Apel

Access e.V. (Germany)

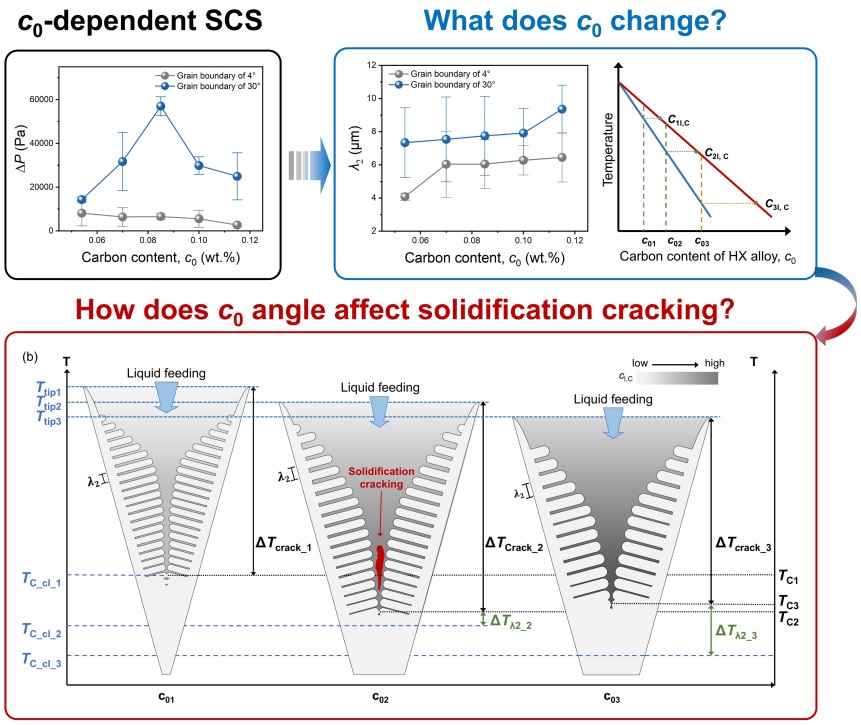
We review the peculiarities of the columnar dendritic growth when, under additive manufacturing conditions, cooling rate and thermal gradient are extreme. Using the dendritic theory, phase-field simulations and experimental observations, we analyze the consequences of the strongly out-of-equilibrium solidification conditions on the characteristics of the growing dendritic array. Our goal is to point the distinctions between the cellular regime, the close-to-equilibrium dendritic regime and the far-from-equilibrium dendritic regime, in terms of morphology, direction of growth or array disorder. Typical grain structures observed within melt pools solidified under LPBF conditions are then discussed using the developed arguments.

Solidification cracking suppression in additively manufactured Hastelloy X by controlling carbon content: Insight from phase-field simulations

Yashan Zhang, Jincheng Wang and Lei Wang

Northwestern Polytechnical University (China)

Lowering carbon content (c0) of powders below the ASTM minimum of 0.05 wt.% is a common approach to producing crack-free additively manufactured Hastelloy X (HX) alloys by narrowing the solidification range. However, this compromises the alloys' mechanical properties. Interestingly, HX alloys with c0 of 0.09 wt.% or higher remain crack-free while maintaining their mechanical properties. This suggests a Λ-shaped relationship between solidification cracking sensitivity (SCS) and c0, and reveals that the carbon's effect on SCS extends beyond merely altering the solidification range. Using a combined phase field and Rappaz-Drezet-Gremaud model, we showed that SCS decreases with increasing c0 in attractive grain boundaries, while it exhibits a Λ-shaped in repulsive grain boundaries, peaking at c0 around 0.085 wt.%. This behavior is primarily attributed to the interplay of two factors: the secondary dendrite spacing (λ2) and the carbon concentration in liquid (cl,C), both of which increase with c0 but have opposing effects on SCS. Increasedλ2 not only narrows the liquid channel width, promoting grain coalescence, but also increases permeability to enhance liquid phase feeding. Together, these factors reduce SCS. Increased cl,C reduces the solid phase fraction to suppress cracking, but broadens the temperature range prone to cracking, ultimately leading to a higher SCS. As the grain boundary angle increases, λ2 increases, which diminishes the role of λ2 in SCS and subsequently alters the trend of c0-dependent SCS. This study provides valuable insights into the complex role of c0 in SCS, offering a pathway for designing crack-resistant superalloys with excellent mechanical properties.



Thu-B-II / Additive manufacturing II

The impact of high cooling rates the solidified microstructure: considering the Al-Si system in casting and additive manufacturing

Indrajeet Katti, Dong Qiu, Duyao Zhang, Matthias Weiss, Joy Forsmark and Mark Easton

University of South Australia (Australia); RMIT University (Australia); University of Bath (UK); Deakin University (Australia); Ford Motor Company (USA)

Increasing the cooling rate is known to have several effects on the microstructure including refining the features including the secondary phases, cell size and the grain size; unless the thermal gradient increases so much that a columnar grain structure is formed. Also at very high cooling rates, there is often an increased solubility of alloying elements in the matrix phase. High cooling rates can also affect the eutectic formation with coupled zones leading to changes in eutectic composition and morphology. By considering the microstructures observed in high pressure die casting and additive manufacturing of Al-10Si alloys we see an increasing proportion of -Al, a reduction in the amount of eutectic and change in the Si morphology along with the microstructural refinement. Furthermore the amount of Si in the -Al, particularly in the eutectic increases. These effects can be explained by the high cooling rates suppressing the eutectic reaction. Hence understanding the kinetic effects on the effective phase diagram is key to explaining the microstructures observed in both high pressure die casting and additive manufacturing.

An Al-Zn alloy with outstanding processability by laser powder bed fusion

Xueze Jin and María Teresa Pérez-Prado

Harbin Institute of Technology (China); IMDEA Materials (Spain)

High strength Al alloys, and in particular the Al-Zn-based 7xxx series, exhibit extensive hot cracking when processed via laser powder bed fusion (LPBF) and this has severely limited their applicability as feedstock for additive manufacturing (AM) [1]. Extensive efforts focused on optimizing key processing parameters such as the laser power, the scan speed, the hatch distance, the scan strategy, or the layer thickness have not been able to avoid the development of columnar grains, which are intimately related to crack formation [2]. Other strategies including the addition of solutes and/or inoculating agents such as Zr, Sc, Si, and ceramic or metallic nanoparticles, as well as the use of ultrasounds and beam shaping during processing, have succeeded to eliminate hot cracking. However, they are only effective in a limited range of processing conditions, usually comprising small ranges of volumetric energy density (VED) [3]. This work investigates the processability by LPBF of an Al-20Zn-0.1Cr (wt.%) alloy. A wide range of processing parameter sets including laser power (P) values between 100 and 400 W and scan speeds (v) ranging from 100 to 1500 mm/s is utilized to manufacture cubic specimens using a pulse-laser source. It will be shown that dense, crack-free, and isotropic polycrystalline microstructures are obtained for an extensive range of VED conditions. While the investigated material is a model alloy, endowed with limited strength, this work might provide guidelines for the design of high strength 7xxx Al alloys with extended processability via LPBF. [1] H.R. Kotadia, G. Gibbons, A. Das, P.D. Howes, Additive Manufacturing 46 (2021) 102155. [2] S. Ghosh, J. Zollinger, M. Zaloznik, D. Banerjee, C.K. Newman, R. Arroyave, Additive Manufacturing 78 (2023) 103845. [3] P.A. Rometsch, Y. Zhu, X. Wu, A. Huang, Mater. Des. 219 (2022) 110779.

Direct Liquid Metal Deposition of Aluminium Alloys

Julie Gheysen, William Le Bas and Andreas Mortensen

EPFL (Switzerland)

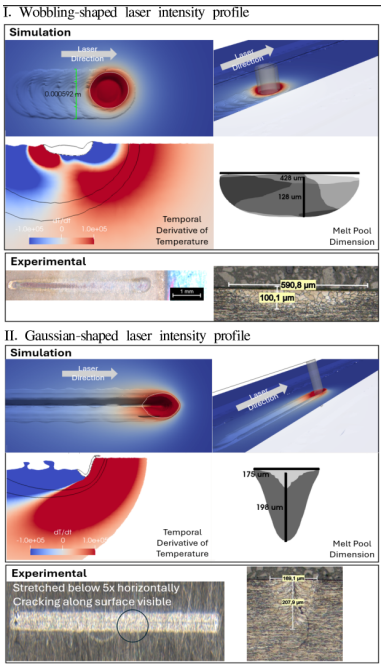
Common metal additive manufacturing technologies require energy-intensive sources such as lasers to achieve the melting and ultimately the bonding of the metallic feedstock. This leads to a sizeable carbon footprint especially for highly reflective materials such as aluminium alloys. Moreover, this high energy input induces complex and turbulent melt pool dynamics leading to stochastic defect formation mechanisms that are hence difficult to suppress. This research aims to propose an alternative technology similar to what is now used with thermoplastic polymers, i.e., Fused Deposition Modelling. An aluminium wire is fed through a nozzle and melted using resistive heating. The molten metal produces then a small droplet between the nozzle and the substrate. Through this droplet metal transits, bonds and solidifies onto the previously deposited layer. This is challenging for metallic materials due to their combination of low viscosity, high capillary forces that induce instabilities such as bulging, and their propensity for reaction with the atmosphere. Commercial eutectic AlSi12 wire was used to manufacture walls using this direct liquid metal deposition (DMLD) process. Hydrogen porosity, which can appear in the parts, was reduced to 0.1% using a combination of proper wire preparation and process parameters selection. The resulting microstructures were characterised as well as their link with the mechanical properties. DLMD AlSi12 shows isotropic mechanical properties with an elongation at fracture of 10 ± 2 %, a yield stress of 94 ± 17 MPa, and an ultimate tensile strength of 176 ± 7 MPa; those properties are higher than those seen in cast AlSi12 [1]. The project is currently expanding to Al-Cu alloys, aiming to fabricate those without hot cracking. [1] Q. Cheng, R., et al., Adv. Eng. Mater., vol. 26, no. 13, p. 2400517, Jul. 2024

Improving the processability of additively manufactured tungsten by laser beam shaping experiments and melt pool flow simulations

Gizem Ersavas Isitman, Aymara Duran Baumann, Tomi Suhonen, Robert Lurbke, Alexander V. Müller, Rudolf Neu, Thomas Stoll, Maximilian Schmitt, Lukas Lohr, Jonas Grünewald, Katrin Wudy, Anssi Laukkanen and Tatu Pinomaa

VTT (Finland); IPP (Germany); TUM (Germany)

Additively manufactured (AM) tungsten is an excellent candidate as a first-wall material for fusion reactors. However, it suffers from excessive cracking after solidification, due to the large cooling rates in the ductile-to-brittle transition temperature (DBTT) regime upon solidification and cooling. In this work, we present strategies to improve laser AM processing of tungsten, by modifying the laser beam shape and adding wobbling trajectories, both of will be shown to reduce the cooling rates in DBTT regime and thereby mitigate cracking, as well as to enhance processing speed and mitigate process faults such as keyhole porosity. This study focuses on an AM melt pool solver developed in OpenFOAM. We investigated three principal laser intensity profiles by simulating the standard Gaussian profile which is prone to cracking, a ring-shaped beam, and a wobbling ring beam, both of which are shown to avoid cracking as observed in experiments. The performed simulations utilize experiments as follows. We quantitatively calibrate melt pool model intensity profile to experimental laser beam caustics. We compare the experimental melt pool depths and widths to the simulated melt pool cross-sections and analyze the degree of cracking in the cross section and along the melt pool surface. The findings demonstrate that the ring-shaped and wobbling laser profiles mitigate the cracking, which can be linked to more stable melt pools with reduced fluctuations compared to the Gaussian profile, and an overall reduced cooling rates and thermal gradients in the DBTT zone. Overall, the results align well with experimental observations and underscore the benefits of using advanced melt pool simulations and beam shaping to optimize the laser beam melting process. This work highlights the critical role of laser profile selection in mitigating cracking and improving the quality of printed components.



Sustainable printing of copper using Laser Powder Bed Fusion

Shishira Bhagavath, Iuliia Elizarova, Kwan Kim, Anna Cm Getley, Yinglun Hong, Samy Hocine, Wei Li, Yuhan Wang, Eduardo Saiz Gutierrez, Chu Lun Alex Leung and Peter Lee

University College London (UK); Imperial College of London (UK)

Laser Powder Bed Fusion (LPBF) Additive Manufacturing (AM) is a groundbreaking digital technology that creates complex components layer by layer using powder feedstocks. LPBF is utilized across various industries, including advanced propulsion, energy, transport, and biomedical. However, its adoption for high-value engineering applications is limited by the availability of suitable feedstocks. This limitation arises from the poor laser-matter coupling efficiency of transparent materials (like glass) and highly reflective powders (such as copper and aluminium), which require high energy inputs to melt. Here, we report the application of an innovative technology of using Chemically Modified Graphene (CMG), which showed a threefold improvement in absorbance compared to pure copper in Near Infrared (NIR) wavelengths, conditions in which commercial LPBF machines typically operate. We assessed the printability of Cu-CMG over a range of laser powerscan velocity (PV) parameters and developed surface roughness and defect process maps. Compared to pure copper, the addition of CMG significantly widen the optimal print regime. Printing is possible at half the laser power (for low scan speeds) and double speeds (for high powers) for various P-V combinations, while micrographs of the printed tracks revealed an improved surface finish with the addition of CMG. Further, using synchrotron X-ray imaging and a custom LPBF rig, we performed in-operando printability studies and identified four melting modes, namely keyhole porosity, keyhole stable, wide vapour depression, and conduction. By processing the in-situ X-ray radiographs, we quantified the melt pool geometry and showed improved melting efficiency with Cu-CMG feedstock. Our CMG additive promises additive manufacturing of dense parts, thus paving the way for the design and development of new applications such as electric motors and heat exchangers.

Influence of laser speed on microstructure of copper enriched steels processed by additive manufacturing

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Université de Lorraine & CNRS, IJL (France)

The increase in copper content in steels is inevitable as recycling becomes more widespread. The very low solubility of this element in the ferrous phases and its tendency to segregate cause difficulties during processing. On the other hand, additive manufacturing makes it possible to reach strongly non-equilibrium conditions, which could be advantageous for the elaboration of copper-rich steels. In this study, we investigate the influence of laser velocity on the microstructure formation of carbon steel with high copper contents (> 5 wt%). Copper trapping is studied for velocities between 100 and 1000 mm/min, which are in the stable processing range. The microstructures are characterised by SEM, EBSD and TEM to quantify phase fractions and microsegregations. The results are compared and discussed with available analytical models for solute trapping.

Thu-B-III / Additive manufacturing III

Microstructure development during laser melting and resolidification; integrated experimental and simulation study

Alexander Chadwick, Guillermo Santos, Arash Samaei, Gregory Wagner, Manas Upadhyay and Peter Voorhees

Northwestern University (USA); IMDEA Materials (Spain); Ecole Polytechnique (France)

Additive manufacturing (AM) is a complex process that involves rapid solidification and remelting. These phenomena are critical to the nature of the final microstructure of AM materials. However, their study is not easy and managing to combine the simulation and experimental aspects of research, can prove to be difficult. The present work constitutes an example of this coupled research. An in situ study of the grain structure formation due to solidification was performed on 316L stainless steel using a continuous wave laser coupled with a scanning electron microscope. Electron back scatter diffraction (EBSD) mapping before laser melting allowed to obtain the initial grain size distribution to input as initial condition in a coupled phase-field/thermal multiphysics modelling framework. Single pass laser scans with different power and velocity were done to mimic bead on plate single tracks. The resolidified microstructure was characterised by EBSD. The predicted resolidified microstructure is in good agreement with the experimental results, suggesting validity of the model. The comparison of the top surface grain morphology of measured and simulated cases is quantitatively apt. According to the predicted three dimensional grain morphology, the major axis length of the resolidified grains is sensitive to laser power and speed, and not that of the minor axis. The orientation of the grain major axis depends on melt pool geometry.

Predicting Columnar to Equiaxed transition during laser-based additive manufacturing of SS316L reinforced by TiN particles

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IIT Bombay (India)

Directionality in heat transfer during fusion based additive manufacturing processes leads to columnar grain growth leading to anisotropy in mechanical properties. SS316L, a popular material choice for fusion based additive manufacturing process finds a variety of applications. In order to reduce the anisotropy in the properties, it is desirable to have equiaxed grains in the solidified material. One of the methods to obtain transition from columnar to equiaxed grains is to increase the nucleation sites by adding particles in the alloy. Different models are available in literature to study the columnar to equiaxed transition during additive manufacturing. This study aims to simulate the Columnar-to-Equiaxed Transition caused by TiN reinforcement in SS316L using the model proposed by Durga et al. The model includes the dendrite growth kinetics that incorporates the multicomponent interactions through the diffusion matrix, rapid solidification effects, dendrite tip radius computations based on marginal stability approach and liquid composition profile computation based on Ivantsov's solution for the growth of a paraboloid. CET is modelled according to Hunt's approach. The inputs to the CET model are from the Dendrite growth kinetics, full nucleation site distribution through Martorano et al. model. Nucleation site size-dependent undercooling required for equiaxed growth is modelled according to Greer's free growth model. Constitutional undercooling arising from the liquid composition profile and the resultant effect on nucleation of equiaxed grains is included as demonstrated by Gäumann et al. Thermal model of processes are simulated using MSC simulation software Simufact using the parameters given in literature for obtaining the thermal properties required as input to CET model. The predictions were compared with the experimental data available in literature. The results emphasize the importance of including the rapid solidification effects, dendrite tip kinetics and multicomponent interactions in the accurate predictions of the Columnar to equiaxed transition.

Effect of laser parameters and layer thickness on the solidification microstructure, texture and variant selection of a laser powder bed fusion produced maraging steel

Adriana Eres-Castellanos, Ana Santana, Jose Antonio Jimenez, Carlos Capdevila and Francisca G. Caballero

Colorado School of Mines (USA); National Centre for Metallurgical Research, CENIM-CSIC (Spain)

Additive manufacturing (AM) offers significant benefits to a wide range of industries. Design freedom for complex geometrical features leads to efficient usage of raw materials and reduced production times (Bayat et al., 2021; Vafadar et al., 2021). Amongst the different types of AM processes available for metals, laser powder bed fusion (LPBF) is widely used for steels (Mirzaali et al., 2019). Materials processed by LPBF are subjected to rapid cooling rates which typically range between 1 and 4x10^6 C/s during solidification (Hooper, 2018). Additionally, previously solidified material experiences cyclic reheating and cooling as subsequent layers are printed. Process parameters such as the laser power, scan speed or layer thickness are known to control these sharp temperature peaks (Kürnsteiner et al., 2017). Grade 300 maraging steels are widely used in AM because the high cooling rates are ideal for maraging steels to obtain a martensitic microstructure. Furthermore, under certain circumstances, the thermal cycling can trigger precipitation without the need of additional heat treatment (Kürnsteiner et al., 2017). Thus, maraging steels present different resultant microstructure compared to traditional counterparts (Jägle et al., 2014). This work aims for a better understanding of phase formation in the solid state and during solidification. The effect of different processing parameters such as the laser power, laser emission mode and layer thickness are considered. Special attention is given to illustrate how processing parameters affect texture and variant selection.

