Einladung zum Seminarvortrag im Aachener Mechanik & Statik Kolloquium

01. März 2017 | 14:00 Uhr

Institut für Allgemeine Mechanik | Templergraben 64 | 1. OG | Raum 112

RWTH AACHEN UNIVERSITY

„Large-scale multiphase-field simulations of microstructures“

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Phase-feld modelling has become a fairly versatile technique for the treatment of microstructure formation and phase tran-sition problems. It usually operates on a mesoscopic length-scale exploring microstructural characteristics at a micrometer resolution. With this scope, the method serves as the bonding chain between atomistic and macroscopic simulation schemes. Herewith, the phase-feld method plays a centrol role in multi-scale materials modelling and naturally desires the exploitation of large representative volume elements. Furthermore, the com-bination of phase-feld modelling with multiphysics applications such as heat and mass transfer, continuum mechanics, fuid fow, micro-magnetism and electrochemistry has been achieved. In-corporating multiscale and multiphysics, phase-feld modelling is central for the future technology "Integrated Computational Materials Engineering (ICME)" as it allows for a medium of information transfer between both, experimen-talists and modellers as well as between diferent materials modelling methods. In the overview talk, we present a novel formulation of a general phase-feld model for multicom-ponent material systems based on a grand potential formalism and discuss techniques to efciently transfer thermodynamic databases to provide direct access to the Gibbs free energies of the diferent phases. Alloy systems with three or more chemical species can form a broad variety of diferent microstructures depending on physical parameters and processing conditions. To investigate the diversity of pattern formations, a full three di-mensional modelling is mandatory and requires intense computational power. We choose a ternary eutectic alloy to demonstrate the power of high performance computations for describing the physical mechanisms of experimentally observed phase ordering dur-ing solidifcation and to derive morphology transition diagrams. Using advanced data analysis tools and principal component algorithms, we illustrate the necessity of mas-sively parallel high performance computing techniques to resolve the microstructures in sufciently large representative volume elements. As another example of large-scale 3D computations, we apply the phase-feld method to study wetting phenomena of immis-ible and compound droplets on fat, porous and chemically structured substrates. By combining the phase-feld method with elasto-plastic models, we show a detailled view into the stress-strain evolution and crack propagation in polycrystalline grain structures.

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