DY 21 Statistical Physics (general) I

Time: Tuesday 10:00–11:45 Room: SCH 251

DY 21.1 Tue 10:00 SCH 251

Multiscale simulations of micro-structure selection in binary alloy solidification — •Heike Emmerich[1] and Matthias Jurgk[2] — [1]RWTH Aachen, Computational Materials Engineering, Center for Computational Engineering Science (CCES), Institute of Minerals Engineering (GHI), Mauerstrasse 5, 52064 Aachen — [2]Max-Planck-Institut for Physics of Complex Systems, Noethnitzerstr. 38, 01187 Dresden

We demonstrate that the competition of dendritic crystals in a solidifying sample gives rise to two qualitatively different micro-structure solutions depending on the density ρ of crystals in the melt. Here we show for the first time, that there is a non-steady transition from one to the other. The precise ρ-dependence of the transition point is determined by the Biot number. Our investigation is based on a scaling analysis for the tip velocity of the dendritic crystals, which we assume to be aligned in an array and to be coupled via the transport of heat. We develop our analytical solutions based upon the asymptotic Kruskal-Segur reduction to a differential equation in the complex plane. It is supported by numerical simulations of a multiscale model of alloy growth. On the one hand this solution can be used to improve the accuracy of applied solidification simulations. On the other hand it yields additional insight in the universality of diffusion limited crystal growth in the presence of competing micro-structures.

DY 21.2 Tue 10:15 SCH 251

Coupled Phase Field/Monte Carlo Simulation for Heterogeneous Crystallization Kinetics — •Jürgen Hubert and Heike Emmerich — RWTH Aachen, Computational Materials Engineering, Center for Computational Engineering Science (CCES), Institute of Minerals Engineering (GHI), Mauerstrasse 5, 52064 Aachen*

Phase field models are a now well established and rapidly growing section within the field of modeling the evolution phase transitions. Among other things they can be used for the simulation of nano crystallization processes, grain growth and heterogeneous nucleation. By combining the phase field method with Monte Carlo Algorithms, the evolution of the crystal orientation can be described with only a slight increase in the necessary computing power.

This entry will show new expansions of existing models, as well as the possibilities and challenges of grain growth simulations with a large number of different crystal orientations.

DY 21.3 Tue 10:30 SCH 251

Size effects in molecular dynamics simulations of nucleation — •Jan Wedekind[1], David Reguera[2], and Reinhard Strey[1] — [1]Institut für Physikalische Chemie, Universität zu Köln, Luxemburger Str. 116, D-50939 Köln, Germany — [2]Universitat de Barcelona, Departament de Física Fonamental, Facultat de Física, Universitat de Barcelona, Martí i Franquès, 1, 08028-Barcelona, Spain

Most molecular dynamics (MD) simulations of vapor-liquid nucleation are performed in a closed, canonical NVT-system. Under these conditions the vapor pressure and thus the supersaturation change during the condensation and growth of a droplet due to the fixed total number of molecules N. Furthermore, the feasibility of observing a nucleation event may depend significantly on the size of the system at hand. We investigate the potential importance of finite size effects in MD simulations of nucleation in the framework of the modified liquid drop model (MLD) [1,2] and the implications of our investigations on the results reported in the literature. Furthermore we show with comparatively simple calculations how it is possible to estimate the system size in terms of N or similarly V, beyond which corrections due to size effects become negligible. By optimizing the system parameters it is possible to save valuable calculation time and extend the range of supersaturations attainable by simulations by several orders of magnitude.

[1] C. L. Weakliem and H. Reiss, J. Chem. Phys. 99 (7), 5374 (1993).
[2] D. Reguera, R. K. Bowles, Y. Dijkaev, and H. Reiss, J. Chem. Phys. 118 (1), 340 (2003).