Laser Powder Bed Fusion of G91: Powder Properties and Microstructural Development

Erick E. Alvarado, Roger Castellote-Alvarez, Isaac Toda-Caraballo, Carlos Capdevila, Pilar Rey, Rebeca Hernández-Pascual, Antonio Fernández-Viña, Marta Serrano and David San-Martin

National Centre for Metallurgical Research, CENIM-CSIC (Spain); AIMEN Centro Tecnológico (Spain); Centro de Investigaciones Energéticas, Medioambientales y Tecnológicas, CIEMAT (Spain)

G91 steel is widely used in the manufacture of components for high-temperature applications within the energy sector, owing to its exceptional mechanical and thermal properties. Consequently, it is also regarded as a promising candidate material for the fabrication of structural components in the next generation of power plants. However, conventional manufacturing processes typically employed to produce these components hold back the creation of complex geometries. Laser Powder Bed Fusion (LPBF) is an Additive Manufacturing (AM) technique that has been brought into play to fabricate components in various alloys. Nevertheless, its feasibility for producing G91 steel components is still being explored. This study focuses on the fabrication of G91 steel samples using the LPBF additive manufacturing technique. A comprehensive characterisation of the G91 steel powders was conducted, assessing aspects such as flowability, microstructure, and composition through various complementary experimental techniques, including X-ray fluorescence (XRF), inductively coupled plasma optical emission spectroscopy (ICP-OES), X-ray diffraction (XRD), scanning electron microscopy with energy-dispersive spectroscopy (SEM/EDS), and electron probe microanalysis (EPMA). Following a detailed optimisation process to reduce porosity, the optimal printing parameters were established: 150-200 W, 750-1000 mm/s, 0.05 mm hatch distance, and 0.03 mm layer thickness. The resulting microstructures were analysed in both as-built and normalised conditions, using optical microscopy (OM), SEM, and XRD. Additionally, mechanical performance was evaluated through microhardness tests and small punch tests, providing insights into the material properties under these conditions.

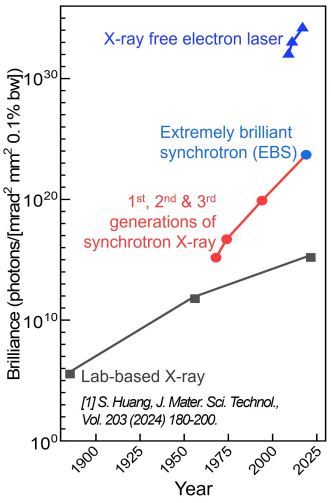
Thu-C-I / Aluminum alloys III

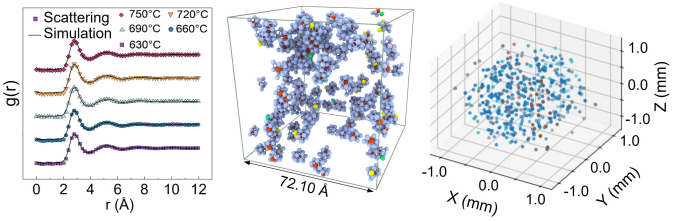
Solidification dynamics across different spatiotemporal scale revealed in operando by the extremely brilliant synchrotron and X-ray free electron laser sources

Kang Xiang, Yueyuan Wang, Hongyuan Song, Kharel Sungcad and Jiawei Mi

University of Hull (UK)

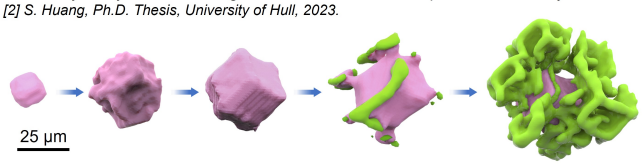
In the solidification of a metal alloy, the nucleation and growth of different structures and their interplays occur at different length (atomic to millimetre) and time (fs to minutes) scale. It has been always an experimental challenge to visualize, in real-time, the dynamic evolutions of those structures in the desired length and/or time scale in in operando conditions, especially difficult when an external field, e.g., ultrasound, magnetic field, laser, etc is involved in the processes. Recently, by exploring the world-leading capabilities of the Extremely Brilliant Source (EBS) of the European Synchrotron Radiation Facility (ESRF) and the X-ray free electron laser of the European XFEL (euXFEL), we are able to study, in operando conditions, the dynamic solidification structures from atomic level all the way up to millimetre scale, and in time scale from ns up to minutes. Here, we present some typical cases to reveal the new scientific insights. At ID11 of the ESRF, we used the ultrafast diffraction and total scattering capability to study the heterogeneous atomic structure evolution of multiple-component Al alloys until the onset of multiphase nucleation. Then we tracked down the location and growth of the multiphases using the 3D X-ray diffraction technique. At ID19 of ESRF, we used the ultrahigh imaging and tomography technique to visualize the growth dynamics of complex multiple intermetallic phases and their interplay in 3D space, in particular, the multiphase co-growth dynamics under the influence of applied ultrasound and pulse magnetic fields. At the SPB of the euXFEL, we used the fs X-ray pulse and MHz imaging to study the dynamic interactions between a pulse laser beam and intermetallic phases of Al alloys in laser welding and additive manufacturing processes. The key findings and new insights from these challenging experiments and the outlook of future research direction are discussed in detail here.



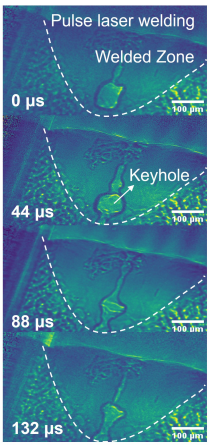


Atomic structure evolution of AlCuFeSi melt in cooling studied by X-ray total scattering and MD simulation. *[2] S. Huang, Ph.D. Thesis, University of Hull, 2023.*

Centre-of-mass map of Al_3Sc phases studied by 3DXRD.



Nucleation and co-growth dynamics of the Chinese-script $Al_{15}Fe_3(SiCu)_2$ phases studied by ultrahigh tomography. *[3] K. Xiang, Acta Mater., Vol. 279 (2024) 120267.*



XFEL MHz imaging of dynamic interactions of pulse laser and Al-20Cu alloy.

Investigating In-Situ Fiber Bragg Grating Responses in Liquid Aluminum Under Applied Stress

Constantin Bauer, Robert Kleinhans and Wolfram Volk

Chair of metal forming and casting (Germany); Fraunhofer IGCV (Germany)

Hot tears are one of many defects in castings and weldings. Especially in weldings, this crack-like defect leads to failure or rejection in production. Nevertheless, castings are also being affected by this phenomenon. Several attempts exist to understand and describe hot tearing, but only a few methods exist to analyze the effect in situ. Fiber Bragg gratings have been used in castings to measure strain and are now used to inspect hot tearing in-situ. With a unique test bench, built of a mirror furnace capable of heating specimens and a tensile testing machine that can pull the prepared specimen simultaneously, it is now possible to analyze the formation of cracks with the optical method of fiber Bragg gratings. This experiment allows a defined application and variation of stress on the aluminum sample made of different alloys and conducting tests to varying temperatures up to liquidus temperature. To get a valid measurement, it is necessary to calibrate the fibers precisely. This task is not trivial since the Bragg grating is sensitive to changes in temperature and strain. In this paper, the authors controlled the furnace to sustain a defined temperature and applied increasing strain steps to the sample. In this way, they can differentiate between the changes caused by the increasing strain and changes from the rise in temperature. This calibration approach makes it possible to detect hot tearing between the solidus line and the liquidus temperature for hypo-eutectic and hyper-eutectic alloys with a wide solidification range. Therefore, the three base alloys AlSi5, AlSi17, and AlCu5 are investigated, and the AlSi9Cu3 served as a cross-validation reference.

Laser-induced breakdown spectroscopy for studying solidification processes

Antonio Vazquez Prudencio, Máni Maghsoudi, Abdul Rahman Mallah, Gudrun Saevarsdottir, Halldor Svavarsson, Georges Salloum-Abou-Jaoude, Snorri Ingvarsson and Kristjan Leosson

DTE ehf (Iceland); Reykjavik University (Iceland); Constellium C-TEC (France)

Laser-induced breakdown spectroscopy (LIBS) analysis offer a promising approach for in-situ measurement of the chemical composition of molten aluminum alloys and the investigation of high-temperature phase transformations within the liquid phase. When analyzing molten metal, LIBS can be used to quantify the dissolved concentration of a given element in the melt, rather than the total concentration in the sample. Hence, LIBS can be used to track the liquidus line in solid-liquid systems, as well as non-equilibrium processes. In this work, we present results of such studies for a variety of binary and ternary aluminum alloys, including real-time investigations of the influence of melt cooling rates on phase formation. The experimental results were compared with thermodynamic databases to assess the agreement between calculations and measurements. The results confirm that LIBS is a powerful tool for characterization of solidification processes.

Precipitation hardening potential in cast Al-Fe alloys

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Brunel University of London, BCAST (UK); King Mongkut's Institute of Technology Ladkrabang (Thailand)

Our recent discovery of precipitation hardening in Al-Fe alloys produced by conventional casting opened an avenue for the development of new alloys as well as exploiting this effect in recycled aluminium alloys. We studied the relationship between the supersaturation of the aluminium solid solution with iron upon solidification at different cooling rates (4 to 60 K/s) and demonstrated a considerable driving force behind the precipitation phenomena. The precipitation products were identified as Al13Fe4 and their lattice coherency with the matrix established. Although the (AlFe) precipitates resulted in some measurable hardening, this effect could be significantly improved by small additions of transition metals such as Zr that were shown to segregate to the interface between (AlFe) particles and the aluminium matrix. The effects of cooling rate, iron concentration in the alloy and additional alloying with Zr are discussed.

Impact of mold constraints on casting shrinkage during the cooling phase in rapid low-pressure sand-casting process

Ahmed Ktari and Mohamed El Mansori

Arts et Métiers ParisTech, MSMP (France)

In the rapid low pressure sand casting (LPSC) process, 3D-printed sand molds (3DPSM) are used to produce complex, near-net-shape castings of high quality. The design of 3DPSM requires consideration of various pattern allowances to ensure that the final part meets the dimensional and geometric requirements specified in the technical data sheets. In this study, a spindle body was cast using rapid LPSC process, considering only the machining and shrinkage allowances for the mold design. Using scanning technology, the 3D surface deviation of the casting was found to have a negative deviation on part of the inner surface. To understand the mechanisms leading to these negative deviations, a coupled thermomechanical FE model of the LPSC process was built using ProCAST software. The effects of mold and core constraints on casting shrinkage during the cooling phase of the process were investigated. The evolution of the mold/cast gap width and the residual stresses generated during the cooling phase were monitored at different locations of the cast and the mold. The effects of the mold stiffness and the mechanical behavior of the casting on the two monitored parameters were also investigated. This study makes it possible to better understand how the mold and cast expand and contract during the LPSC process. The results enable better optimization of pattern allowances and then the mold design, leading to a reduction in machining time and resource consumption.

Low-Pressure Die Casting of Aluminum Alloy Components for EV Battery Enclosures

Jaime Lazaro-Nebreda, Erdem Karakulak, Pavel Shurkin and Geoff Scamans

Brunel University London (UK)

The production of battery boxes for electric vehicles typically relies on extrusions joined by welding, riveting, or adhesives, with minimal use of casting components due to their lower performance and higher defect rates. This study aims to enhance the structure and properties of battery box corner nodes, making them more reliable and viable for broader use in electric vehicle manufacturing. We employed low-pressure die casting (LPDC) to produce the corner nodes, replacing previous sand casting method known for higher porosity. A new die design, developed in collaboration with Sarginsons, allows for the simultaneous casting of four corner nodes, reducing die filling turbulence and improving casting integrity. Additionally, we use electric heating for the die and furnace to lower CO2 emissions compared to traditional gas burning methods. Advanced characterization techniques, including X-ray tomography and Profilometry-based indentation plastometry (PIP), were used to evaluate the internal structure and properties of the castings. Our findings indicate excellent mold filling with minimal porosity defects and good mechanical properties, though with some variability. This variability correlates with the presence of porosity within the casting structure, demonstrating a clear relationship between local defects and local mechanical properties. This research contributes to the development of optimized castings with reduced weight and low rejection rates, enhancing the potential for aluminum alloy cast components in electric vehicles.

Thu-C-II / Steels

Modeling and experimental evaluation of as-cast structure and macrosegregation in steel ingot from a rotating mold

Menghuai Wu, Haijie Zhang, Christian Gomes-Rodrigues, Abdellah Kharicha, Alexander Scheriau, Thomas Holzgruber and Harald Holzgruber

University of Leoben (Austria); INTECO Melting and Casting Technologies GmbH (Austria)

The concept of using a rotating mold for casting steel ingots was proposed 50 years ago, and it was demonstrated that this technique can promote a center equiaxed structure and eliminate centerline shrinkage. However, it has never been implemented in practice. The reason for this is that the complex multiphase flow during solidification in the rotating mold, along with the flow-solidification interactions, were not fully understood, leading to a lack of control over the engineering casting process. Recently, the research group at the University of Leoben adapted their mixed columnar-equiaxed solidification model for this process, incorporating two significant improvements: (1) the model was transitioned from an inertial to a rotational frame, explicitly accounting for centrifugal, Coriolis, and Euler forces acting on each phase; and (2) the mechanism of equiaxed crystal formation through fragmentation was included. This enhanced model was systematically evaluated through parameter studies, comparisons with existing literature, and laboratory casting experiments. The novel findings are as follows: 1.The formation of equiaxed crystals in steel ingots is primarily driven by crystal fragmentation, rather than by heterogeneous nucleation. 2.The rotating mold technique for promoting the center equiaxed structure can only be achieved with alternating mold rotation and is highly sensitive to the process parameters of mold rotation. 3.The classical A-segregation can be suppressed using the mold rotation technique. 4.While centerline shrinkage porosity and A-segregation are eliminated, vertical segregation along the centerline can intensify due to the gradual accumulation of equiaxed crystals. Therefore, addressing this unwanted axial segregation requires precise 'design' of the multiphase flow, achieved by optimizing the mold rotation parameters and implementing other complementary measures.

2.5D thermo-mechanical strong-form meshless travelling slice model of continuous casting of steel billets

Gašper Vuga, Tadej Dobravec, Boštjan Mavrič and Božidar Šarler

University of Ljubljana (Slovenia)

This study introduces a novel strong-form meshless method for solving the thermo-mechanical solidification process of the continuous casting of steel. A two-dimensional slice of zero thickness, moving in the casting direction, is modelled in the Lagrangian framework. The mechanical model is one-way coupled with the thermal model, where heat fluxes from the mould, sprays, and rollers are applied to solve heat conduction within the strand. The resulting temperature and ferrostatic pressure drive the mechanical Kozlowsky IA viscoplastic model, which calculates the shrinkage of the solid shell and the resulting residual stresses. These results are utilised to identify critical regions prone to hot-tearing formation. The mechanical model employs a generalised plane strain assumption (2.5D), incorporating linear strains perpendicular to the slice, facilitating the computation of strand straightening. The thermo-mechanical model is spatially discretised using the radial basis function generated finite differences (RBF-FD). The mechanical part incorporates a novel hybrid approach that combines RBF-FD with classical finite differences, enhancing the method's stability. This study examines the influence of process parameters such as casting velocity, material composition, and impact of electromagnetic stirring on solid shell shrinkage and the probability of hot-tearing occurrence in the strand. The study represents the first 2.5D strong-from meshless thermo-mechanical model successfully used in a complex industrial process.

Numerical issues of the liquid/solid interface determination at continuously cast slab solidification using effective heat capacity and enthalpy methods

Anna Ivanova and Brian G. Thomas

Colorado School of Mines (USA)

Numerical accuracy in predicting growth of the solidified shell during metal alloy solidification is a key aspect of computational modeling of heat transfer during casting processes. An accurate model of shell temperature and growth dynamics is essential for predicting both micro- and macro- behavior. In continuous casting of steel, shell formation controls the surface integrity and grain structure, which affects defects such as breakouts, cracks, and segregation. Many different numerical methods exist for solving the governing differential equations and calculating the position of the moving liquidus and solidus temperature interfaces, including the effective heat capacity and enthalpy methods. All of these methods experience numerical errors, including fluctuations of the shell thickness, which are sometimes mistaken for real growth variations by inexperienced researchers. These fluctuations are also important because they greatly aggravate errors in the calculation of gradients, such as front velocity and cooling rate, which control microstructure formation. This work investigates these numerical fluctuations, in the context of a classic one-dimensional solidification test problem involving continuous casting of steel slabs. The results confirm that these fluctuations arise in all methods investigated and are associated with the computational grid. Movement of the phase transition boundaries between two-phase and single-phase regions speed up and slow down as the front passes through each grid node in a solidifying cell. Numerical difficulties increase with decreasing temperature range between the liquidus and solidus temperatures. The wiggles can be used to identify the numerical errors, which are quantified in this work. Numerical procedures to improve computational accuracy and to minimize the magnitude of the errors associated with these fluctuations are discussed.

Influence of the fragmentation on the microstructure and segregation in a 110 t steel ingot

Ahmed Kaci Boukellal and Hervé Combeau

Université de Lorraine & CNRS, IJL (France)

Steel ingot solidification is a challenging problem that has been studied for more than five decades. Indeed, it involves different phenomena at the macroscale such as fluid flow, heat and mass transfer, coupled to phenomena at the microscale. At this last scale, the dendritic structures columnar or equiaxed develop. In the present work, we focus on the influence of the microstructure on the macrosegregation in a 110 t steel ingot. More precisely, we study the influence of the fragmentation phenomenon on the microstructure and notably the location of the columnar to equiaxed transition and the carbon segregation. To do so, we use the multi-scale and multi-physics homemade developed software SOLID© to span a wide range of (1) the fragments fluxes, (2) the critical gradients below which fragmentation is triggered along the columnar front, and (3) heights, the location at which fragmentation occurs. Comparison of our numerical results, namely the carbon segregation maps and the microstructures maps, to the experimental ones show that the equiaxed grains originate mainly from the fragmentation in the hot top part of the ingot. Moreover, the carbon segregation along the ingot centerline reproduces well the experimental profile on the lower part of the ingot when the solid movement is taken into account. However, a better agreement with experiments is observed on the upper part when the grains are assumed to be fixed. The discrepancy between experiments and numerical simulations on the upper part of the ingot, when the solid movement is taken into account is discussed. We suggest that this discrepancy is related to the law of permeability used in the model to describe the flow through the equiaxed structures.

Characterisation of centimetric scale segregation in large steel ingots

Jacob R. Kennedy, L Gutman, F Roch, A Marceaux-Dit-Clement, M Zaloznik and J Zollinger

Université de Lorraine & CNRS, IJL (France); Framatome (France)

During the solidification of large steel ingots segregations can occur at multiple scales. The traditional techniques used for the characterisation of micro and macrosegregation patterns are not suitable for the centimetric meso-scale segregations which are known to form. Micro X-Ray Fluorescence (μXRF) was optimised for characterising steel samples and applied to samples serial sectioned from a large ingot. The chemical maps obtained showed evidence of three scales of segregation, intradendritic (microsegregation between secondary dendrite arms), interdendritic (between dendrites/grains) and a third scale which was continuous between samples. These continuous segregations can be tracked between samples and reconstructed, appearing in the form of segregation channels in 3D. To the authors knowledge this is the first instance in which what may possibly be the classical A segregates have been characterised in 3D, allowing an analysis of their size shape and composition evolution to be conducted. It was shown that these characteristics remain similar between the continuous channel segregates and the interdendritic segregates, which were not continuous between maps. The solidification of the ingot was also simulated in order to extract the local conditions of the experimental sample, such as the thermal history, evolution of the solid fraction and liquid flow. Comparison of the simulations and experimental data allow the identification of when during solidification the channels form.

