MM 17: SYM Phase Transformations in Metallic Melts VI

Time: Tuesday 11:30–13:00 Location: H 1058

MM 17.1 Tue 11:30 H 1058

Modeling elasticity effects in pattern formation during alloy solidification — Bo Liu[1], •Klaus Kassner[2], Robert Spatschek[3,4], and Clemens Müller-Gugenberger[4] — [1]AG Mathematische Modellierung, MPI für Marine Mikrobiologie, Bremen — [2]Institut für Theoretische Physik, Otto-von-Guericke Universität, Magdeburg — [3]Center for Interdisciplinary Research on Complex Systems, Northeastern University, Boston, Massachusetts, USA — [4]Institut für Festkörperforschung, Forschungzentrum Jülich

We have developed a series of phase-field models allowing to simulate various aspects of strain-induced effects on alloy solidification. On the one hand, we include compositionally induced stresses in a phase-field model describing growth of dilute alloys. Special care is taken to obtain a viable thin-interface limit, i.e., we eliminate artificial effects of interface stretching, surface diffusion, and interface dissipation by an appropriate choice of phase-field functions and parameters. Simulations of directional solidification in a parameter range discussed by Spencer et al. [1] in terms of a linear stability analysis reveal oscillatory standing wave modes as the preferred dynamic state. On the other hand, after realizing that past models are flawed, we have created asymptotically correct phase-field models for the simulation of surface diffusion under stress, which may become important in solidification when micro-crack formation plays a role.

[1] B.J. Spencer, P.W. Voorhees, S.H. Davis, G.B. McFadden, *Acta metall. mater.* **40** 1599 (1992).

MM 17.2 Tue 11:45 H 1058

Elastic effects on phase transitions in multicomponent alloys — •Denis Pilipenko, Robert Spatschek, Efim Brener, Heiner Mueller-Krumbhaar, and Clemens Mueller-Gugenberger — Institut für Festkörperforschung, Forschungszentrum Jülich, 52425Jülich, Germany

We report on our activities concerning the influence of elastic effects on multicomponent alloys, which can lead to long-range interactions and the appearance of unexpected dynamical behaviors. We present a continuum theory to describe elastically induced phase transitions between solid and melt phases, which is simulated both by phase field and sharp interface methods. For the particular case of diffusionless phase transitions in solids, where structural and density differences provoke significant strain effects, we predict the macroscopic growth in a strip geometry, which can lead to the emergence of twin boundaries. In the limit that one phase is very soft, we obtain a self-consistent macroscopic model for fast fracture processes, which is based on the Asaro-Tiller-Grinfeld instability. Here we demonstrate that sharp-interface and phase field predictions are in very good agreement despite the large lengthscale gaps that are intrinsic to this problem. Finally, we briefly present recent results concerning the diffusion-limited propagation of a melt phase along an inter-phase boundary and melting in eutectic and peritectic systems.

MM 17.3 Tue 12:00 H 1058

Nonequilibrium crystal growth: a comparison of molecular dynamics and phase-field simulations — •Denis Danilov[1], Britta Nestler[1], Alexander Mirzoev[2], and Ilya Maltsev[2] — [1]Hochschule Karlsruhe, Karlsruhe, Germany — [2]South-Ural State University, Chelyabinsk, Russia

Melting and crystallization are of fundamental interest in condensed matter physics. We employed molecular dynamics (MD) simulations to investigate nonequilibrium behavior of crystallization with a simple system: the Lennard-Jones (LJ) 6-12 potential. Although quantitatively, LJ model at best applies to noble gases, it is used as a generic model for simple close-packed systems. Simulations of crystal growth from the melt were performed in the (100) direction, measuring the growth velocity as a function of the undercooling. Different definitions of the order parameter that discriminates between the solid like and liquid like particles in the simulation box have been considered. The influence of the termostat type on the growth kinetics has been tested, showing the crucial role that the approximation of the release of the latent heat plays in MD modeling of crystal growth. The MD results are compared with phase-field simulations where input model parameters were obtained from atomistic simulations.