DY 21.4 Tue 10:45 SCH 251

Hole crystallization in semiconductors — •Michael Bonitz[1], Vladimir Filinov[2], and Holger Fehske[3] — [1]Institut for Theoretical Physics and Astrophysics, University Kiel, Leibnizstr. 15, 24098 Kiel — [2]Institute for High Energy Density, Russian Academy of Sciences, Izhorskay 13/19, Moscow 127412, Russia — [3]Institute of Physics, University Greifswald, 17487 Greifswald

Electrons and holes in a solid are normally delocalized over the crystal lattice. However, it has been speculated [1,2] that, for a sufficiently large mass ratio $M = m_h/m_e$, hole localization and even crystallization should be possible. We present a theoretical analysis of the conditions of hole crystallization which yields a critical mass ratio M of about 80 and predictions of the possible density and temperature range. We also discuss the close relation of the hole crystals to ion crystals in classical plasmas and in ultradense stellar objects such as White Dwarfs and neutron stars.

A phase diagram of Coulomb crystals in electron-hole plasmas which is applicable to generic plasmas with two charge components is presented. The analytical results are confirmed by extensive first principle path integral Monte Carlo simulations which cover the transition from an excitonic gas to a hole crystal embedded into a Fermi gas of electrons.

[1] B.I. Halperin, and T.M. Rice, Rev. Mod. Phys. 40, 755 (1968);
[2] A.A. Abrikosov, J. Less-Comm. Metals 62, 451 (1978);
[3] M. Bonitz, V.S. Filinov, V.E. Fortov, P.R. Levashov, and H. Fehske, Phys. Rev. Lett. (2005), accepted

DY 21.5 Tue 11:00 SCH 251

Mesoscopic fluctuations and intermittency in aging dynamics — •Paolo Sibani — Fysisk Institut, SDU, Campusvej 55, DK5230 Odense M

Mesoscopic aging systems are characterized by large intermittent noise fluctuations. In a *record dynamics* scenario [P. Sibani and J. Dall, Europhys. Lett. 64, 2003] these events, or quakes, are treated as a Poisson process with average $\alpha \ln(1 + t/t_w)$, where t is the observation time, t_w is the age and α is a parameter. Assuming for simplicity that quakes constitute the only source of de-correlation, we present a model for the probability density function (PDF) of the configuration autocorrelation function. Beside α, the model has the average quake size $1/q$ as a parameter. The model autocorrelation PDF has a Gumbel-like shape, which approaches a Gaussian for large t/t_w and becomes sharply peaked in the thermodynamic limit. Its average and variance, which are given analytically, depend on t/t_w as a power-law and a power-law with a logarithmic correction, respectively. Most predictions are in good agreement with recent data from the literature and with the simulations of the Edwards-Anderson spin glass carried out as a test.

DY 21.6 Tue 11:15 SCH 251

Lineabatic treatment of periodically driven stochastic systems — •Mykhaylo Evstigneev and Peter Reimann — Universität Bielefeld, Unviversitätsstr. 25, 33615 Bielefeld

A periodically driven noisy system in the limit of long times is considered. To deduce its asymptotic time-periodic probability distribution, two approaches are commonly used: adiabatic theory, valid if driving is very slow, and linear response theory, applicable when driving is weak. A novel approximation scheme - the lineabatic approximation - is introduced, which combines these two approaches to yield the driven probability distribution even when driving is moderately strong and fast, so that both linear response and adiabatic approximations break down. The accuracy of the lineabatic scheme is discussed based on specific examples.

DY 21.7 Tue 11:30 SCH 251

A connection between an exactly soluble stochastic control problem and a nonlinear reaction-diffusion equation — •Roger Filliger[1], Max Olivier Hongler[2], and Ludwig Streit[1] — [1]CCM, Universidade da Madeira, Portugal — [2]IPR, EPF-Lausanne, Switzerland

We present an exactly soluble optimal stochastic control problem involving a diffusive two-state random evolution process and connect it to a non-linear reaction-diffusion type of equation by using the technique of logarithmic transformations. The work generalizes the recently established connection between a discrete two velocities, non-linear Boltzmann equation and the optimal control of a two-state random evolution process.

We further show that the cost structure associated to the control problem is connected to the large deviations probabilities of the uncontrolled dynamics.