Development of Maraging Steels from Mixes of Commodity Alloys

Sama Safarloo, Tobias Edtmaier, José M. Torralba and Juan Alberto Meza

Universidad Carlos III de Madrid (Spain); IMDEA Materials (Spain); Vienna University of Technology (Austria)

The development of high-performance maraging steels using commodity alloys containing the essential alloying elements was investigated. An arc melting process was employed to consolidate compositions as close as possible to a maraging type steel, including 18Ni-300, MAR-50 Co-free, and MAR-60 grades. A characterization of the structural and microstructural characteristics and mechanical properties (including tensile features) was carried out to evaluate the quality of the produced steels. This approach offers a sustainable and cost-effective method as it would allow the development of very high performance steels without the need to start from critical alloying elements but from highly available scrap from commodity alloys.

Thu-C-III / Nickel alloys

Gravity effect on the freckle formation during directional solidification of Ni-based superalloys

Haijie Zhang, Dexin Ma, Yunxing Zhao, Abdellah Kharicha and Menghuai Wu

University of Leoben (Austria); Central South University (China)

The formation mechanism for freckle defects is well understood. With the gravity effect during an upward directional solidification, thermosolutal convection caused by liquid density inversion in the mushy zone accounts for the onset of freckles. The solute-enriched liquid with a lower density tends to rise, forming the plumes and segregation channels. The upwelling flow within the channels fragment some high-order side arms around the segregation channels, leading to the formation of misoriented grains. One idea to suppress this gravity effect is to solidify the casting in a downward direction [T. Cheng, et al., Mater. Charact. 202 (2023) 112992]. The objective of this work is to study the freckling tendency during a downward directional solidification process. The underlying idea of this technique is to align the solidification direction with gravity, thereby allowing the solute-enriched liquid with lower density, located in the deepest part of the mushy zone, to stabilize the interdendritic liquid flow. A previously developed multiphase volume-average solidification model is used to model the directional solidification process. The spurious grains are merely originated from dendrite fragmentation. Two directional solidification experiments were conducted in an industrial-scale Bridgman furnace. One is cast with upward solidification, and the other is cast with downward solidification. The purpose of the experiments is to validate the numerical model. The main findings are as follows: Freckles were observed in castings solidified upward, whereas castings solidified downward were free of freckles. This study demonstrates that downward directional solidification effectively suppresses freckle formation by aligning the solidification direction with gravity, thereby counteracting solutal-buoyancy-driven flows. However, due to the shadow effect of the Bridgman furnace, thermal-buoyancy-driven flows cannot be completely eliminated. When the lateral temperature difference within the casting exceeds a certain threshold, the casting quality is significantly degraded as a result of the formation of numerous spurious grains.

Freckle Formation in directional solidification of IN718 alloy

Ibrahim Sari, Menghuai Wu and Abdellah Kharicha

Montanuniversitaet Leoben (Austria)

In industrial processes involving molten metals, freckles are a common defect in nickel-based superalloy castings, which negatively impact mechanical performance. Castings with freckles are often discarded, leading to significant economic losses, as these defects cannot be eliminated through post-casting or thermomechanical treatments. Despite advancements in understanding the mechanisms behind these defects, reliable theories and empirical guidelines to inform engineering design remain scarce. This study investigates the formation of freckles during the directional solidification (DS) of IN718 alloy. A two-phase solidification model, coupled with fluid flow, heat transfer, and solute transport, is employed to simulate the solidification of IN718 alloy in a 3D cylindrical geometry with a diameter of 25 mm and a length of 150 mm using the finite volume method. The simulation captures critical phenomena, including thermo-solutal convection, buoyancy-driven flow, and macro-segregation during solidification. The results reveal the development of freckles aligned in the vertical direction, with distinct segregation patterns, including upward flow channels, observed post-solidification. A comparison with a published experimental setup, which closely resembles the classical Bridgman furnace used in industry, demonstrates good agreement with the simulation results.

Prediction and control of the casting defects in the directional solidification of single-crystal nickel-based superalloys

Jun Li, Neng Ren, Luwei Yang, Mingxu Xia, Hongbiao Dong and Jianguo Li

Shanghai Jiao Tong University (China); University of Leicester (UK)

Freckles and low angle grain boundaries are always formed on the turbine blade castings. The formation of freckles is believed to be the result of solute transport and remelting induced dendritic fragmentation at multiple scales, while low angle grain boundaries are regarded as the stress induced dendritic deformation. Numerical prediction is rather challenging to couple the heat transfer, fluid flow, nucleation, grain growth, solute partition, and strain-stress. We develop a microstructure prediction model combining the Eulerian multiphase framework and cellular automaton model. Stress and deformation of the dendritic structure are further analyzed using finite elemental method. Simulation results reveal that solute channels prone to be formed in the near-wall region and sharp features, while the solute plumes can hardly develop continuously under the perturbation of the melt flow. Radial heat flux of the directional solidification greatly promotes the formation of solute plumes. The overgrowing dendritic trunk is partially remelted in the swaying solute plume, and thus the isolated dendritic tip becomes floating grains in arbitrary orientation, which is the origin of the freckle grains. The flow-induced dendritic stresses were found to develop with the height of the primary dendrite tip and to reach a steady state with the stabilisation of the width of the mushy zone. The higher-order branches of the dendrites are the weak locations for flow-induced dendrite deformation. The dendritic stresses near the solidification front were found to be concentrated on the first layer of dendrites at the surface and transferred to the interior through dendritic bridging. Measures (such as adaptive withdrawal rate) are also proposed to reduce the unexpected radial heat flux in the directional solidification process in the Bridgman furnace.

Phase-Field Modelling of Microstructure Evolution and Heat Treatment Optimization in Multi-Component Ni-Based Superalloy

Murali Uddagiri, Yuxun Jiang, Lorenz Grafe, Jochen Tenkamp and Ingo Steinbach

Ruhr University Bochum (Germany); MAN Energy Solutions SE (Germany)

Ni-based superalloys are widely used in aerospace and energy sectors due to their exceptional mechanical properties and ability to withstand high temperatures. The performance of these alloys is strongly influenced by their microstructural evolution during solidification and heat treatment processes, particularly during homogenization and precipitation. This study uses phase-field simulations coupled with CALPHAD-based thermodynamic and kinetic databases to model the microstructural evolution of Ni-based superalloys. The phase-field approach provides a detailed understanding of nucleation, growth kinetics, and solute diffusion, capturing the key physical processes active at the microscopic scale. The first part of the study focuses on CMSX-4, a single-crystal Ni-based superalloy, to simulate dendritic growth, solute redistribution, and segregation of alloying elements under rapid solidification conditions. These simulations provide insights into the rapid solidification process, including the morphology and scale of the resulting microstructure. The second part extends the analysis to study the effects of heat treatment on microstructure evolution in LPBF-fabricated IN718. The as-built microstructure, characterized by eutectic Laves phases and a solid solution γ matrix, is subjected to various heat treatment strategies. The study investigates how the LPBF-produced microstructure influences the formation, volume fraction, and spatial distribution of γ', γ", and δ precipitates in IN718. The findings are validated against experimental results obtained from the same material, ensuring the reliability of the simulations.

Parallel sessions

Day 4 / Friday June 13, 2025

Fri-A-I / Rapid solidification

Crystallization waves and explosive crystallization of liquid helium

Peter Galenko and Nikolay Kropotin

University of Jena (Germany)

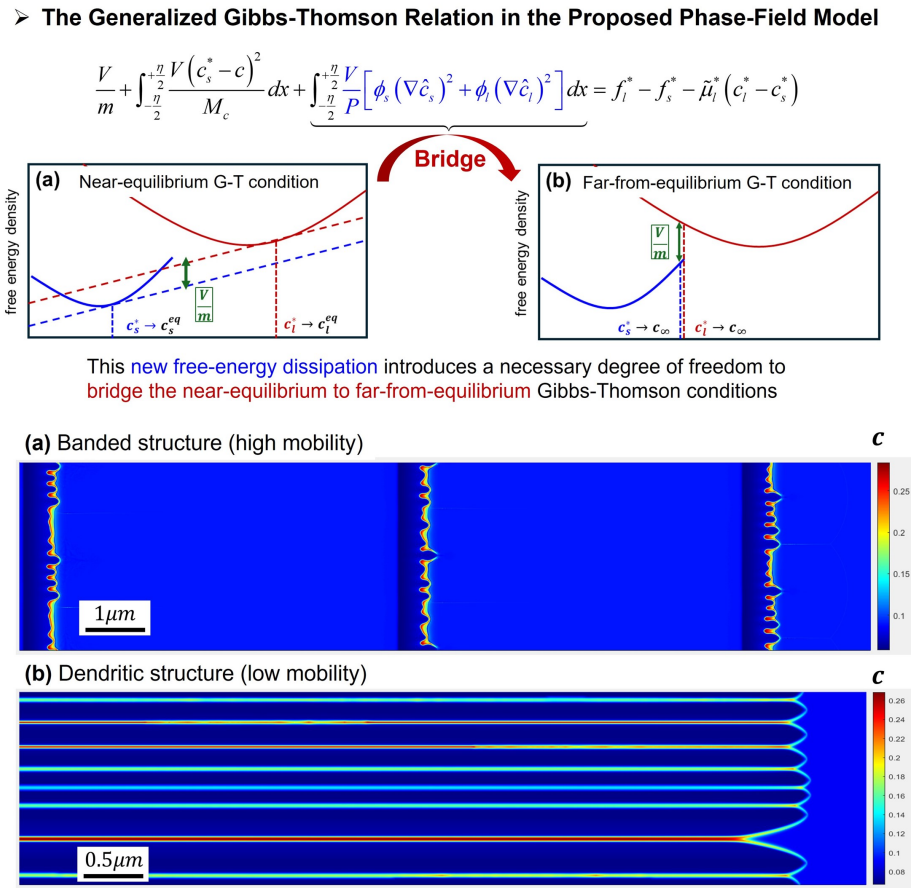
Explosive crystallization of liquid helium is one of manifestations of rapid solidification processes. The liquid helium, as a quantum macroscopic object exists in a narrow range of ultra-low temperatures and exhibits superfluidity with a cascade of various metastable states as the pressure changes. Features of the transition from a liquid superfluid state to a solid crystalline state are explained in the present theoretical modeling within the framework of a single description based on the kinetic phase field theory. To describe the peculiarities of crystallization of the liquid helium the hodograph equation is used as the equation for the sharp interface limit of the kinetic phase field. The change in the growth shape of quantum crystals, the appearance of crystallization waves, and fast explosive crystallization are described consistently with experimental data on phase transformations in superfluid helium.

A phase-field model bridging near-equilibrium and far-from-equilibrium alloy solidification

Yue Li, Lei Wang and Zhijun Wang

Northwestern Polytechnical University (China)

Mapping to the appropriate GibbsThomson (GT) condition is essential for phase-field modeling to produce reliable and realistic solidification microstructures. However, existing phase-field models face challenges in simultaneously satisfying both near-equilibrium and far-from-equilibrium GT conditions. This limitation restricts the applicability of phase-field methods in scenarios with a wide range of interface velocities, such as those observed in additive manufacturing. In this work, we propose a phase-field model that bridges both regimes by redefining each interfacial concentration field into two components: a conservative term representing long-range diffusion and a non-conservative term accounting for short-range redistribution within the diffuse interface. This formulation makes the model fully variational and analytically traceable through thin-interface analysis, allowing for accurate mapping to the GT condition and determining model parameters. A key advancement of this model is the inclusion of free energy dissipation for short-range redistribution fluxes in the thin-interface limit, providing the necessary degree of freedom to reconcile both near-equilibrium and far-from-equilibrium GT conditions. This capability is demonstrated by applying the model to simulate banded structures, effectively capturing the transition between near-equilibrium and far-from-equilibrium states.



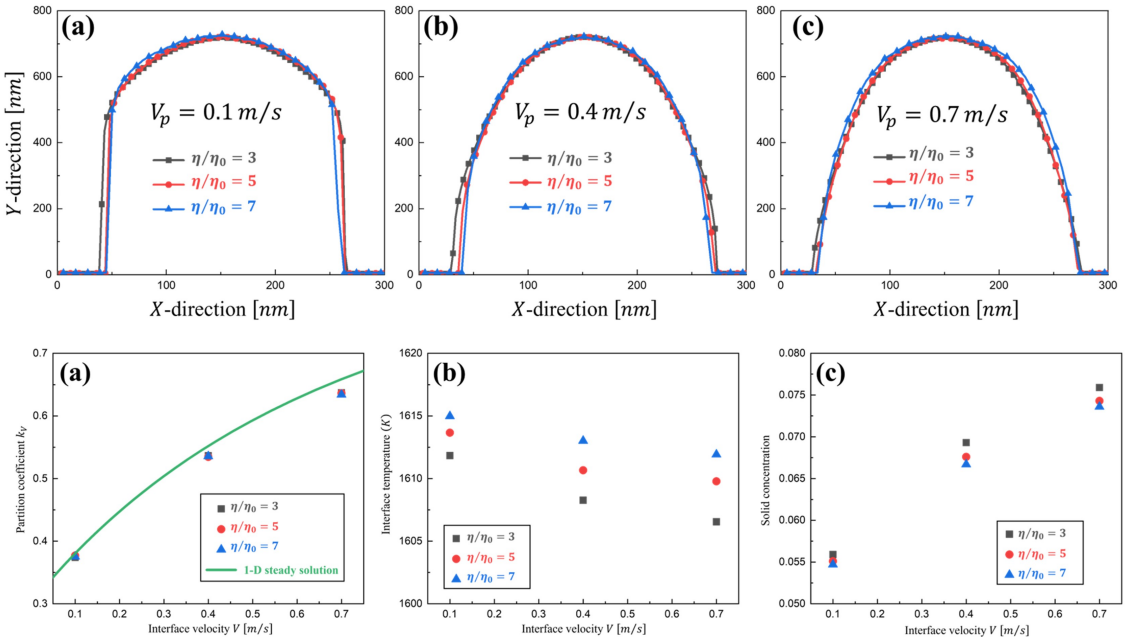
Quantitative phase-field modeling of solute trapping and solute drag in rapid solidification

Yue Li, Lei Wang and Zhijun Wang

Northwestern Polytechnical University (China)

Solute trapping and solute drag are key non-equilibrium phenomena observed during rapid solidification. To provide a practical numerical tool for investigating their impact on solidified microstructures, we propose a novel phase-field model that quantifies rapid solidification by introducing an interfacial short-range solute redistribution flux and enhancing interfacial solute diffusivity. The model incorporates three major advancements: (i) The short-range redistribution transitions two distinct concentration fields from equilibrium partitioning to non-partitioning conditions as the interface velocity increases. This feature not only prevents the formation of spurious phases but also enables high-velocity asymptotic behavior independent of the alloy's thermodynamic properties. (ii) By employing tensor solute diffusivity and correcting the normal component with local curvature, all artificial interface effectssuch as solute trapping, surface diffusion, and interface stretchingcan be simultaneously suppressed by enlarging the interface thickness. (iii) Due to the alloy-independent asymptotic solution, an analytical relation between normal solute diffusivity, interface thickness, and local curvature can be derived for arbitrary binary alloy. Two-dimensional directional solidification simulations further demonstrate that this model successfully reproduces the expected solute trapping and solute drag behaviors and is effective for describing non-dilute alloys.

Quantitative phase-field modeling of solute trapping and solute drag in rapid solidification

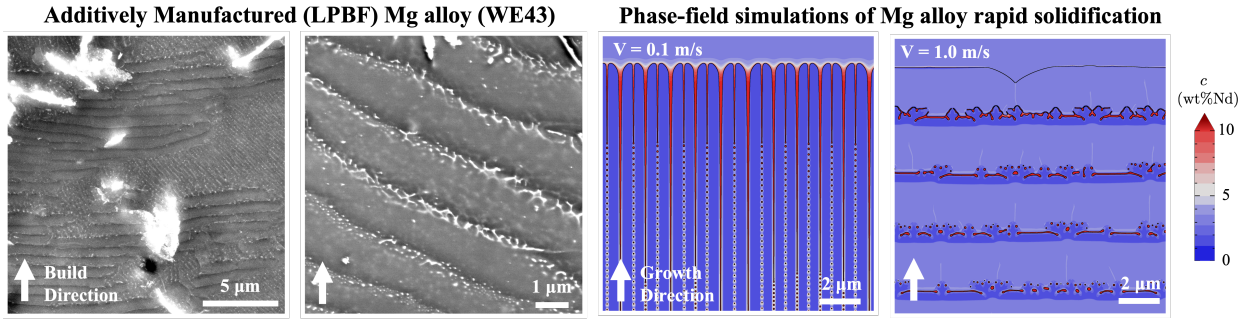


Emergence of Banded Microstructures in Rapid Solidification of Biomedical Mg Alloys

Damien Tourret, Rouhollah Tavakoli, Adrian Boccardo, Ahmed Kaci Boukellal, Muzi Li, Jon Molina and Javier LLorca

IMDEA Materials (Spain); Sharif University of Technology (Iran); University Rey Juan Carlos (Spain); Nancy University IJL (France); Universidad Politecnica de Madrid (Spain)

Laser powder-bed fusion (LPBF) is often described as a rapid solidification process due to the high cooling rates involved. However, direct evidence of far-from-equilibrium solidification phenomena such as solute trapping, kinetic undercooling, or morphological transitions remains limited. Recent observations of ”banded” microstructures in LPBF-printed biomedical WE43 Mg alloys offer compelling evidence of rapid solidification in LPBF of this alloy. These microstructures, characterized by alternating segregation-free and patterned regions normal to the growth direction, are hallmarks of rapid solidification under far-from-equilibrium conditions. Here, we use computational simulations to investigate the physical origins and evolution of these banded structures. We use quantitative phase-field modeling of rapid solidification, applied to a model Mg-Nd system under thermal conditions relevant to LPBF additive manufacturing. These simulations reveal that LPBF-relevant conditions indeed favor the development of banded microstructures, driven by instabilities in the dendritic interface. In Mg alloys with hexagonal close-packed symmetry, these instabilities originate predominantly from fast-growing dendritic sidebranches at 60° angles from the primary growth direction. This work offers promising perspectives toward the rational design of 3D-printed biomedical implants with spatially tailored properties through process-informed microstructural control.



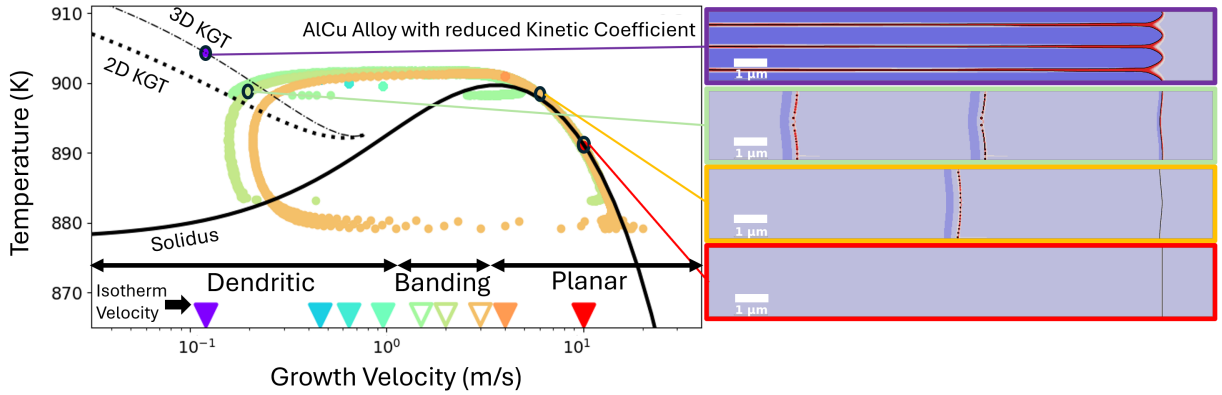
A phase-field study of the effect of kinetic undercooling on the occurrence of banding in rapid solidification of alloys

José Mancias, Rouhollah Tavakoli, Raymundo Arroyave and Damien Tourret

Texas A&M University (USA); IMDEA Materials (Spain); Sharif University of Technology (Iran)

Solidification, a key process in manufacturing and materials science, governs the formation of microstructures and, consequently, material performance. During rapid solidification, banding microstructures may emerge, which are characterized by periodic oscillations between planar and dendritic or cellular morphologies, significantly affecting alloy properties. These patterns are driven by instabilities in the solid-liquid interface under certain thermal and solutal conditions. Within the broad relevant welding and additive manufacturing literature, some alloys (e.g., Al, Mg) are known to exhibit banding in the high-velocity range transitioning from dendritic to planar beyond absolute stability, while others (e.g., Fe, Ni) do not. However, the fundamental properties that promote or suppress this banding regime remain unclear. We explore which alloy parameters influence the occurrence (or absence) of banding. To do so, we use the phase-field model proposed by Ji, Dorari, Clarke, and Karma [Physical Review Letters 130, 026203, 2023], which enhances computational efficiency by calibrating solute diffusivity through the interface. In particular, we focus on the mobility parameter μ, which controls interface kinetic undercooling. By varying μ, we identify critical conditions governing the transition between banding and non-banding behavior. For alloys prone to banding, we establish a threshold μ below which banding disappears. For alloys typically not prone to banding, increasing μ can induce band formation. These findings provide a framework for predicting banding behavior during rapid solidification and contribute to advancing the understanding of rapid solidification phenomena to guide the development of materials with tailored properties.

