DY 16 Growth Processes and Surface Properties

Time: Monday 16:15–18:15 Room: HÜL 186

DY 16.1 Mon 16:15 HÜL 186

Crack Propagation as a Free Boundary Problem — •Denis Pilipenko, Robert Spatschek, Efim Brener, and Heiner Mueller-Krumbhaar — Institut fuer Festkoerperforschung, Forschungszentrum 52425 Juelich

We demonstrate a macroscopic theory of fracture in the spirit of nonequilibrium growth processes in pattern formation. The theory is based only on the dynamical theory of elasticity, surface energy and elastically induced phase transitions between a hard and a soft solid phase. Alternatively, crack growth can be described by surface diffusion along the crack. Although it is commonly believed that crack growth is dictated by the microscopic details in the vicinity of the tip, and despite the simplicity of our continuum theory, it predicts many important features of fracture. Among them is the limitation of the steady state growth velocity to values appreciably below the Rayleigh speed (the speed of sound) and tip blunting. We present a multipole expansion technique to solve numerically the problem of steady state growth in a very efficient way, using a sharp interface description of the propagating crack front. The results are discussed and compared to phase field simulations.

DY 16.2 Mon 16:30 HÜL 186

Phase Field Modeling of Crack Propagation — •Robert Spatschek, Clemens Mueller-Gugenberger, Efim Brener, and Heiner Mueller-Krumbhaar — Institut fuer Festkoerperforschung, Forschungszentrum 52425 Juelich

The phenomenon of fracture is of extraordinary relevance for our life. Cracks occur on all scales from nano- to kilometers, from tiny microcracks in material failure to the geological scales of earthquakes. Therefore, it is not surprising that a full modeling of rupture requires to separate a whole hierarchy of lengthscales, from the detailed structure of the tip region to the macroscopic scale of stress relaxation. Obviously, this leads to enormous numerical calculations. We present a simple theory that describes the entire fracture process in the framework of a macroscopic continuum theory of pattern formation, based only on the dynamical elasticity and phase transition dynamics. A phase field model is employed to solve the equations numerically on massively parallel computers with many hundreds of processors. We discuss predictions, limitations and possible extensions to the model.

DY 16.3 Mon 16:45 HÜL 186

Effect of a forced flow on dendritic solidification — •Thomas Fischaleck and Klaus Kassner — Otto-von-Guericke-Universität Magdeburg, FNW/ITP, PF 4120, 39016 Magdeburg

The effects of convective flow on dendritic crystal growth and pattern formation have been an active research topic for many years, but have not been fully understood on the theoretical side. This is mainly because the governing equations are considerably more complicated than without flow and microscopic solvability theory, successfully describing a single free crystal growing into its quiescent supercooled melt, is no longer applicable in its original formulation.

Introducing an asymptotic decomposition scheme to nonlinear solvability theory we substantially extend the range of this concept and present a new approach to dendritic growth phenomena based on a free boundary formulation. This technique is demonstrated for dendritc growth in a forced potential flow.

DY 16.4 Mon 17:00 HÜL 186

KMC simulations of sintering nano-clusters including grain boundaries in 3D — •Martin Fendrich, Ruslan Zinetullin, and Dietrich E. Wolf — Institut der Physik, Universität Duisburg-Essen, Campus Duisburg, Germany

Thermal sintering processes of two nano-clusters are simulated using the Kinetic Monte-Carlo (KMC) method. By letting two independent fcc-lattices interpenetrate each other and allowing atoms to exchange between them, a grain boundary is modeled. We developed a hybrid simulation scheme combining the atomistic KMC method with a numerical integration of the equations of motion for the two particles in contact. The simulations show that the qualitative sintering process may be divided into two stages. In the first stage a fast reorientation of the grains takes place leading to special classes of mutual torsions with misorientation angles between 0 and $\approx 80°$. The frequencies in which orientations of the characteristic classes occur can be understood in terms of a coherent site lattice analysis. The evolution of the cluster's shape and the duration of the subsequent coalescence stage strongly depends on the adopted orientation of the grains.

DY 16.5 Mon 17:15 HÜL 186

Simulation of binary alloy cluster growth: Segregation, exchange processes, magnetic interactions and magnetic field effects — •Mario Einax[1], Stefan Heinrichs[1], Philipp Maass[2], and Wolfgang Dieterich[1] — [1]Fachbereich Physik, Universität Konstanz, D-78457 Konstanz — [2]Institut für Physik, Technische Universität Ilmenau, D-98684 Ilmenau

We present detailed kinetic Monte Carlo (KMC) simulations of growing nanoclusters on a weakly interacting substrate within a fcc-type binary alloy model. This model is designed to describe recent molecular beam epitaxy experiments on $CoPt_3$ nanoclusters that develop perpendicular magnetic anisotropy (PMA) [1]. As a consequence of Pt surface segregation (driven by exchange processes) and cluster shape we find a growth-induced structural anisotropy, located near the cluster surface, which is compatible with experimentally observed magnetic properties [2]. Analytic approaches are discussed to clarify the competition between the incoming flux and surface equilibration processes leading to kinetically limited surface segregation.