MM 17.4 Tue 12:15 H 1058

Modelling of dendrite growth and fragmentation in multicomponent melts — Peter Galenko and •Dieter Herlach — Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt, 51170 Köln, Germany

A progress reached in direct experimental measurements of non-equilibrium solidification allows for developing and verifying theoretical models in a wide range of undercooling. Both sharp-interface model and diffuse interface model are applied to solidification of pure (one component) melts, binary alloys (both dilute and concentrated), and ternary diluted alloys. The current theories of dendritic growth based on these models correlate the undercooling to the dendrite growth velocity. It is shown that the sharp-interface model reasonably predicts kinetics of dendritic solidification in agreement with the experimental data obtained by the methods of in situ diagnostic (e.g., using high-speed camera). In addition to the predominant effect of diffusion transport of atoms and conductive transport of heat on growth kinetics, convection of the liquid may quantitatively influence on the growth and fragmentation of dendrites. Combined with in situ diagnostic of solidification, advanced computer modelling of microstructure formation on the basis of experimentally proven physical models allows for developing the perspective of virtual materials design of high functional materials. Financial support by DFG under SPP-1120 through the project DFG-HE1601/13 is acknowledged.

MM 17.5 Tue 12:30 H 1058

Dendritic solidification in the diffusive regime and under the influence of buoyancy driven melt convection — •Ingo Steinbach and Markus Apel — RWTH-Aachen, Access e.V.

Simulations of dendritic solidification in binary and ternary alloys in the diffusive regime and under the influence of buoyancy driven melt convection are performed using a quantitative phase-field model. At first, in the diffusive regime rapid solidification into a highly undercooled melt of ternary Ni-Al-Zr is investigated and compared to levitation experiments and sharp interface calculations. Secondly, the stability of dendritic arrays dependent on the primary spacing is investigated for a binary Al-Cu alloy under directional solidification conditions. Thirdly, melt convection driven by solutal buoyancy is introduced to the latter case and the influence of buoyancy on the spacing selection is discussed. A scaling relation for the dependence of primary spacing on the gravity level is derived and compared to experimental results from centrifugal casting under increased gravity.

MM 17.6 Tue 12:45 H 1058

Stationäre und instationäre Morphologieentwicklung bei gerichteter Erstarrung ternär-eutektischer Legierungen — •Bernd Böttger, Victor Witusiewicz, Markus Apel, Ulrike Hecht und Stephan Rex — access, Aachen, Germany

In diesem Beitrag werden Ergebnisse zu Erstarrungsexperimenten, zum thermodynamischen Assessment sowie zur Phasenfeld-Simulation in ternär-eutektischen Legierungssystemen vorgestellt. In einem ersten Schritt wurde die vollständige thermodynamische Beschreibung der Systeme Ag-Cu-Zn und Bi-In-Sn erarbeitet, für die nur bruchstückhafte Informationen vorlagen. Hierfür wurden Experimente durchgeführt. Diese Daten stehen somit als CalPhaD-Datenbanken zur direkten Ankopplung an die Simulation zur Verfügung.

Experimente zur gerichteten Erstarrung wurden sowohl in der klassischen Bridgman-Technik als auch als pseudo-2D-Experimente in dünnen Glaskapillaren durchgeführt. Für letztere Technik wurde eigens ein Mikro-Bridgman-Aufbau entwickelt, der eine in-situ-Beobachtung der Gefügebildung erlaubt. Dadurch wurden insbesondere die Durchführung transienter Experimente und die Beobachtung instationärer Mikrostukturen im Legierungssystem In-Bi-Sn möglich.

Die Anwendung der Phasenfeldmethode zur Gefügesimulation führte zu einem neuen Verständnis der stationären und instationären Erstarrungsprozesse in 2D und 3D. Für In-Bi-Sn konnte ein quantitativer Vergleich mit pseudo-2D-Experimenten durchgeführt werden, der auch die indirekte Bestimmung von Diffusionskoeffizienten und Grenzflächenenergien ermöglichte.