Effect of Kinetic Coefficient and Isotherms' Velocity on Rapid Solidification Banding Instability



Fri-B-I / Additive manufacturing IV

Multi-mode imaging and analysis of solidification behaviour in metal additive manufacturing

Wajira Mirihanage, Fan Wu, Da Guo, Renan Kindermann, Adnan Ditta, Zhe Cai, Matthew Roy and Stefan Michalik

University of Manchester (UK); Henry Royce Institute (UK); Diamond Light Source (UK)

Additive manufacturing enables the rapid production of large-scale components with intricate geometries. However, the rapid solidification characteristics inherent to arc and laser-based additive processes introduce significant challenges, particularly in defect formation and microstructural control. Time-resolved in situ synchrotron X-ray imaging and diffraction techniques provide a powerful means to investigate melt pool evolution and the solidification processes involved in wire arc direct energy deposition-based metal additive manufacturing. Unique experimental setups and configurations allowed real-time visualization and investigation of melt pool dynamics and phase transformations during melting and solidification. Multi-modal data comprising time-resolved imaging, diffraction patterns, and post-solidification high-resolution microscopy provide details across multiple spatiotemporal length scales. Processing, quantification, and analysing the extensive volumes of data generated in these experiments presented substantial challenges. This work highlights the methods employed to handle and analyse multi-stream data, enabling the extraction of insights into solidification microstructure formation. The analysis of the imaging data and extracted results reveals the influence of various external forces on heat and mass transfer within the highly transient melt pool, which ultimately shapes solidification microstructures and defect formation.

On the origins of fine equiaxed microstructure in additively manufactured 316L stainless steel Inconel 718 bimetals

Sourav Goswami, Manas V. Upadhyay, Sushil Mishra and Shyamprasad Karagadde

Indian Institute of Technology Bombay, Mumbai (India); Ecole Polytechnique, LMS (France)

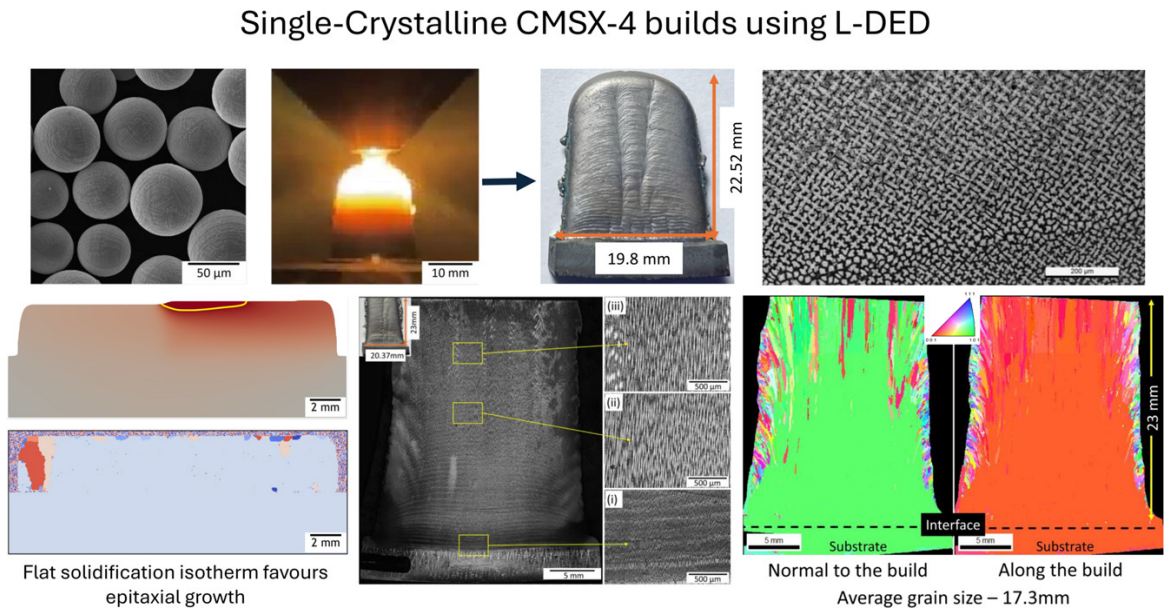
Bimetallic structures of 316L stainless steel and Inconel 718 were deposited by laser directed energy deposition using wire feedstocks and identical deposition parameters for both materials. The interfaces formed between the two materials varied with the sequence of deposition addition of Inconel 718 on pre-deposited 316L stainless steel produced flat, regular interfaces (Type 1 interfaces), while depositing 316L stainless steel on Inconel 718 led to wavy, irregular interfaces (Type 2 interfaces). Electron backscatter diffraction-based analysis revealed epitaxial grain growth and discontinuous grain growth across the Type 1 and Type 2 interfaces, respectively. Further, regions near the Type 2 interface possessed a fine equiaxed microstructure with a high density of Σ3 twin boundaries, with clusters of neighboring grains exhibiting multiple-twin orientation relationships with a five-fold symmetry around a common <110> axis. Insights were drawn from a computational fluid dynamics-based heat transfer and fluid flow model of the system to explain the unique solidification microstructure.

A Multi-Scale Framework for Achieving Single-Crystal Growth in Ni-based Superalloy Using Laser-Directed Energy Deposition

Swapnil Bhure, Divya Nalajala and Abhik Choudhury

Indian Institute of Science, Bengaluru (India)

Additive manufacturing (AM) has emerged as a transformative technology for producing complex geometries, making it an attractive choice for manufacturing critical aerospace components. High-pressure turbine blades in jet engines represent a quintessential example, as they combine intricate geometries with stringent microstructural requirements, such as single-crystallinity, to ensure superior performance in extreme environments. However, achieving single-crystal structures in such components through AM remains a significant challenge due to the interplay between thermal conditions, solidification behavior, and geometric complexity. This work presents a comprehensive multi-scale framework for identifying process parameters that enable the fabrication of single-crystalline CMSX-4 superalloy builds using Laser-Directed Energy Deposition (L-DED). At the melt-pool scale, a diffuse-interface-inspired model is developed to simulate the shape and thermal dynamics during multi-layer deposition. The simulated thermal histories are subsequently used in a Potts-based grain-structure model to predict solidification textures and assess the conditions necessary for single-crystal growth. The parameter space derived from these simulations is experimentally validated, demonstrating the successful realization of single-crystalline microstructures. Additionally, the thermal histories are employed in phase-field simulations to evaluate the primary dendrite arm spacing (PDAS) for the CMSX-4 alloy, which serves as a critical indicator of microstructural fidelity. These simulated PDAS values are compared with experimental measurements, providing validation and further insights into the solidification conditions under various process parameters. The results reveal a strong correlation between optimized thermal gradients, solidification rates, and the preservation of single-crystal growth. This integrated approach not only highlights the critical process parameters for achieving epitaxial growth but also establishes a pathway for designing strategies to build complex shapes while maintaining desired microstructural attributes. The insights gained from this study have broader implications for advancing the application of AM in producing high-performance components for aerospace and other industries.



CMSX-4 Superalloy Builds: A Comparative Study of Directional Solidification and Additive Manufacturing with Optimized Heat Treatment Strategies

Divya Nalajala, Swapnil Bhure and Abhik Choudhury

Indian Institute of Science - Bangalore (India)

Single crystalline Ni-based superalloys are preferred in the hottest parts of the aero-engine due to absence of the grain boundaries which improves high temperature creep strength. Conventionally, Directional solidification processing (DS) is used to produce columnar and single crystalline (SX) microstructures in Ni based superalloys. However, traditional manufacturing involves multiple complicated steps and requires long-term homogenization heat treatments before the component can be used in the final application. Additive manufacturing (AM) has revolutionized the manufacturing sector because of its ability to produce near-net-shaped components in a single step using a computer-aided design (CAD) model of the part. In addition to that, high thermal gradients and solidification rates associated with the AM processing favour epitaxial growth and results in microstructural refinement compared to the conventional processing. The objective of this study is to understand and compare the microstructure, segregation behaviour and mechanical properties of the CMSX-4 superalloy single crystals manufactured through DS and laser based directed energy deposition (DED) AM routes. Additionally, the study aims to optimize the heat treatment strategy specifically for AM samples to enhance their microstructural and mechanical performance. In-house developed vertical Bridgman furnace is used to generate the superalloy single crystals through seeding technique as a function of thermal gradient and solidification velocities. Laser based DED machine is used to manufacture superalloy single crystals of [001] orientation by epitaxial growth from the substrate using bi-directional scan strategy. Microstructural analysis of DS and AM processed single crystals revealed a dendritic microstructure with a larger dendrite arm spacing in the former case. Compositional analysis of DS single crystals revealed severe segregation of Re and W to the dendritic regions; Ta, Al and Ti to the inter-dendritic regions compared to AM builds. Additionally, heat treatment strategies are optimized for AM samples to improve their microstructural homogeneity and thereby mechanical properties.

Multiple physical fields of laser powder bed fusion of nickel-based superalloys

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Shanghai Jiao Tong University (China); Queen Mary University of London (UK); University of Leicester (UK)

Multiple physical fields in the laser powder bed fusion of nickel-based superalloys, including temperature field, flow pattern, solute distribution, are of great importance to estimate the properties and performances of the built parts. However, it is really hard to get the information in situ with experiments. In this case, numerical modelling could be a powerful approach to conduct the corresponding study. At the macro scale, that is the full dimensional of the melt pool, a thermal-fluid-solute model is developed to real the evolution of these multiple fields. In particular, solute transport during rapid and repeated thermal cycle in additive manufacturing (AM) leading to non-equilibrium, non-uniform microstructure remains to be studied. Here, a fully-coupled fluid dynamics and microstructure modelling at the microstructural scale is developed to rationalise the dynamic solute transport process and elemental segregation in AM, and to gain better understanding of nonequilibrium nature of intercellular solute segregation and cellular structures at sub-grain scale during the melting-solidification of the laser powder bed fusion process. It reveals the solute transport induced by melt convection dilutes the partitioned solute at the solidification front and promotes solute trapping, and elucidates the mechanisms of the subsequent microstructural morphology transitions to ultra-fine cells and then to coarse cells.

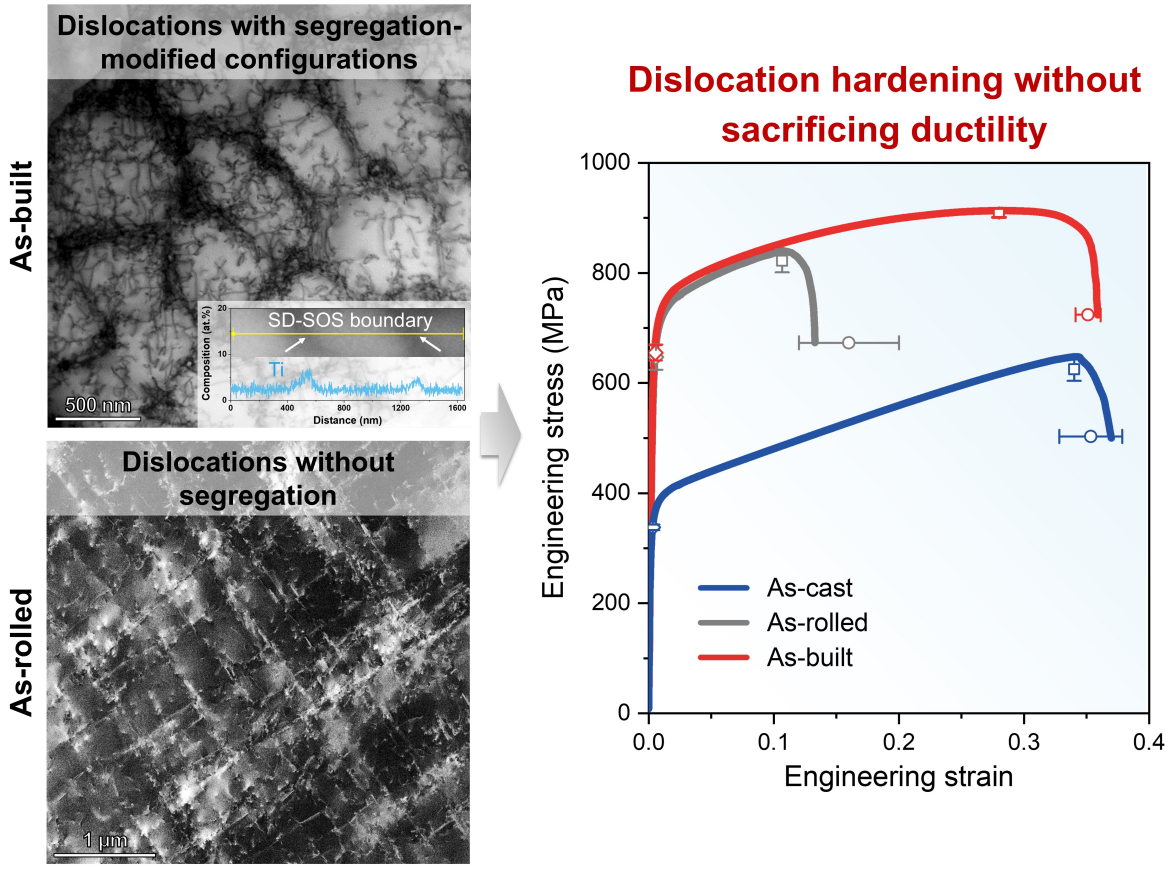
Fri-C-I / Complex alloys & Alloy design

Segregation-dislocation self-organized structures ductilize a work-hardened medium entropy alloy

Bojing Guo, Feng He and Jincheng Wang

Northwestern Polytechnical University (China)

Dislocations are the intrinsic origin of crystal plasticity. However, initial high-density dislocations in work-hardened materials are commonly asserted to be detrimental to ductility according to textbook strengthening theory. Inspired by the self-organized critical states of non-equilibrium complex systems in nature, we explored the mechanical response of an additively manufactured medium entropy alloy with segregation-dislocation self-organized structures (SD-SOS). We show here that when initial dislocations are in the form of SD-SOS, the textbook theory that dislocation hardening inevitably sacrifices ductility can be overturned. Our results reveal that the SD-SOS, in addition to providing dislocation sources by emitting dislocations and stacking faults, also dynamically interacts with gliding dislocations to generate sustainable Lomer-Cottrell locks and jogs for dislocation storage. The effective dislocation multiplication and storage capabilities lead to the continuous refinement of planar slip bands, resulting in high ductility in the work-hardened alloy produced by additive manufacturing. These findings set a precedent for optimizing the mechanical behavior of alloys via tuning dislocation configurations.



Design of a novel FeNiCrAl multi-component alloy based on phase selection mechanism

Jianbin Wang and Zhijun Wang

Northwestern Polytechnical University (China)

With excellent compressive mechanical properties, FeNiCrAl medium entropy alloys with multi-components have attracted extensive attention in recent years. However, the limited tensile ductility of FeNiCrAl medium entropy alloys is the bottleneck for their industrial applications. In this work, dual-phase of FCC+B2 and BCC+B2 were modulated in FeNiCrAl medium entropy alloys for excellent tensile behaviors. In the as-cast state, the tensile yield strength and ultimate tensile strength are 1140 MPa and 1423 MPa, respectively, with a uniform elongation of 6.0%. Furthermore, the minor alloying behaviors of W and Mo in FCC+B2 dual-phase FeNiCrAl alloy were explored. For tensile properties at ambient temperature, as-cast Fe36Ni36Al17Cr10Mo1 alloy exhibited higher yield strength and fracture strength compared with Fe37Ni36Al17Cr10 alloy. Then, dual-phase alloys with Mo content of 2 and 3 at% were further designed and carefully studied. It is found that a nano-scale structure occurred in as-cast Fe35Ni36Al17Cr10Mo2 alloy, where a large number of spherical BCC precipitates are distributed in the dendrite region of B2 phase. Meanwhile a mixture of irregular B2 phase and FCC phase is contributed to the inter-dendrite area. The Fe35Ni36Al17Cr10Mo2 alloy exhibited the most excellent and comprehensive mechanical properties due to the fine structure and its high work hardening ability. The yield strength, ultimate tensile strength and fracture elongation of as-cast Fe35Ni36Al17Cr10Mo2 alloy are 863 ± 20 MPa, 1285 ± 17 MPa and 16.0 ± 1.0 %, respectively, which is higher than the most of reported dual-phase as-cast FeNiCrAl multi-component alloys.

Generating alloy thermodynamic and thermophysical data using CALPHAD

A. Nicholas Grundy, Johan Jeppsson and Qing Chen

Thermo-Calc Software AB (Sweden)

Numerical simulation of solidification processes requires alloy properties in function of temperature and composition. CALPHAD databases are a well-established and widely used source of both thermodynamic properties as well as -more recently- thermophysical data such as thermal conductivity, liquid viscosity, surface tension, elastic properties and more. In the last years Thermo-Calc has been developing models for thermophysical properties and has been adding them to their commercial alloy CALPHAD databases. But having phase-by-phase descriptions of thermophysical properties in the database is only one side of the story. The other is deciding on assumptions that best represent the state of the alloy. For very slow cooling rates one can assume the alloy is in thermodynamic equilibrium and overall thermophysical properties can be calculated by rules of mixture using the fractions and compositions of all phases making up the alloy. For faster cooling rates a popular choice to describe the state of the alloy is the Scheil solidification model, that allows solute redistribution (segregation) to be accounted for. Quantitatively accounting for back-diffusion in the primary solidification phase and (specifically for steels) accounting for the decomposition of delta-ferrite further improve the accuracy and applicability of the Scheil model. Calculating thermophysical properties from a Scheil solidification simulation again requires applying rules of mixture, with the added complexity that the primary solidification phase will have a varying composition. Both equilibrium and Scheil assume thermodynamic equilibrium as the solid-liquid interface. For even faster cooling rates -typical for example for additive manufacturing- this assumption breaks down requiring other models, such as solute trapping models or models for dendrite tip undercooling, to describe solidification.