In a second step our model is generalized to include an external magnetic field in the growth direction, which is found to induce bulk structural anisotropy favorable for PMA. Moreover, magnetic interactions are shown to have a significant influence on the bulk transition temperature for the onset of $L1_2$-ordering [3].

[1] M. Albrecht et al., Europhys. Lett. **56**, 884 (2001)
[2] S. Heinrichs et al., cond-mat/0510196
[3] M. Einax et al., to be published

DY 16.6 Mon 17:30 HÜL 186

Surface processes during low energy ion bombardment of glassy metallic thin films — •Sebastian Vauth and S. G. Mayr — I. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

Thin glassy metallic $Zr_{65}Al_{7.5}Cu_{27.5}$ films are prepared by cocondensing the three components by electron beam evaporation under UHV conditions. After that the sample is irradiated in situ with keV-Kr^+-ions and the surface topographies are analyzed by scanning tunneling microscopy (STM) with respect to structure formation and smoothing. The studies are performed as a function of irradiation conditions, viz. ion energy and fluence. The STM data are numerically analyzed by calculating the root mean square roughness and spectral power densities to track down the underlying surface mechanisms of structure formation. To get insight on a microscopic level we perform molecular dynamics (MD) simulations of glassy CuTi and Si films. We investigate temperature activated processes in comparison with processes caused by ion bombardment. To model the experimental results on a mesoscopic level we make use of stochastic rate equations describing the surface morphology. In similarity to equations to model film growth we develop an equation for irradiation based on our experimental and MD data. This work is financially supported by the DFG Sonderforschungsbereich 602, TP B3.

DY 16.7 Mon 17:45 HÜL 186

The isotropic-nematic interface in suspensions of platelets — •Tanja Schilling[1], Paul van der Schoot[2], and David van der Beek[3] — [1]Institut für Physik, Johannes Gutenberg-Universität, 55099 Mainz, Staudinger Weg 7, Germany — [2]Eindhoven University of Technology, Applied Physics, PO Box 513, 5600 MB Eindhoven, The Netherlands — [3]Van 't Hoff Laboratory for Physical and Colloid Chemistry, Utrecht University, 3584 CH Utrecht, The Netherlands

Suspensions of plate-like particles phase separate into an isotropic and a nematic phase at sufficiently high concentrations. The reasons for this are identical to those for the formation of a nematic phase in suspensions in rod-like colloids: a strongly anisotropic excluded-volume interaction between the particles favours parallel alignment. However, there is a crucial difference between the nematic ordering of rods and platelets: Rods

may be quantitatively understood at the level of second virial theory whereas this is not the case for platelets. Presumably this is the reason why in the theoretical literature so much more emphasis has been on nematics of rods than on that of platelets. Also, experimentally it seems to be easier to supress gelled states in rod dispersions than in plate ones. Recently, however, significant progress in the experimental study of suspensions of platelets has been made, making it timely to consider the issue in more detail.

We present a combined theoretical, simulational and experimental study of the isotropic-nematic interface. In particular, we show that its interfacial tension can be extracted from the capillary rise of the interface without knowledge of the elastic constants of the nematic phase.

DY 16.8 Mon 18:00 HÜL 186

Heat capacity of quasi-one-dimensional atomic adsorbates deposited in the groves of carbon nanotube bundles — •Konstantin Chishko, Tatiana Antsygina, and Igor Poltavsky — B. Verkin Institute for Low Temperature Physics and Engineering, 47 Lenin Ave., Kharkov 61103, Ukraine

The model taking into account both the formation of one-dimensional (1D) condensate at the bottom of the external grooves on carbon nanotube bundles and also the promotion of two secondary 1D chains over primary one (three-chain quasi-one-dimensional structure) is developed to describe the thermodynamics of rare gas adsorption on the nanobundle surface. The Gibbs free energy and the heat capacity of the system under study have been obtained within a universal lattice gas approach using both two-time Green functions and transfer matrix methods with regard to interparticle interactions in the primary and secondary chains. So, the model is adequate for treatment of a rather wide range of coverages on the initial stage of deposition. The heat capacity has been found as functions of both temperature T and low-dimensional adsorbate density n_{ads} at different values of interpartical energies and the interaction energy between adsorbed atoms and the substrate nanobundle. As a function of n_{ads}, the heat capacity demonstrates non-monotonic behavior with peaks localized near $n_{ads} \simeq 1$ and $n_{ads} \simeq 3$ which correspond to completed occupation of the positions in the primary and secondary chains. The height and width of the peaks are determined by the magnitudes of the interaction energies in the system. All the effects predicted by the theory are accessible for the experimental observation.