# MM 42: Materials design II

Time: Friday 12:30–13:30 Location: H16

MM 42.1 Fri 12:30 H16

**A coupled meso-macro-scale simulation of solidification in Al-Cu alloys** — •Ivaldo Leao Ferreira[1], Britta Nestler[1], and Amauri Garcia[2] — [1]Institute for Computational Engineering, Karlsruhe University of Applied Sciences, Karlsruhe, Germany — [2]Fac. Engenharia Mecanica, UNICAMP, Brasil

The macroscopic heat transfer modelling associated to fluid flow is frequently used in prediction of ingots defects, while mesoscopic modelling is applied for the studies of alloy changes in relation to a typical microstructure. By combining a meso-scale model for the extraction of local alloy concentrations and a macro-scale model able to predict temperature, solute concentration, velocity fields and pressure profiles, it is possible to conduct cast process simulations for a large range of space and time scales. An extension of a 2D macro-scale model proposed for predicting inverse macrosegregation profiles during solidified alloy ingots is coupled with a meso-scale phase-field model for simulating microstructure formation processes. The phase-field model can provide parameters such as the phase fractions, primary/secondary arm spacings and microsegregation profiles. The approach will help to understand the effects exerted by the kinetics of solidification on the form of microstructure and consequently on microsegregation and macrosegregation profile in ingots or casting parts in commercially available alloys.

MM 42.2 Fri 12:45 H16

**Parallel algorithms for microstructure simulations with fluid flow** — •Michael Selzer and Britta Nestler — Institute for Computational Engineering, Karlsruhe University of Applied Sciences, Karlsruhe, Germany

Fluid flow has an important effect on the formation of microstructures and on the properties of materials. Our numerical method for solving the Navier-Stokes equations coupled with the microstructure model is based on a finite difference method on a staggered grid including a successive overrelaxation iteration for the pressure update. Simulations modelling the ripening process of a fine distribution of liquid droplets embedded in a fluid medium have demonstrated the necessity of developing parallel and optimized algorithms for solving the set of nonlinear partial differential equations in order to reduce computing times. The parallelization is realized by a domain decomposition using the message passing interface (MPI) library for data exchanging between computing nodes. To homogenize the load distribution, a dynamic redistribution of the domain decomposition is implemented. We apply the parallel simulator to microstructure formation processes with fluid flow and systematically analyze the computational performance depending on the configuration setup and on the optimization methods.

MM 42.3 Fri 13:00 H16

**Thermoelectric currents in weld pools** — •Adrian Lange and Eckhard Beyer — Fraunhofer Institut für Werkstoff- und Strahltechnologie, Winterbergstraße 28, D-01277 Dresden

In order to achieve higher welding speeds and a better quality of the weld seam, external static magnetic fields are tested for laser beam welding. Experiments with fine grained steels and aluminium alloys show a reduction of the so called humping effect, an improvement of the top seam quality, and an influence on the cross section of the seam [1,2]. These phenomena depend on the orientation of the magnetic field. To explain that dependence, the existence of thermoelectrical currents was proposed in [1,2]. The interaction of that proposed currents with the external field shall generate a Lorentz force distribution in the weld pool which may be the reason for the observed phenomena.

Based on the Onsager relation for the thermoelectrical current density and the appropriate boundary conditions for the laser beam welding, thermoelectrical currents can be determined analytically [3]. Results for iron and aluminium are presented in a approximative two-dimensional geometry. Since measurements for the values of the thermoelectrical (Seebeck) coefficient of both materials are spare, different hypothetical material sets are tested and discussed.

[1] M. Kern, P. Berger, and H. Hügel, Schweißen & Schneiden **52**, 140 (2000).
[2] M. Kern, P. Berger, and H. Hügel, Welding Journal **79**, 72s (2000).
[3] J. Paulini, G. Simon, and I. Decker, J. Phys. D **23**, 486 (1990).

MM 42.4 Fri 13:15 H16

**XANES-Messungen zur atomaren Umgebung von Mg in AlMgSiCu-Legierungen** — •Torsten Staab[1], Karl Maier[1], Hartwig Modrow[2] und Esther Dudzik[3] — [1]Universität Bonn, Helmholtz Institut für Strahlen- und Kernphysik, Nussallee 14-16, 53115 Bonn — [2]Universität Bonn, Physikalisches Institut, Nussallee 12, D-53115 Bonn — [3]Hahn-Meitner Institut Berlin/Bessy, Albert-Einstein-Str. 15, 12489 Berlin

Größe und Verteilung nanoskaliger Cluster — sogenannter Guinier-Preston-Zonen — bestimmen die Festigkeit von Aluminiumlegierungen. Diese Cluster behindern die Bewegung von Versetzungen. Schweißbare Al-Legierungen für den Flugzeugbau (Airbus A380) enthalten neben Mg und Si als Hauptlegierungsbestandteile auch Kupfer. Nachdem XANES-Messungen an der Cu k-Kante Hinweise auf die atomare Umgebung von Kupfer liefern konnten, zeigen neuere XANES/NEXAFS-Messungen an der Mg k-Kante auch die atomare Umgebung dieses Legierungselementes durch den Vergleich von ab-initio Rechnungen mit experimentellen Daten. Während des Alterungsprozesses der Legierung ändert sich die chemische Zusammensetzung der Ausscheidungen und damit die lokale atomare Umgebung der Legierungselemente Kupfer und Magnesium.