Phase field simulation study of solidification morphologies and microsegregation in high entropy alloy thin films

Alexandre Viardin, Anna Schönell, Thomas Bähr and Markus Apel

Access e.V. (Germany)

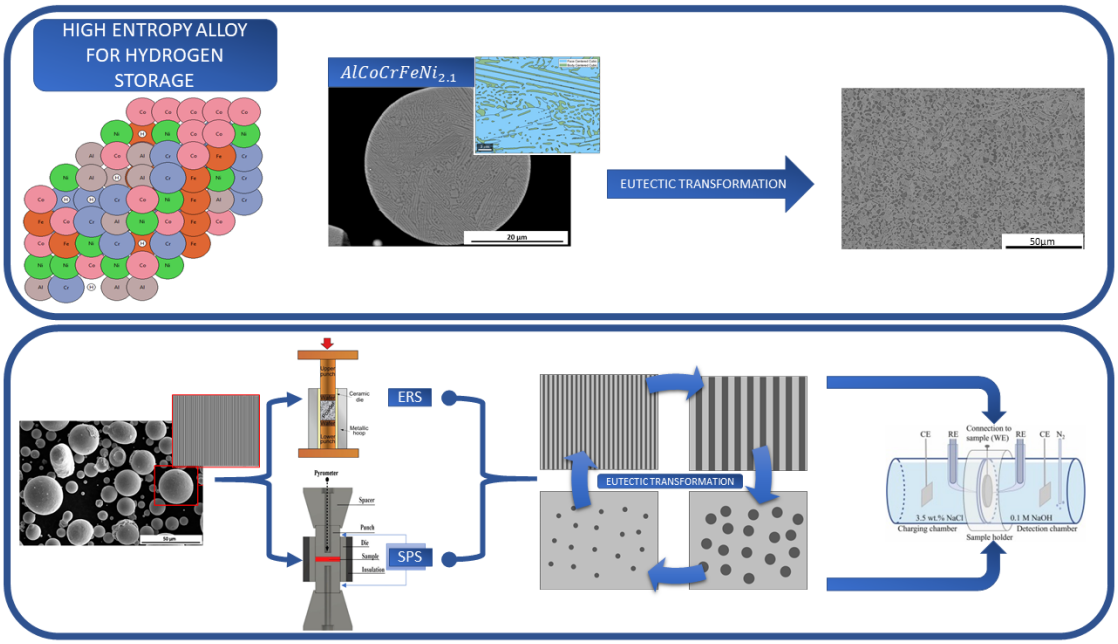
High entropy alloys offer great potential for producing high performance coatings while minimising or eliminating the use of toxic or critical elements. To realise this potential, a thorough understanding of the solidification morphologies and microsegregation patterns in thin films is essential to select appropriate alloy compositions according to the desired phase or elemental distributions in the coating. A wide range of alloy compositions in the five element alloy system of iron, cobalt, chromium, manganese and nickel have been investigated using CALPHAD coupled phase field simulations. It is shown how variations in composition affect solidification dynamics and the resulting microstructures. The results shed light on composition depending phase selection, solidification ranges and morphologies in high entropy alloy thin films.

Microstructural control in eutectic high-entropy alloys: solidification pathways for hydrogen storage applications

Daniel Guerrero Sánchez, Mónica Campos Gómez, Paula Alvaredo Olmos and José Manuel Torralba

Universidad Carlos III de Madrid (Spain); IMDEA Materials (Spain)

The use of hydrogen as a clean energy source offers a promising solution to reduce greenhouse gas emissions associated with fossil fuels. However, hydrogen embrittlement (HE) remains a significant challenge for materials used in hydrogen storage, such as stainless steels and aluminum. Although their FCC structure limits hydrogen permeation, defects within these materials promote embrittlement. Therefore, controlling hydrogen permeability is essential to enhance material resistance to HE and ensure the safety of hydrogen storage systems. In this context, eutectic high-entropy alloys (EHEAs) offer a novel alternative due to their ability to modulate hydrogen permeability through precise microstructural control. The present study focuses on the AlCoCrFeNi2.1 alloy, where solidification processes during powder atomization and subsequent sintering play a critical role in defining the final microstructure. Atomized powders, characterized by rapid solidification, exhibit refined and homogenous microstructures. These powders are consolidated using two sintering techniques: Spark Plasma Sintering (SPS), enabling rapid sintering, and Electric Resistance Sintering (ERS), achieving ultra-rapid sintering. The solidification conditions during atomization and sintering allow fine-tuning of the morphology of the microconstituents, transitioning from globular to lamellar structures. This microstructural modulation not only impacts mechanical properties but also plays a key role in hydrogen permeability and resistance to embrittlement. Furthermore, the control of interlamellar spacing as a function of the solidification and sintering parameters enables the optimization of the material's behavior in hydrogen-rich environments. By linking solidification processes, microstructural features, and hydrogen resistance, this study provides a pathway for the design of robust EHEAs tailored for safe and efficient hydrogen storage applications, addressing key challenges in clean energy technologies.



Posters

Validation of a Freeze-Lining Solidification Model Using Laboratory Experiments Under Static and Dynamic Conditions

Christian M G Rodrigues, Menghuai Wu, Haijie Zhang, Zilong Qiu, Annelies Malfliet, Muxin Guo, Anton Ishmurzin, Gernot Hackl, Clemens Lind and Abdellah Kharicha

University of Leoben (Austria); Katholieke Universiteit Leuven (Belgium); RHI Magnesita, Leoben (Austria)

The solidification and remelting of slag have traditionally received limited attention within the broader field of solidification. However, freeze-lining (FL) formation, a solidified slag layer, has recently gained significant interest from researchers due to its critical role in protecting refractory linings and its significant impact on overall energy efficiency. As such, FL formation has become a key consideration in the design and operation of numerous pyrometallurgical processes. This study investigated FL formation through both laboratory cold finger experiments and computational modeling. Static cold finger experiments were conducted to measure slag bath temperature, FL growth, and associated wall heat fluxes during the immersion of a gas-cooled probe. These data were used to validate a computational model framework that coupled a single-phase flow model with a mixture continuum solidification model. The model agreed well with the experimental results. Subsequently, the cold finger experiments were extended to a rotating crucible setup to explore the impact of forced flow on FL development. The model framework was modified to account for the additional rotational flow and successfully replicated the experimental results, including slag temperature distribution and FL growth. The validated simulations provided valuable insights into the mechanisms governing FL formation under both static and dynamic conditions. Differences in outcomes were interpreted using the computational model. The findings advance the understanding of FL behavior and offer valuable guidance for optimizing industrial pyrometallurgical processes. Despite its effectiveness, the mixture-continuum model oversimplified the FL crystal morphology by treating it as static. Future work will extend the model framework by incorporating a mobile morphology, allowing for a more accurate representation of the FL structure and dynamics.

Role of buoyancy flows in the remelting and solidification process of VAR

Chenbo Xu, Haijie Zhang, Christian Gomes-Rodrigues, Abdellah Kharicha and Menghuai Wu

University of Leoben (Austria)

Vacuum arc remelting (VAR) is one of the most important processes to refine metal alloys and is widely used in the production of superalloys, high-performance steel, and titanium alloys. The key feature of this process is the controlled upward quasi-unidirectional solidification, which reduces shrinkage pores and macrosegregation. However, depending on the alloys and alloy compositions, segregation defects such as freckles can still occur in VAR-produced ingots. This study uses a volume average based solidification model to study the flow phenomena and their interaction with columnar solidification during the VAR process. The flow is driven by self-induced electromagnetic forces, as well as thermo- and solutal buoyancy. Special focus is given to the solutal effect of specific alloy elements (lighter or heavier) and their impact on macrosegregation. A mixed columnar equiaxed model, which was developed by the current authors, is used [Wu et al., Metals 9 (2019) 229]. Here, only the formation of the columnar structure is considered, while the formation of equiaxed crystals is ignored. The model is coupled with ANSYS Maxwell to account for the electromagnetic forces. Two model alloys are considered: Ti-Zr and Ti-Si. These alloys were chosen because the atomic mass of the solute element Zr is significantly heavier than Ti, whereas Si is much lighter. The VAR model ingot has a diameter of 300 mm and a maximum length of 1000 mm. The simulation results show how the solute elements, whether lighter or heavier, influence molten pool flow dynamics, solute distribution, macrosegregation, and freckle formation inside the ingot. These insights contribute to a deeper understanding of the VAR process and can offer guidance for improving ingot quality. Acknowledgement: This work was financially supported by Austrian Research Promotion Agency (FFG) -Austrian Space Application Program (ASAP) through the project FLOWSICONS - II (FO999900538).

Combinatorial development of Al-based alloys using DED technology

Eduardo Reverte Palomino and Julien Zollinger

Institut Jean Lamour - Université de Lorraine (France)

The use of additive manufacturing technologies has greatly expanded the capabilities of metallurgical research for the development of new high-performance alloys. In particular, laser additive manufacturing (LAM) and direct energy deposition (DED) technologies provide a powerful combinatorial approach for the rapid evaluation of alloy compositions. However, many well-established alloys, such as aluminium alloys, still require further optimisation of their AM processing compared to traditional casting methods. In this work, we present and discuss a systematic combinatorial framework designed for combinatorial screening of metallic alloys via laser DED. Rapid development of metal alloys is achieved through high-throughput screening, which integrates combinatorial strategies and efficient evaluation to improve alloy properties. The material feeding system uses powder as the source, allowing in-situ powder mixing to produce on-demand compositions. First, the methodology of alloy screening and its optimisation are presented. Then, the effects of DED process parameters on manufacturing defects such as pores or cracks have been investigated. In addition, crack-free and high-density samples were further evaluated by microstructural, structural and hardness tests, allowing the mapping of binary to multicomponent systems for Al-Mn-Fe-Zr alloys.

Freckle Formation and Freckle Criterion of Directionally Solidified Alloys Under Various Solidification Conditions

Lisa Philipp, Ibrahim Sari, Menghuai Wu and Abdellah Kharicha

Montanuniversitaet of Leoben (Austria)

Freckles are macrosegregations that form during the directional solidification of alloys, significantly compromising their structural integrity. To address this challenge, we developed a numerical model to investigate melt and mushy zone behavior under thermosolutal convection and predict freckle formation under various casting conditions. The model simulates fluid flow in a two-dimensional Hele-Shaw-like cell during upward directional solidification, employing a two-phase mixture approach with the Boussinesq approximation to account for convective flow driven by density variations. The mushy zone is treated as a porous medium, with its permeability defined by the Karman-Cozeny relation. Initial studies focused on a linear horizontal solidification front with a rejected solute lighter than the solvent, analysing the effects of growth rate, temperature gradient, and solute expansion coefficient. To enhance the model, the influence of a convex interface was introduced by tilting the solidification front at an angle relative to the horizontal plane. This modification amplifies thermosolutal convection, increasing mushy zone permeability and primary dendrite arm spacing, thereby elevating the risk of freckle formation. Additionally, variations in the initial solvent composition were examined. [1][2][3] The combined effects of these factors are analysed using a Rayleigh criterion, offering valuable insights into freckle formation mechanisms under complex casting conditions. This work contributes to the development of predictive tools for optimizing alloy solidification processes and improving material quality. [1] J. Valdés, P. King, X. Liu. On the Formulation of a Freckling Criterion for Ni-Based Superalloy Vacuum Arc Remelting Ingots. Metallurgical and Materials Transactions A. 41 (2010) [2] C. Beckermann, J.P. Ramirez. Development of a freckle predictor via Rayleigh number method for single-crystal nickel-base superalloy castings. Metall Mater Trans A 31, 25452557 (2000) [3] W. Yang, KM. Chang, W. Chen, et al. Freckle criteria for the upward directional solidification of alloys. Metall Mater Trans A 32, 397406 (2001)

Physical simulation of the practical solidification process by chill-plate experiments

András Roósz, Arnold Rónaföldi, Zsolt Veres and Maria Svéda

University of Miskolc (Hungary); HUN-REN-ME Materials Science Research Group (Hungary)

During the practical solidification processes (like the continuous casting of steel, semi-continuous casting of aluminium, and mould casting), the solid/liquid front velocity and the temperature gradient continuously change, moving away from the chill plate or the wall of the mould. One of the methods of experimental solidification testing, which is most similar to practical solidification processes, is the chill-plate casting when the heat is removed from one direction, while it is restricted in the other one. Solidification experiments were performed with a self-built solidification facility that used three different heat extractions to determine the front velocity (v) and temperature gradient (G) values at which the columnar structure changes to equiaxial (CET). As the new facility has an RMF inductor, the effect of melt flow generated by the RMF was also investigated. The used Al-4wt% Cu alloys were provided by Hydro Aluminium Rolled Products GmbH, now Speira GmbH, manufactured from high-purity Al and Cu material without and with 0.5 wt.% of master alloy AlTi5B for grain refinement. The sample's length and diameter are 60 and 20 mm, respectively. The temperature distribution was measured by seven K-type thermocouples. During the solidification of the sample, both the front velocity and the temperature gradient were changed. Without RMF, if $G/v < 1$ Ks/mm2, the grain structure was equiaxed, while at 15 mT and 30 mT, it is 2,5 Ks/mm2 and 25 Ks/mm2, respectively.

Metadynamics of solid-liquid interface for alloy

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University of Tokyo (Japan)

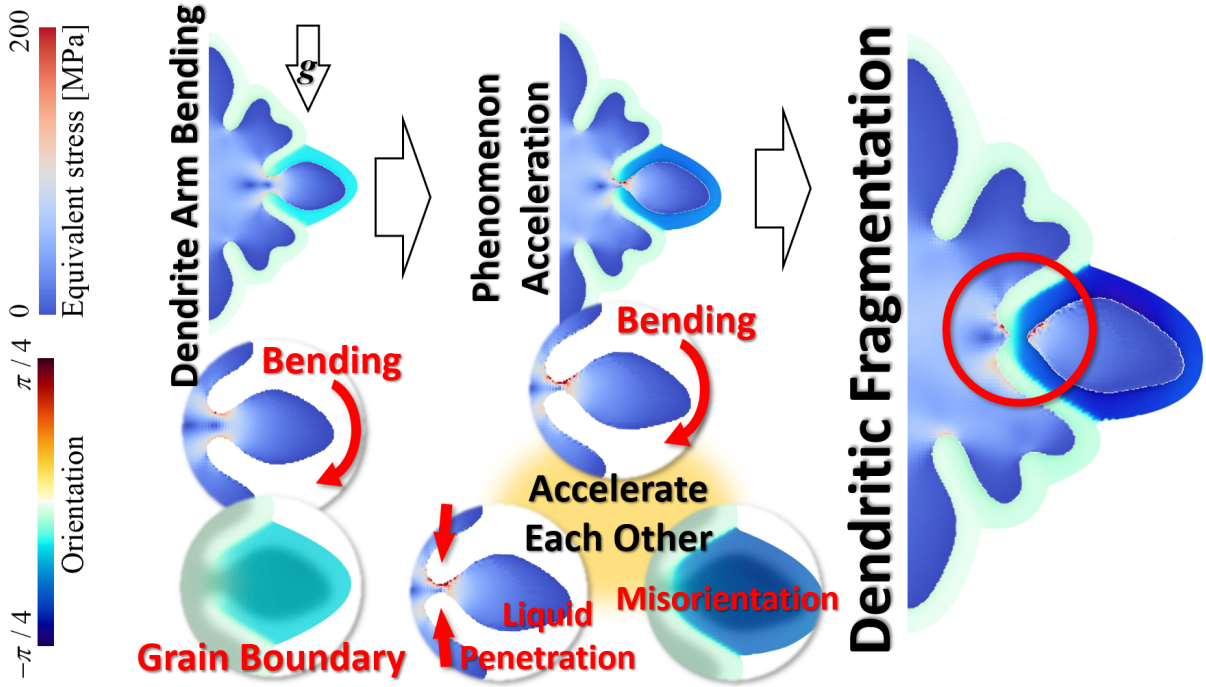
The solid-liquid interfacial energy is closely related to the solidification growth of structural materials. Determining the solid-liquid interfacial energy is essential for understanding this process. However, it is not easy to experimentally determine the solid-liquid interfacial energy with high accuracy. Therefore, theoretical approaches to determine the interfacial energy were developed. One method to calculate this value is metadynamics, an acceleration technique for molecular dynamics simulations. In this method, we employ collective variables to represent the state of the system (i.e. solid, liquid, etc.). By applying bias based on the collective variables, the probability of finding unexplored states increases. Using this method, we could observe a wide variety of states from solid to liquid during the simulation. From the applied bias, the free energy surface is calculated. Using metadynamics, previous studies have derived the free energy surface for pure metals with FCC and BCC structures, whereas there are few studies for binary alloy. In this study, we focused on the metadynamics for alloy systems to derive the free energy surface and the solid-liquid interfacial energy. The obtained free energy surface of the system was explained based on the change of free energy for each phase with carbon concentration change. In our method, the solid-liquid interfacial energy for alloys was calculated considering the solute distribution effect. This is done by using the free energy surfaces of two systems with different system sizes. The behavior of the free energy surface obtained from metadynamics is consistent with the thermodynamics for Fe-C binary-alloy system. Therefore, we concluded that metadynamics simulations are effective for analyzing the solid-liquid interfacial energy for binary alloys.

Phase-field multi-physics modeling and simulation of granular and dendritic fragmentation induced by solid deformation during solidification

Gensei Kobayashi, Mitsuteru Asai, Shinji Sakane and Tomohiro Takaki

Kyoto Institute of Technology (Japan); Kyushu University (Japan)

Microstructure refinement is a key approach to enhance the mechanical properties of metals. Near the melting temperature, grains or dendrites can easily fragment under the application of external forces. This fragmentation significantly contributes to microstructure refinement; however, the underlying mechanisms triggered by external forces remain poorly understood. To address this gap and identify optimal conditions for fragmentation, simulation studies are essential. In this study, we developed a multi-physics model to simulate granular or dendritic fragmentation induced by solid deformation during solidification. The model incorporates solidification and melting processes, grain boundary formation resulting from solid deformation, and liquid flow dynamics. Solid morphological changes and grain boundary formation were represented using the phase-field method, liquid flow was modeled with the lattice Boltzmann method, and solid deformation was captured using the material point method. The performance of the proposed model was validated through multiple simulations.



Large-Scale Data Assimilation for Estimating Interfacial Properties Using Quantitative Phase-Field Model

Aoi Watanabe, Ryuhei Sato and Yasushi Shibuta

University of Tokyo (Japan)

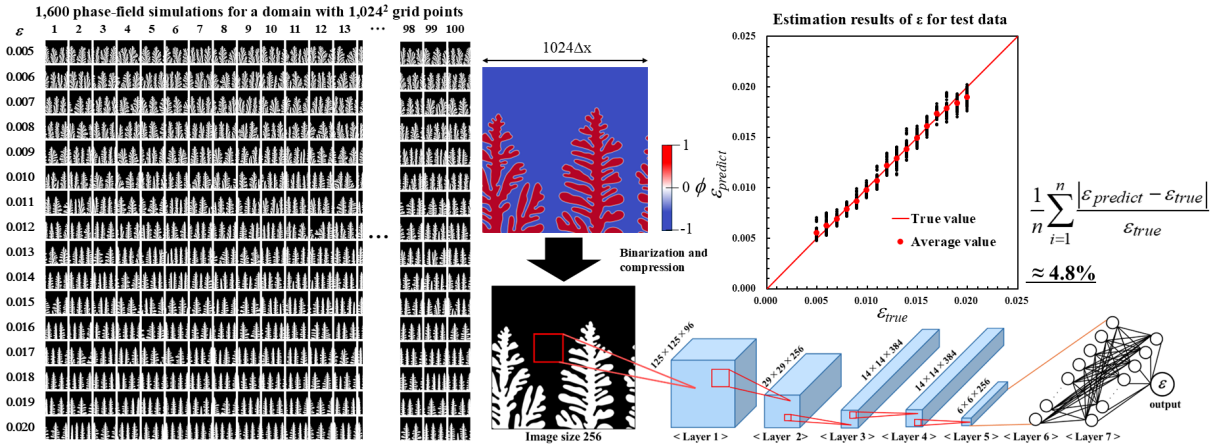
The interfacial physical properties are important for the microstructure control during the solidification of metals. However, it is challenging to directly determine these interfacial properties from experiments. In this study, we introduce the data-assimilation method, integrating both theoretical simulations and experimental data, to quantitatively evaluate such interfacial properties. The capillary anisotropy ε_c and kinetic anisotropy ε_k were determined through the quantitative phase-field simulation of Ni solidification with the data-assimilation technique. This phase field model is a time-nonlinear simulation model, requiring the ensemble approximation for data assimilation. Thus, the accuracy of the estimated physical properties depends on the number of ensembles. So, we conducted the large-scale data assimilation simulation with ensemble numbers, N=1024. We employed a phase-field simulation with known interfacial properties (ε_c=0.018, ε_k=0.130) as a reference instead of experimental one. This technique is referred to as twin experiments. Specifically, the field variable representing the solid-liquid phase state were taken every 1.85 ns as the observational data set. These observational data were incorporated into the simulation model using the Ensemble Kalman Filter method during the data assimilation. As a result, the parameters of the simulation model were improved to explain the observational data well. After the data assimilation with 18.5 ns phase-field simulations, the capillary anisotropy and kinetic anisotropy converge to 0.018±2.36×10^3 and 0.013±5×10^4, respectively. This result demonstrates that the data assimilation can estimate physical properties, that are difficult to directly determine from experiments.

Material property prediction from dendrite images using systematic phase-field simulations and convolutional neural network

Haruki Yano, Ayano Yamamura, Shinji Sakane and Tomohiro Takaki

Kyoto Institute of Technology (Japan)

The morphology of dendrite structures observed in general casting and solidification processes is determined by material properties and solidification conditions. This morphology has a significant impact on the properties and defect formation of solidified products. Therefore, numerical simulation studies have been actively conducted to predict dendrite structures. Although, for highly accurate solidification simulation, correct material properties are required, the number of materials for which the material properties are clear is limited, and the lack of material properties is a major problem. In this study, we aimed to build a machine-learning model using dendrite images as training data, which can infer material properties from experimentally obtained 2D cross-sectional dendrite images. Machine learning requires a large amount of training data, which is difficult to obtain experimentally. Therefore, we obtained training data from 2D phase-field simulations by systematically changing material properties. A convolutional neural network specialized for image recognition was used as the machine-learning model. We estimated the solidliquid interface energy and its anisotropic strength, which significantly affect dendrite morphology and are difficult to obtain experimentally. We employed a quantitative phase-field model and simulated the dendrite structures in the directional solidification of an Al-3wt% Cu alloy by systematically changing the solidliquid interface energy and its anisotropic strength. For the simulation results, we collected dendrite images as a training dataset. The training dataset was divided into training and validation data. After training with the training data, the material properties of the unlearned validation data were estimated. The average absolute error rate was approximately 5.5%, which is close to the true value, confirming the effectiveness of the model.

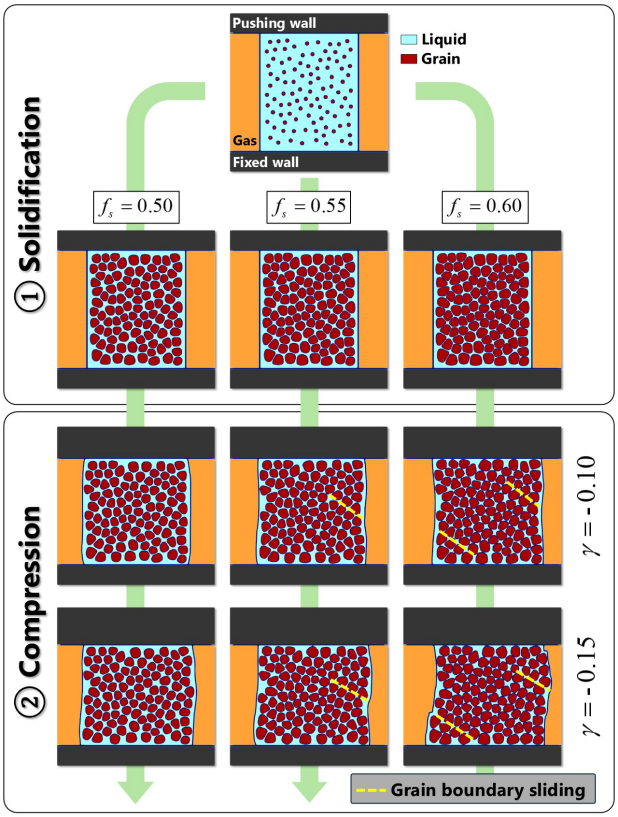


Multi-phase-field lattice Boltzmann simulations for semi-solid compressive deformation

Tomoki Uchiyama, Namito Yamanaka, Konosuke Ikeda, Shinji Sakane and Tomohiro Takaki

Kyoto Institute of Technology (Japan)

Semi-solid deformation during casting has a strong influence on the formation of various solidification defects such as pores, cracks, and macrosegregation. Therefore, a detailed understanding of the deformation behavior and highly accurate prediction of defect formation during semi-solid deformation are extremely important. Previously, void formation has been examined by in situ observation of the uniaxial compression deformation of semi-solid bodies. Regarding the mechanism of void formation, it is thought that the re-arrangement of crystal grains caused by compression generates a pressure difference between the liquid and gas phases, and the gas phase then intrudes into the semi-solid body. However, the details of void formation remain unclear. In our previous study, a multi-phase-field lattice Boltzmann model has been developed that can reproduce polycrystalline solidification by considering the motion of the solid phase and the flow of the liquid phase [Comp. Mater. Sci., 197 (2021) 110658], thereby helping to evaluate the deformation of semi-solid bodies [Materialia, 38 (2024) 102295]. In this study, we introduced a gas-liquid interface in the model and simulated the uniaxial compressive deformation of a semi-solid body. The macroscopic deformation of the body and the microscopic particle re-arrangement behavior depending on the solid fraction and deformation rate were demonstrated. In addition, the occurrence of shear bands at high solid fractions was confirmed, where slippage occurred across multiple particles.

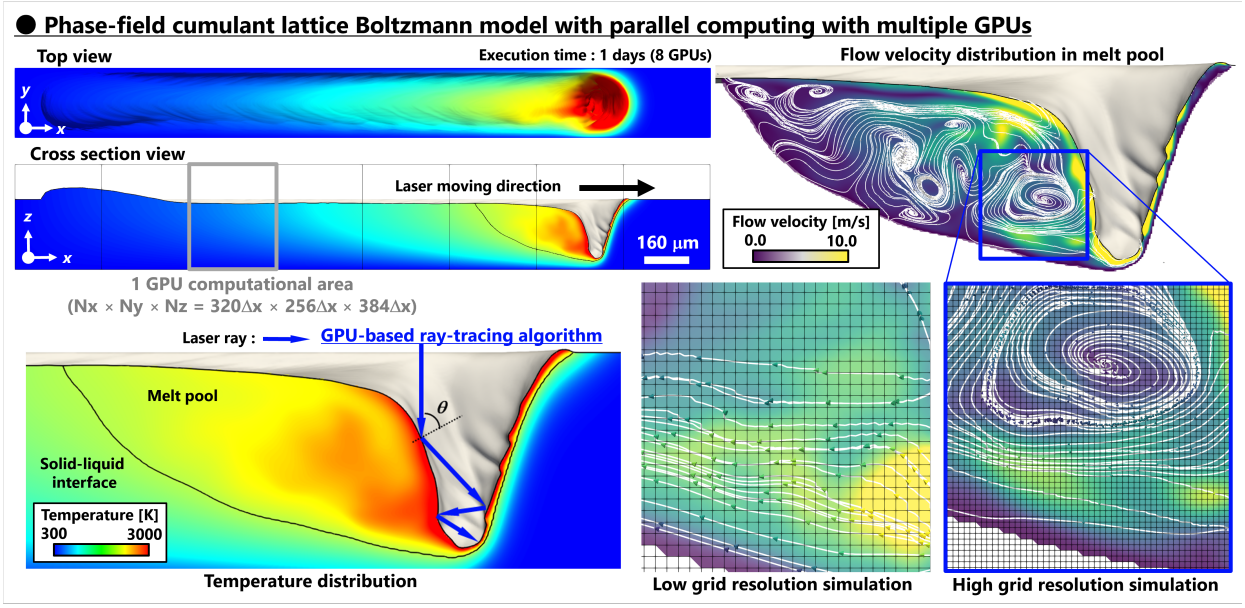


High-performance phase-field lattice Boltzmann simulations for accurate thermal fluid flow in metal additive manufacturing

Konosuke Ikeda, Shinji Sakane, Takayuki Aoki and Tomohiro Takaki

Kyoto Institute of Technology (Japan); Institute of Science Tokyo (Japan)

Metal additive manufacturing (AM) has attracted significant attention for its ability to create complex three-dimensional products of arbitrary shape through repeated melting and solidification using selective laser scanning. Enhancing the performance of AM products requires scanning parameter optimization to achieve precise control over solidification structures. To achieve this, numerical simulation is essential. Here, thermal fluid flow in a melt pool significantly influences material microstructure formation. However, conventional thermal fluid flow simulations have some problems such as lack of computation accuracy and space-time resolution. In this study, we developed a computational method for accurately predicting thermal fluid flow in the melt pool. The cumulant lattice Boltzmann method was employed for efficient and stable flow computation, while a phase-field (PF) method was utilized for precise representation of solid-gas-liquid interface migration. The PF method for interface modeling enabled accurate laser ray reflection on metal surfaces. In addition, the GPU-based ray-tracing algorithm achieved high-speed computation. Furthermore, parallel computing with multiple GPUs was implemented and three-dimensional large-scale simulations were successfully conducted on a GPU supercomputer. These simulations provided detailed insights into flow patterns within the melt pool and accurately reproduced the keyhole formation process.



Complex characterising of primer Si and eutectic in Al-Si alloys

Éva Kócsák, Dimah Zakaraia, András Roósz, Arnold Rónaföldi and Zsolt Veres

University of Miskolc (Hungary); HUN-REN-TKI Materials Science Research Group (Hungary)

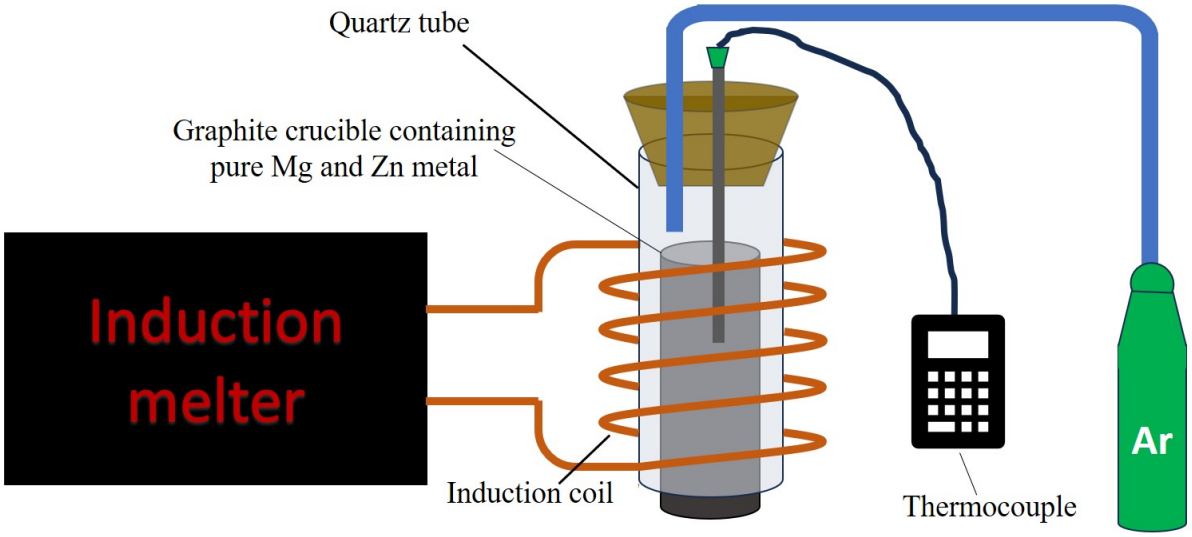
The microstructure of the primary and eutectic phases significantly affects the mechanical and physical properties of metallic alloys. Understanding the effects of solidification parameters is essential to characterise the microstructure of the samples. Investigation of the regular eutectics and the dendritic primary phases are considered ordinary. However, describing the irregular eutectics, like the Al-Si eutectic, and classifying primary silicon is not entirely solved. We developed a complex method that helps qualify the Al-Si alloys' microstructure. Our process involves measuring the average eutectic lamellae distance, the apparent length of lamellae and, the angle between the lamellas and the solidification direction. The shape and the size of the primary silicon are investigated. All our manner steps can be performed using ImageJ or a similar image analysis software. The angle of the lamellas and the size of the eutectic lamellas and primary Si can be measured easily in some steps by the software. To measure the average lamellae distance, an equation was created, which calculates what the average distance between lamellae would be if the structure were regular with the same number and length of lamellae. The shape of the primary silicon phases can be described by their circularity and roundness. We determined the critical value of these shape factors with which we can separate the polyhedral, dendritic and star-like shapes. Our method makes characterising the primer Si and the irregular eutectic in Al-Si alloys easy.

Casting of magnesium alloys for microgravity space experiments

Geetanjali Srivastava, Yanuar Rohmat Aji Pradana, Fan Wu, Wajira Mirihanage, Mert Celikin, Wim Sillekens and David J. Browne

University College Dublin (Ireland); University of Manchester (UK); ESA-ESTEC (Netherlands)

Magnesium alloys are lightweight materials with very high specific strength and good electromagnetic shielding properties, making them increasingly important. The low density of magnesium alloys renders them useful in various aerospace and automotive applications, facilitating the development of lightweight vehicles, and their biocompatibility is attracting new interest for use in temporary medical devices. However, casting magnesium alloys presents significant challenges due to their high reactivity and propensity for oxidation in molten form, necessitating an inert atmosphere during processing. This research is focused on casting of magnesium-zinc alloys for use as sample materials for future in-situ studies of their solidification. The binary alloy was prepared using induction melting of the two components in an inert atmosphere, ensuring chemical uniformity prior to casting into steel moulds. The microstructures of the magnesium alloys were observed using metallography. This research aims to synthesise and test Mg-Zn alloy samples in a controlled manner; these will be used in a future microgravity experiment to be conducted on ESA's MASER 17 sounding rocket to develop knowledge of the effects of gravity on alloy solidification. Equiaxed solidification will be monitored using in situ X-ray imaging of the alloy solidifying in the specially designed XRMON-SOL furnace. This research will contribute to the broader understanding of the alloy solidification process.



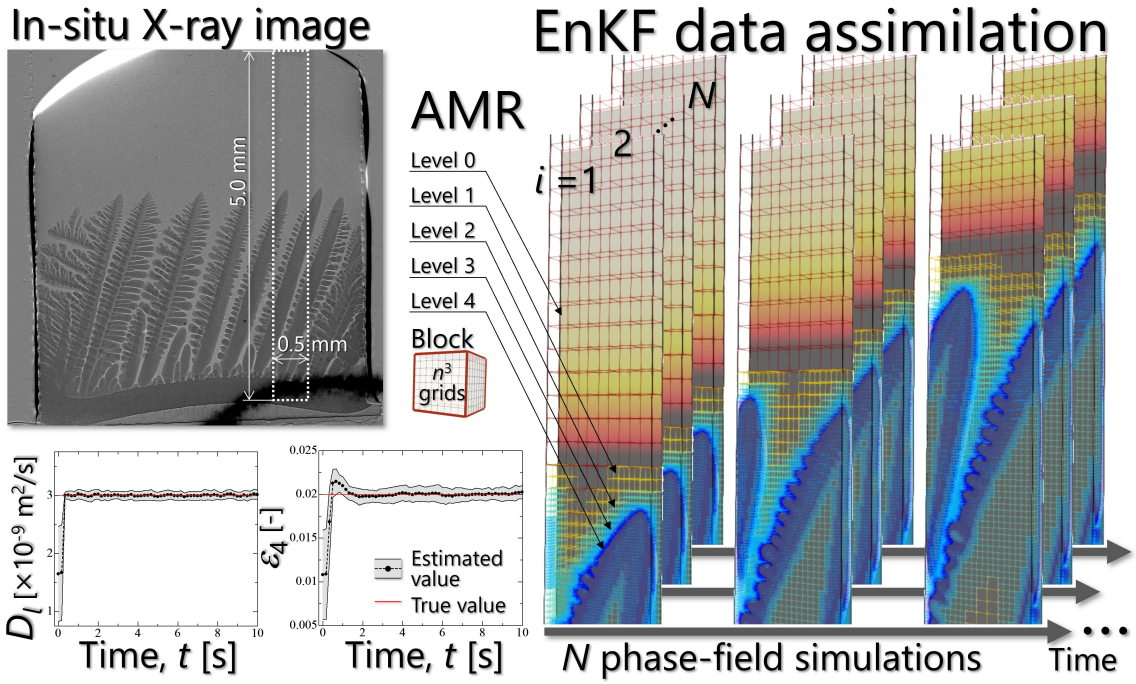
Experimental setup for the casting of Magnesium alloy

AMR-accelerated phase-field data assimilation for dendrite solidification

Ayano Yamamura, Shinji Sakane, Hideyuki Yasuda and Tomohiro Takaki

Kyoto Institute of Technology (Japan); Kyoto University (Japan)

Data assimilation holds significant potential for integrating experiments and simulations. In our previous study, we developed a sequential data assimilation system to estimate material properties and crystal orientations during dendritic growth under alloy solidification, validated through twin experiments. However, sequential data assimilation requires tens to hundreds of simultaneous simulations be performed, which restricted our twin experiments to solidification conditions in which data assimilation was manageable. To enable more computationally intensive data assimilation with actual in-situ X-ray observation data, additional efforts to reduce computational costs are essential. In this study, we address this challenge by introducing an adaptive mesh refinement (AMR) method. The AMR technique assigns finer computational grids to solid-liquid interface domains. Consequently, in data assimilation utilizing the AMR method, each ensemble features varying mesh divisions based on its dendrite morphology. To facilitate data assimilation with AMR, we performed mesh refinement and coarsening operations tailored to the different dendrite morphologies of all ensembles. This approach results in a changing number of components in the state vectors at each filtering step, depending on the changes of the number of grid points. We conducted twin experiments for directional solidification in both a thin film and cylinder using AMR and validated the effectiveness of the method. The results demonstrated that the AMR method can significantly reduce computational memory usage and costs, particularly during the initial stages of dendritic growth. Thus, this method serves as an effective tool for data assimilation with in-situ X-ray observation data.

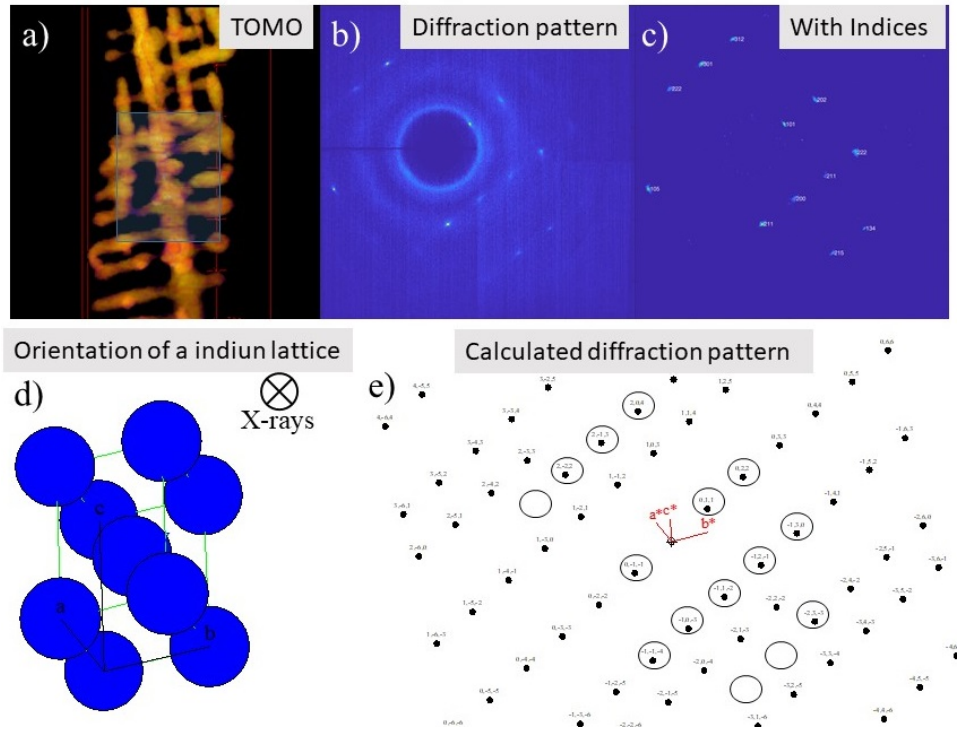


Combining in-situ synchrotron X-ray techniques to study the dendritic growth in GaIn alloys

Natalia Shevchenko, Joerg Grenzer and Sven Eckert

Helmholtz-Zentrum Dresden-Rossendorf (Germany)

The direct investigation of specific solidification phenomena (morphological transitions, local branch evolution, defect accumulation, etc.) is a complex process requiring high spatial and temporal resolution, as well as a high sensitivity of the detector. In this work, in-situ X-ray synchrotron imaging (e.g. radiography or tomography) and (local) diffraction methods are combined to study dendritic microstructures of solidifying Ga-In alloys. X-ray diffraction techniques are well suited to the analysis of lattice constant variations, lattice orientations and misorientation defects. However, to combine these techniques, precise control of the position of the X-ray beam on a selected dendrite or microstructure feature needs to be maintained. The tomography/diffraction experiments are performed at the ID19 beamline (ESRF, France) with a spatial resolution of ~1 µm and a diffraction spot size of 250 µm. A capillary cell with an inner diameter of 400 µm was used. Our measurements show that the diffractograms obtained from a single indium dendrite are equivalent to TEM (Transmission Electron Microscopy) pattern, but at a different size scale. It is notable that not all groups of diffraction reflections appear on the indium diffractogram, a phenomenon that may be attributed to the fact that a single dendrite represents a single crystal with a certain mosaicity. The majority of the indium dendrites grow along the <110> orientation typically observed in body-centered metals. Alternatively, the indium crystal lattice could be considered close to a slightly distorted FCC structure, with the major growth direction being the <100> orientation. These results demonstrate that the combination of these X-ray techniques can provide additional data, spatially resolved, especially on the orientation distribution, lattice spacing and mosaicity of a dendrite single crystal and could help to validate microstructural solidification models.

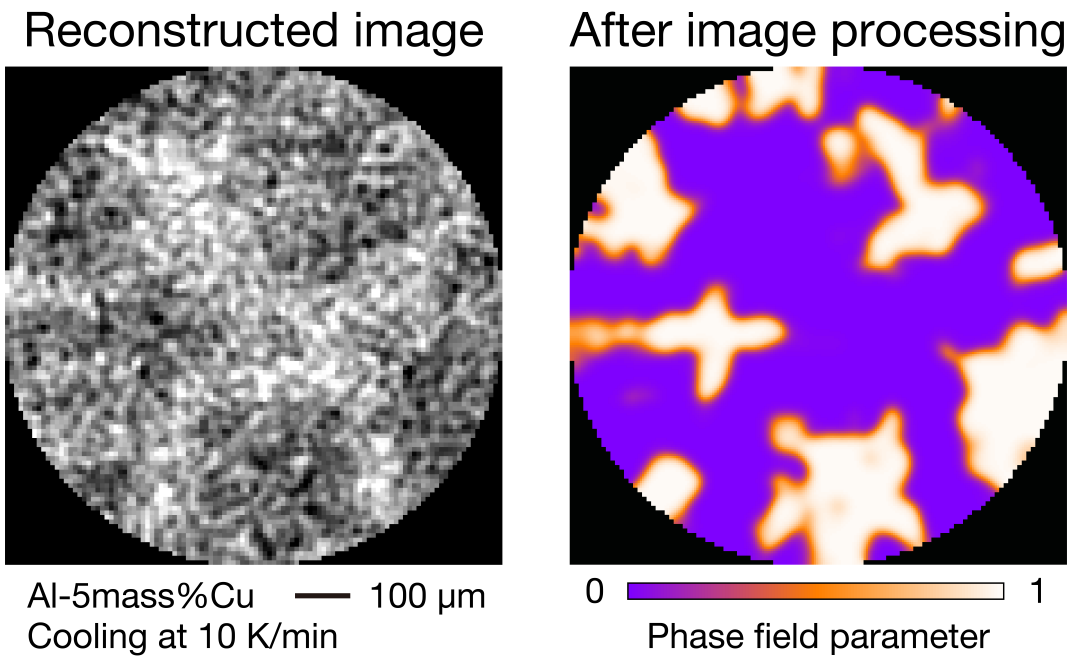


Observation of equiaxed dendrite growth and motion in Al-Cu alloy using 4D-CT

Taka Narumi, Takahiro Shimokawa, Sota Nakano, Ryoji Katsube and Hideyuki Yasuda

Kyoto University (Japan); Nagoya University (Japan)

During casting process, motion (i.e., floating and settling) of equiaxed grains due to melt flow and buoyancy force is associated with latent heat release and solute transport, affecting the thermal and concentration fields surrounding equiaxed grains. Furthermore, their sedimentation gives rise to mechanical interaction between them. In such a semisolid region, shear deformation can be localized, forming segregation bands and porosity. Thus, understanding grain structure evolution and defect formation requires elucidating the equiaxed grain motion in conjunction with their dendritic growth. Time-resolved tomography using synchrotron radiation X-rays (4D-CT) is an indispensable tool for directly understanding microstructure evolution in metallic materials during solidification. However, 4D-CT is subject to a fundamental compromise between spatial and temporal resolution; while temporal resolution as short as a few seconds is necessary to track the equiaxed grain motion, a degradation in image quality is inevitable, raising challenges in evaluating dendritic shape evolution. Here we report an application of image processing technique based on a phase field model that addresses these challenges. An equiaxed solidification process in Al-Cu alloy (5-15 mass%Cu) was observed in-situ using 4D-CT at BL20B2 in SPring-8. The voxel size of the 4D-CT data was 5.5 μm x 5.5 μm x 5.5 μm, and the temporal resolution ranged from 0.5-2 s. The phase field parameter was calculated under specified conditions using the brightness distribution of the CT image as the initial condition. The calculation was iterated until the solid fraction converged to that evaluated from the brightness distribution of the CT image. Consequently, the dendritic morphology of equiaxed grains was successfully restored, enabling quantifying their motion. Their velocity in the vertical direction ranged 100-200 μm/s. The onset of the sedimentation was detected as the solid fraction reached 0.1-0.2, which is smaller than the typical coherency point.



Phase-field modelling of dendrite growth in undercooled Ti-6Al-4V

Victoria Kaban, Mingming Tong and David Browne

University College Dublin (Ireland); University of Galway (Ireland)

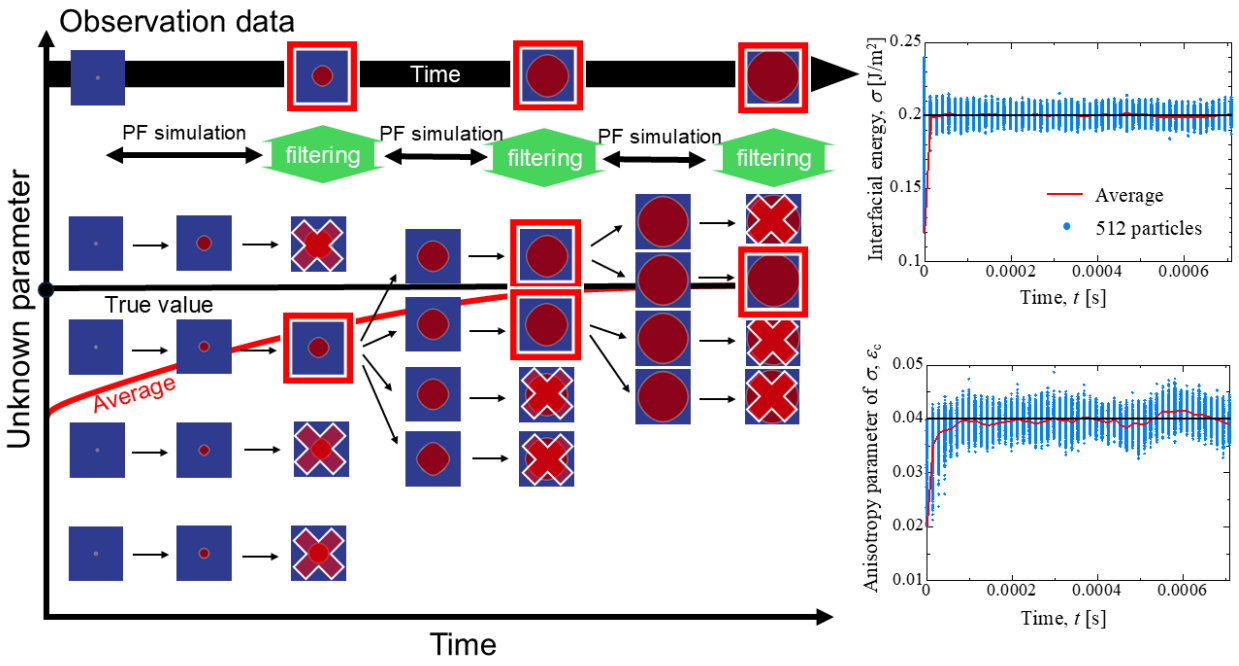
Ti-6Al-4V is the most popular Ti alloy widely used in various applications ranging from medicine to aerospace industry. It is also one of the most interesting alloys for additive manufacturing (AM) which provides sustainable fabrication of three-dimensional parts of almost any shape. Investigations of crystal growth under non-equilibrium conditions are required in order to understand microstructure evolution in AM. In this work the dendrite growth of the beta-phase in Ti-6Al-4V is modelled for different degrees of melt undercooling with the phase-field method. Model predictions are analysed with respect to experimental data on growth velocity values obtained in electromagnetic levitation experiments.

Particle filter-based phase-field data assimilation for estimating material parameters in solidification

Aya Maruhashi, Ayano Yamamura, Shinji Sakane and Tomohiro Takaki

Kyoto Institute of Technology (Japan)

In the phase-field simulation of dendritic growth, the absence of material properties is a significant issue. Data assimilation is a promising approach for obtaining unknown properties, and it incorporates experimental data into simulations. Previously, we used data assimilation using an ensemble Kalman filter (EnKF); however, when modifying the estimated values during filtering, the phase-field variables change, leading to disturbances in the interface morphologies and making data assimilation difficult. To address this issue, we introduce particle filter (PF)-based data assimilation. This method does not alter the phase-field variables during filtering; therefore, it is expected to suppress disturbances in interface morphologies. To investigate the PF-based data assimilation, we conducted twin experiments using time series data of a solid-liquid interface morphology obtained from isothermal solidification simulations of pure aluminum as the observation data. Here, we compared PF and EnKF by varying the number of particles and the filtering interval in the estimation of the interface energy and its anisotropy strength. EnKF achieved high-accuracy estimation even with a few particles, whereas increasing the filtering interval caused disturbances in the interface morphologies. With PF, the estimation accuracy decreased slightly with fewer particles, whereas increasing the number of particles allowed it to achieve a same accuracy as that of EnKF. Moreover, increasing the filtering interval did not disturb the interface morphologies. These results confirm that PF can achieve highly accurate material property estimation without disturbing the interface morphologies, provided that sufficient particles are used. In the future, we intend to develop data assimilation methods by leveraging the advantages of PF and EnKF.



Characterization of Additively Manufactured Stainless Steel with In-Situ Heat Treatment

Amber Schneeweis and Md. Thariqul Islam

Technische Hochschule Rosenheim (Germany)

As additive manufacturing (AM) continues to grow in commercial importance, the necessity of optimizing mechanical properties with minimal cost and time increases as well. Because of the thermal conditions experienced during AM, subsequent heat treatment is often necessary to achieve the desired properties. In hopes of bypassing the additional step of subsequent heat treating in a separate chamber, recent efforts have been made to incorporate various forms of heat treating directly into the printing process. This study makes use of the two lasers in a dual laser, powder bed fusion system, with one laser being used to print as usual and the second laser programmed to follow the same path with a time delay and lower power. This decreases the cooling rate and thermal gradient experienced by the part with the goal of reducing residual stress, one of the primary reasons for heat treating AM parts. Samples of a common stainless steel (316L) were printed with a Trumpf TruPrint 1000, some using the standard optimized parameters for this material and other with the addition of the second laser to perform the in-situ heat treatment. Samples were compared in terms of porosity, microstructure, melt pool size and shape, hardness, and tensile parameters. Tensile parameters obtained by standard tensile testing were compared with a promising new technique capable of obtaining accurate values for yield strength, ultimate tensile strength, and elongation via indentation. Initial results show that in-situ heat treatment produces a measurable improvement in mechanical properties. The effect of laser power and offset time between lasers on microstructure and properties was also investigated.

Icosahedral order in an AlZr alloy: insights from first principle calculations

Jonathan Chapignac, Elise Garel, Philippe Jarry and Noel Jakse

University Grenoble Alpes & CNRS, SIMaP (France); Constellium C-TEC (France)

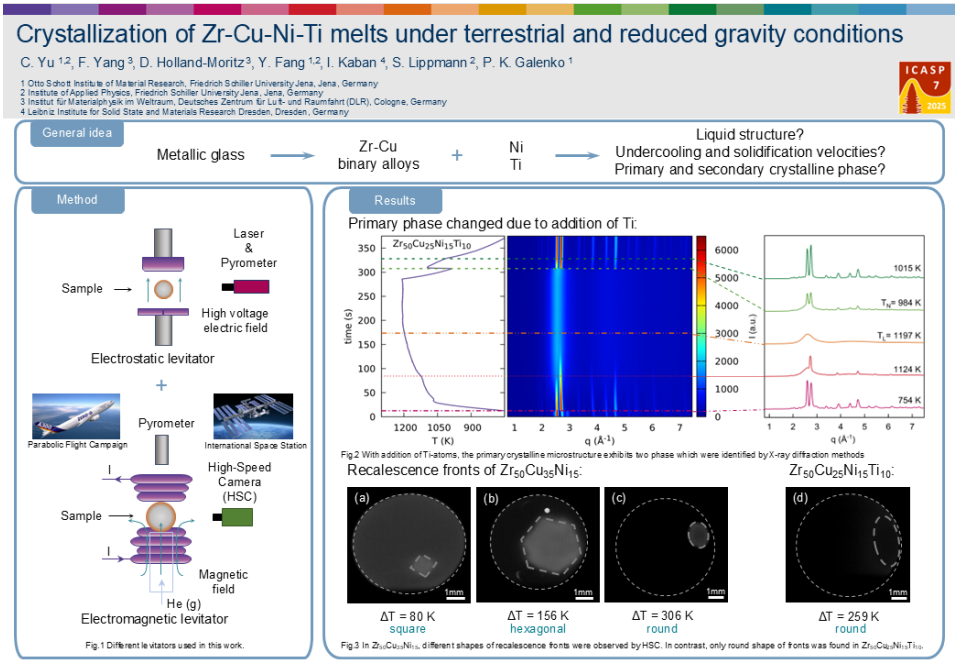
Icosahedral ordering is known to play a pivotal role in the alloy's solidification dynamics, as was shown experimentally by Rappaz et al.[1] that trace elements in metallic alloys have a dramatic effect on their solidification behavior, particularly when they induce icosahedral short-range ordering (ISRO) of atoms in the liquid. Furthermore, this ordering develops into an icosahedral medium-range order (IMRO) as the undercooling increases, thereby possibly affecting both nucleation and growth mechanisms, as its presence was found to act as a diffusion barrier, effectively reducing atomic mobility during the solidification process. Atomistic simulations have been used by Pasurel et al.[2] to help study the role of icosahedral order on experimentally challenging properties like diffusion and enable detailed analysis of atomic-scale structures such as short and medium range order. In this study, we investigate the structural and dynamic behavior of an Al-Zr binary alloy in the liquid and undercooled phases using first-principle simulations conducted via ab initio molecular dynamics simulations. Our results reveal that the addition of 3%at of zirconium in aluminum leads to the formation of Frank-Kasper icosahedral order in the melt phase, which reinforces upon undercooling and reduces the diffusion. As diffusion together with capillary governs the formation of solidification patterns, the parameters governing melt dynamics at the atom scale is further discussed.

Crystallization of Zr-Cu-Ni-Ti melts under terrestrial and reduced gravity conditions

Chu Yu, Fan Yang, Dirk Holland-Moritz, Yindong Fang, Ivan Kaban, Stephanie Lippmann and Peter Galenko

Friedrich Schiller University Jena (Germany); Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt, DLR (Germany); Leibniz Institute for Solid State and Materials Research Dresden(Germany)

Zr-Cu based alloys are well-known glass forming systems exhibiting a transition from heat-and-mass diffusion-limited solidification to kinetically-limited growth of crystals. The previous and latest results on theoretical modelling and experimental investigation of crystal growth kinetics are discussed for rapidly solidifying glass-forming Zr-Cu-Ni(-Ti) alloys: when 15 at% Ni replaces part of Cu in Zr50Cu50, crystal growth velocities of this Zr50Cu35Ni15 alloy first increase in dependence of undercooling, then keep at the plateau when the undercooling is between 260K-320K, while the primary phase (B2-CuZr) does not change. As a result of the addition of Ti-atoms, the primary solidifying phase is different from that in Zr-Cu-Ni alloys, which was proven using in-situ X-ray diffraction during solidification. The crystal growth velocity has been evaluated by the observation of the propagating growth front with a high-speed video camera in an electromagnetic or electrostatic levitation (EML / ESL) facility with recording of temperature using fast pyrometry. We have compared the samples processed by EML facilities, which are installed under terrestrial conditions and during parabolic flight campaigns. We found that only the samples processed by EML on the ground had a spiral structure on the surface, which is caused by convective flow. With increasing undercooling of the melted samples below the equilibrium liquidus temperature, the crystal growth velocity first increases but then slows down due to the transition to the kinetically limited growth regime as a result of the strong decrease of the atomic mobility. We used X-ray diffraction to identify the selection of phases during crystallization of the samples. The obtained experimental data are planned to be used as an input for modelling of the solidification kinetics in glass-forming alloys.

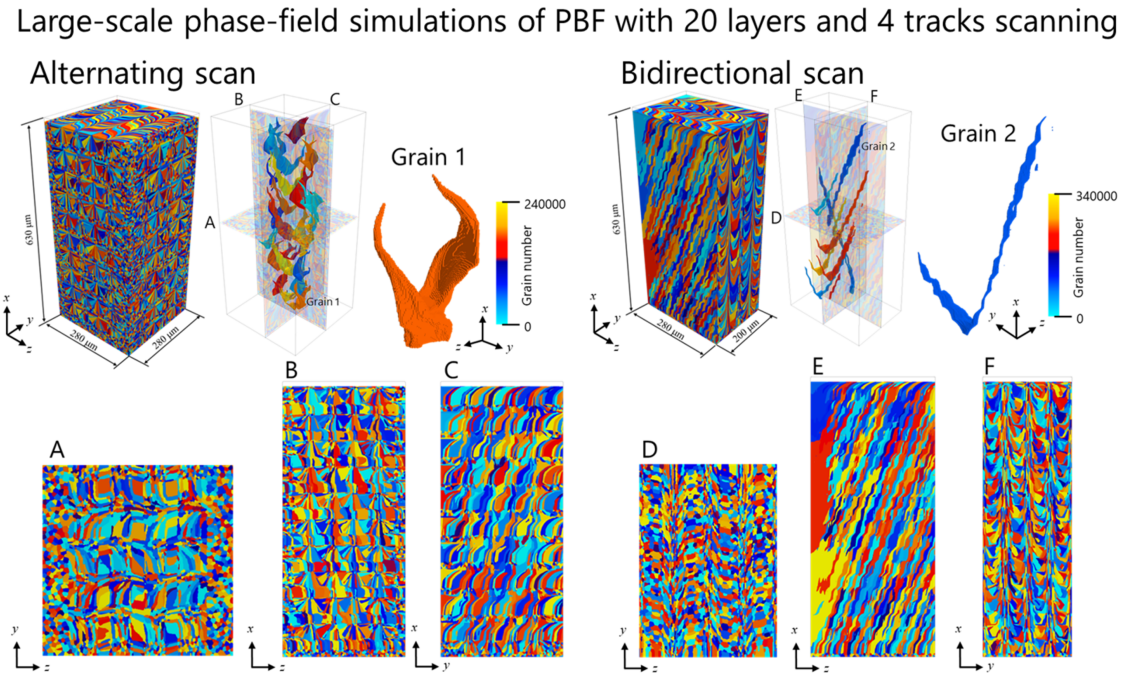


Multi-phase-field microstructure prediction for multiple layers and tracks in metal additive manufacturing

Yuki Takahashi, Shinji Sakane and Tomohiro Takaki

Kyoto Institute of Technolog

Metal additive manufacturing (AM) has garnered significant attention for its ability to create complex three-dimensional parts. In selective laser melting (SLM), a representative AM technology, product performance is largely influenced by the microstructures formed during processing. These microstructures can be controlled by altering the laser scanning pattern, known as the scanning strategy. Understanding the relationship between scanning strategies and the resulting microstructures is critical, yet the vast number of possible strategies makes numerical simulation indispensable. To predict microstructures resulting from various scanning strategies, we combined Rosenthal's equation, which describes the theoretical spatiotemporal temperature variation caused by a moving point heat source, with the multi-phase-field (MPF) method for accurately modeling microstructure evolution. This approach enabled microstructure predictions across multiple layers and tracks using parallel computations on multiple GPUs [Mater. Trans., 64 (2023) 1150-1159]. However, the melt-pool shape in SLM often deviates from predictions made by Rosenthal's equation, particularly at high laser power. To address this limitation, we investigated the applicability range of Rosenthal's equation in SLM by comparing microstructures derived from this model with those obtained from thermal fluid simulations. Additionally, we extended microstructure predictions to many layers and tracks in SLM using the MPF method.



Nucleation in Al-Si: a molecular dynamics study with machine-learning interatomic potential

Quentin Bizot and Noel Jakse

University Grenoble Alpes & CNRS, SIMaP (France)

Aluminium alloyed with silicon is particularly interesting due to its properties, such as good corrosion resistance, excellent weldability, and low density. These advantages, combined with the abundance and low cost of silicon, make this alloy widely used in various applications. Furthermore, the Al-Si binary is characterized by a eutectic in the Al rich part, with no stable intermetallic compounds across the entire composition range. Solidification control is crucial in manufacturing technologies, as it determines the microstructure and, consequently, the performance of the final product. Al-Si alloys demonstrate phase separation between α-Al and Si during the solidification, which can take on globular or lamellar morphologies. Solidification starts with nucleation, where small solid regions form within the liquid. However, investigating the mechanisms occurring during the early stages of nucleation is experimentally challenging due to the short duration, the small size of the structures involved, and the stochastic nature of nucleation. One way to address these challenges is through molecular dynamics simulations. However, existing classical interatomic potentials for Al-Si often lack the accuracy needed to describe the material's properties effectively. To overcome this limitation, we developed a machine learning interatomic potential using a high-dimensional neural network trained on ab initio molecular dynamics (AIMD) calculations for liquid and supercooled liquid states. We focused on validating the dynamic, thermodynamic, and structural properties in the liquid phase, which represent significant experimental challenges for this binary system. Moreover, this potential enables us to study the nucleation mechanisms occurring at the early stages from the liquid phase near the eutectic composition.

On the effect of solidification induced segregation on austenite formation and grain growth during re-heating of a forged steel part

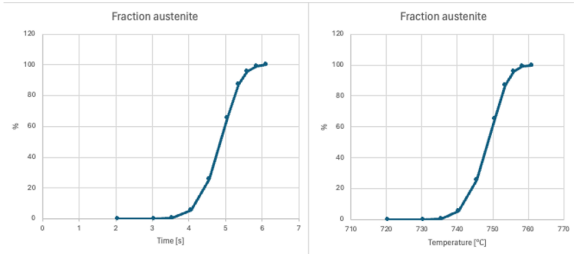
Aarne Pohjonen, Rishabh Bharadwaj, Oskari Seppälä and Mahesh Somani

University of Oulu (Finland)

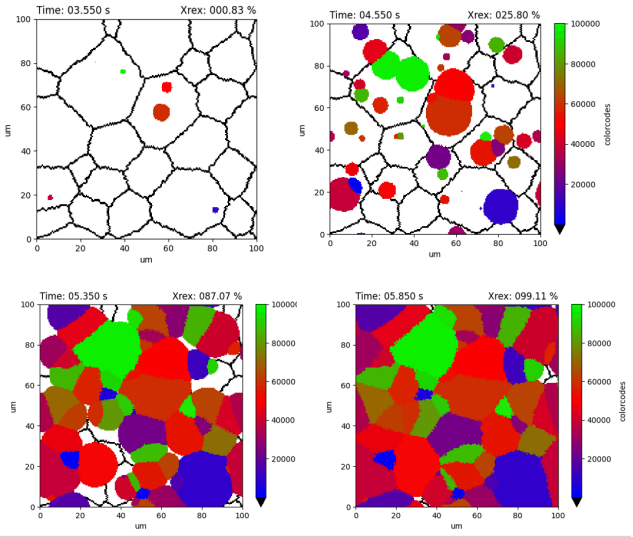
We present initial results from a cellular automata (CA) model, which has been constructed to incorporate effect of elemental segregation to the austenite nucleation and growth as well as grain growth during re-heating of a forged large scale steel object. The model has been constructed on the notion that there is position dependent variation in austenite grain structure of a quenched sample, which was obtained from re-heated forged object. The variation is thought to be a result of elemental segregation that has occurred during casting. The parameters of the previously developed CA model are adjusted for both alloy rich and alloy poor regions to mimic the experimentally observed grain structure.

Cellular Automata (CA)

Nucleation, growth, impingement, grain growth



Austenization during heating



Nucleation $N = \omega C \exp\left(\frac{\Delta G^*(T)}{RT}\right) \exp\left(-\frac{Q_N}{RT}\right)$

Growth $G = A\exp\left(-\frac{Q_G}{RT}\right)$

Insights into melting dynamics and microstructural evolution in multiphase peritectic alloys

Mehdi Medjkoune, Thomas Schenk, Guillaume Boussinot and Julien Zollinger

Université de Lorraine, Institut Jean Lamour (France); Access e.V. (Germany)

Melting exhibits unique and complex behaviors, far from being a simple reverse process of solidification. Recent phase-field simulations have highlighted key phenomena such as Temperature Gradient Zone Melting (TGZM) and Liquid Film Migration (LFM), which provide insights into steady-state configurations and solute dynamics at trijunctions. To experimentally validate these findings, we focus on melting dynamics and microstructural evolution in multiphase peritectic alloys, aiming to understand pattern formation and microstructure selection during melting and melting/solidification processes. Experiments are conducted on Cu-Sn and Al-Ni alloys. Cylindrical samples (~5 mm in diameter, ~10 cm in length) are directionally melted in a Bridgman furnace at controlled velocities or subjected to isothermal heating, followed by quenching to preserve mushy zone microstructures. SEM-EDS characterizations and EBSD analyses are employed to study the influence of pre-existing microstructures on phase interactions, anisotropic growth, and solute redistribution. Both directional melting without prior solidification and melting of pre-patterned samples are investigated to assess memory effects and the role of initial microstructures on melting dynamics. Key results highlight the role of faceted and non-faceted phases, anisotropy, and solute concentration on microstructure evolution. Observations confirm the importance of TGZM and LFM in peritectic systems, where melting initiates at interphase boundaries and is driven by solute diffusion in the liquid. Preliminary evidence also suggests a new mechanism for fragmentation induced by the reverse peritectic reaction during remelting. This work offers novel insights into melting processes in multiphase alloys, emphasizing the dynamic coupling between phase transformations and solute redistribution, with implications for casting and metallurgical applications.

Computational Modelling of Initial Temperatures within a Vacuum Induction Melting (VIM) Furnace

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Computational modelling is an important tool for the continued development of a modern foundry and offers a method for investigating furnace design changes at an accelerated pace, allowing options to be explored before committing to costly and time-consuming experimental trials. In addition, modelling the flow, heat transfer and microstructural evolution allows for assessing the design change on the as-cast product. Without modelling many more experiments would be required resulting in increased waste, cost and material losses. Modelling of a casting process requires accurate boundary conditions without which the model cannot provide an adequate reflection of the process. Some input parameters required are more readily available than others i.e., materials data. Others, such as initial temperatures can be more difficult to accurately specify due to temperature gradients within the casting furnace and would require many thermocouples to measure experimentally. This limits the usefulness of the model unless the heating cycle can be accurately modelled. In this work, ProCAST's was used to model a Vacuum Induction Melting (VIM) furnace, containing an upper and lower heating coil running at 22 and 19 kHz respectively. These results were subsequently compared to experimental data obtained running the heating coils at 25% and 100% of maximum input power. It was found that the crucible assembly exhibited temperatures close to the experimental data. However, for the mould assembly, large temperature differences were shown. This preliminary work will be presented here. Future development work includes: -Further refinement of the electromagnetic properties, including the effects of temperature variation of properties. -The use of further EMAG calculations steps, and a variation in the voltage input. -The use of separate frequencies in the upper and lower heating regions. -The impact of using a heating model rather than single-volume temperatures on solidification behaviour.

Study of the mechanisms of the non-equilibrium solidification in the alumina-zirconia binary system

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Electro-fused alumina-zirconia-silica ceramics are attracting growing interest because of their outstanding thermal and corrosion-resistant properties. These properties result from the cooling and solidification process. In this work, aerodynamic levitation coupled with a CO2 laser heating was used to understand the microstructure formation. However, the complex microstructures obtained during their synthesis due to the high cooling rate make their study difficult. This study aims to perform a first simplified approach, focusing on the understanding of the out-of-equilibrium solidification mechanisms of the alumina-zirconia binary system, by focusing research on the microstructures and atomic environments correlated to synthesis conditions. Rapid cooling experiments were carried out using the aerodynamic levitation synthesis to reveal the out-of-equilibrium character of the different compositions of the binary system. The characterization of the different samples was performed by SEM, NMR and XRD. The ex-situ NMR analysis was first performed followed by in-situ NMR analyses coupled with an aerodynamic levitation synthesis. These methods were correlated with solidification videos and temperature measurements obtained during the syntheses. Due to the extreme conditions of syntheses, out-of-equilibrium phenomena appear involving the presence of atomic environments AlO4 and AlO6 while an AlO6 environment is expected and of eutectic morphologies and structures within microstructures. In-situ characterization clearly shows that the progression of the solid phase as well as thermal events during the change of state have an impact on the onset of these phenomena. In order to highlight these out-of-equilibrium phenomena, the different in situ and ex-situ characterization methods used will be coupled with machine learning models.

Non-equilibrium solidification of Al2O3 MgO ZrO2 system

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Electrofused oxides from the AlO-ZrO-MgO (AZM) system are expected to play a crucial role as refractory materials due to their excellent thermal, mechanical, and chemical stability in extreme conditions. The solidification of oxides leads to key processes such as the nucleation & crystal growth, which are critical in determining the final microstructure, & thus properties of the material. The formation of spinel MgAlO crystals is particularly interesting due to its contribution in the thermo-mechanical resistance. However, electrical melting of oxides is challenging because the technology must operate at temperatures above 1800°C. Additionally, the change in density from liquid to solid results in a volume contraction of approximately 15%, leading to voids and cracks in the fused cast blocks. The aim of the current project is to address these challenges by consolidating knowledge on the solidification mechanisms & developing innovative AZM-based refractory systems. The primary objectives of this research are to formulate & melt oxides using aerodynamic levitation combined with laser heating. This method reaches temperatures above 2000°C & enables rapid cooling (~300°C/s). Such cooling induces deviations from equilibrium states, leading to various solidification pathways. To elucidate the structural and microstructural changes during non-equilibrium solidification, various advanced characterization techniques are utilized, including scanning electron microscopy, X-ray diffraction, & 27Al solid-state nuclear magnetic resonance. By enabling the investigation of unexplored areas of knowledge, this project is expected to offer valuable insights for designing high-performance, sustainable refractories. Ultimately, these advancements support the broader objective of enhancing the durability & efficiency of refractory materials.

Modelling and Simulation of Atomic-Scale Solid/Liquid Interface under an External Magnetic Field Using Phase Field Crystal Method

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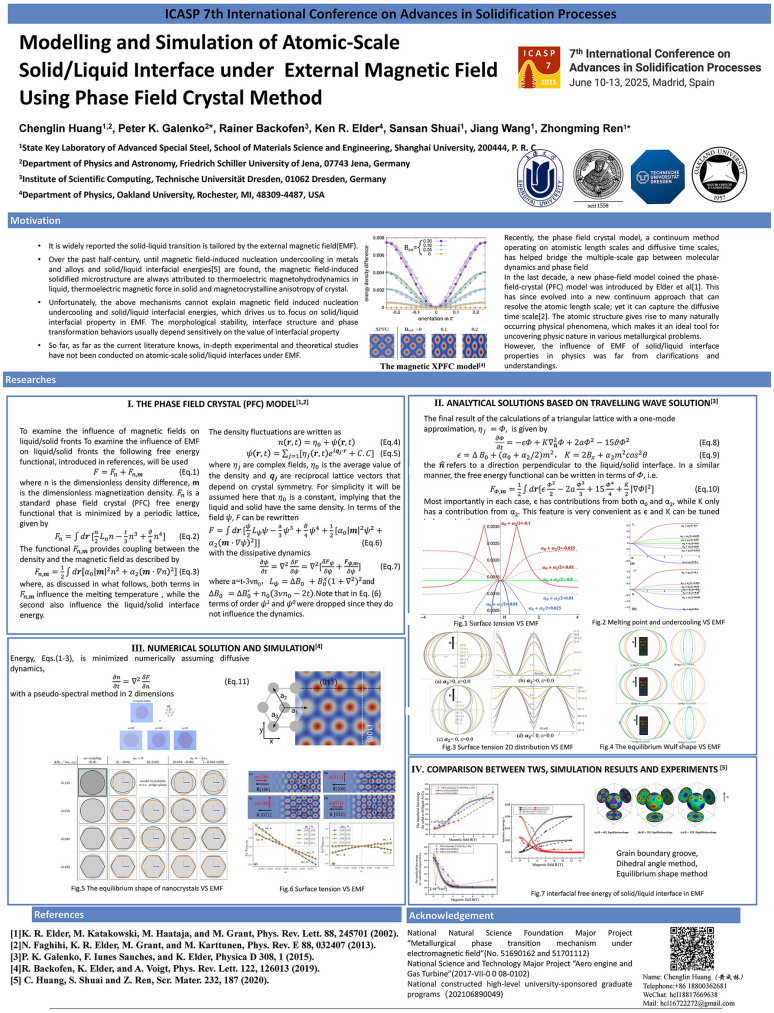
External magnetic field affects the polycrystalline microstructure of magnetic samples. Using the basic ideas developed by phase field crystal method [Phys. Rev. Lett., 122, 126103 (2019); Comput.Methods Appl. Mech. Eng., 371, 113310 (2020)], an influence of magnetic field on the morphology and energy of solid-liquid interface is studied analytically and numerically. The coupling of the magnetic field with the atomic density is analyzed for the equilibrium state of the interface and by the traveling waves for the interface dynamics given by the methodology described in the work. Attribution to previous experiments and comparison with the results of laboratory studies described in the literature are made in comparison with the theoretical advancements and numerical simulations of the present works are discussed in details.



Unraveling the Dynamics of Eutectic Melting: An In Situ Study of CBr-CCl Microstructures

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Multiphase melting/solidification processes are essential in novel material elaboration, yet eutectic melting dynamics remain poorly understood. We present an in situ experimental study of directional melting in the CBr-CCl eutectic, a transparent alloy that follows physical laws governing metallic eutectics while enabling direct visualization. Building upon previous work on this model system, we examine pre-solidified lamellar microstructures with controlled morphologies through real-time optical observation of the solid-liquid interface. Our research reveals complex melting behavior highly dependent on parameters including melting velocity, imposed lamellar spacing, and alloy concentration. We observe distinct asymmetries between solidification and melting kinetics that challenge current theoretical frameworks, with particular sensitivity noted in compositions away from the eutectic point. These findings address a significant knowledge gap in the materials elaboration literature and offer insights into processing techniques such as zone melting and additive manufacturing where controlled partial melting is essential for microstructural development.

Mechanisms of Defect Formation in High Pressure Die Casting

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High Pressure Die Casting (HPDC) is a manufacturing technique which involves injecting molten metal into a metal die cavity, where it solidifies within seconds under high pressures. Due to the rapid manufacturing rate and good surface finish, HPDC is widely employed in the production of automative components. However, HPDC products are prone to number of defects including shear bands and porosity, the origins of which can be traced to the complex semi-solid flow and solidification during HPDC. In this study we investigated the role of semi-solid flow on eutectic and porosity band formation using synchrotron imaging. By quantifying the gas porosity growth during the deformation of the semi-solid and cooling, we identified two sources of hydrogen flux, namely (a) dilatancy-driven advection of hydrogen and (b) rejection of hydrogen during solidification. We further estimated the strain fields using digital image correlation. Based on the local stress state, pore and liquid fraction, four defect zones were defined namely: plug flow zone, dead zone, shear zones and the bulk. The above-mentioned two mechanisms are being integrated into physics-informed machine learning porosity predictions.

A component-scale Machine Learning framework for prediction of porosity in High Pressure Die Casting

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High Pressure Die Casting (HPDC) is a rapid manufacturing process mainly used in mass production of intricate automotive components. Due to the high cooling rates and high pressures, coupled with thin wall sections, the metal solidifies rapidly, leading to the formation of unique features such as porosity and shear bands. Most prediction approaches either involve local pore-centric models with accurate predictions or component-scale simulations, which require significant computational time with lower accuracy. This work combines a local, micro-scale model with a macro-scale model using a Machine Learning (ML) framework based on a transfer learning approach. The ML model is trained using a deformable-grid one-dimensional finite volume model of combined gas and shrinkage pore growth as a function of pressure, temperature, and cooling rate; values which are predicted from a transient component level CFD simulation. The model is then further re-trained using a combination of macroscopic field variables and porosity measured from X-ray microtomography (XMT) scans of an industrial HPDC component. The model successfully predicts pore sizes and locations on a component level, spanning the entire range of measured pore radii, and highlighting a new predictive potential for a large class of problems in manufacturing.