SKM-SYMF 1: Heterogenous Nucleation and Microstructure Formation: Steps towards a System- and Scale-bridging Understanding

Time: Thursday 14:30–17:00 Location: TRE Ma

Invited Talk SKM-SYMF 1.1 Thu 14:30 TRE Ma
Visualizing the structural solid-liquid transition with colloidal suspensions — •Peter Schall — University of Amsterdam, Amsterdam, The Netherlands

Crystal-liquid interfaces offer unique insight into the structural transition from solid to liquid, which is of key importance for understanding crystal nucleation and growth. These interfaces are, however, difficult to access experimentally because they are buried between two dense phases. We used a colloidal crystal-fluid equilibrium to obtain direct images of the structural solid-liquid transition: the individual particles in colloidal suspensions can be conveniently imaged and tracked in time using optical microscopy. We grow large colloidal crystals, and image their flat interfaces with the colloidal melt in three dimensions with confocal microscopy. We elucidate changes in the three-dimensional short range order across the interface, and determine the interfacial free energy directly from these configurational changes. Finally, we follow thermally excited fluctuations of the interface to measure the interfacial tension and its anisotropy, which are important parameters of crystal nucleation and growth.

Invited Talk SKM-SYMF 1.2 Thu 15:00 TRE Ma
Crystallization process in suspensions of hard spheres — •Tanja Schilling[1], Hans-Joachim Schoepe[2], Martin Oettel[2], George Opletal[3], and Ian Snook[3] — [1]Theory of Soft Condensed Matter, University of Luxembourg, Luxembourg — [2]Institut fuer Physik, Universitaet Mainz, Germany — [3]School of Applied Sciences, RMIT University, Melbourne Australia

We report on a computer simulation study of crystal nucleation in hard spheres. Through a combined analysis of real and reciprocal space data, a picture of a two-step crystallization process is supported: First dense, amorphous clusters form which then act as precursors for the nucleation of well-ordered crystallites. This kind of crystallization process has been previously observed in systems that interact via potentials that have an attractive as well as a repulsive part, most prominently in protein solutions. In this context the effect has been attributed to the presence of metastable fluid-fluid demixing. Our simulations, however, show that a purely repulsive system (that has no metastable fluid-fluid coexistence) crystallizes via the same mechanism.

Invited Talk SKM-SYMF 1.3 Thu 15:30 TRE Ma
Homogeneous bulk, surface, and edge nucleation in crystalline nanodroplets — •Kari Dalnoki-Veress and Jessica Carvalho — McMaster University, Hamilton, Canada

We present a study on the homogeneous nucleation of dewetted poly(ethylene oxide) droplets on a substrate that is itself crystallisable. While the chemical properties of the substrate prepared in either the amorphous or crystalline state are identical, the surface landscape varies widely. We observe a large difference in the substrate's nucleating ability depending on how it is prepared. Furthermore, the scaling dependence of the nucleation rate on the size of the droplets depends on the substrate surface properties. The birth of the crystalline state can be directed to originate predominantly within the bulk, at the substrate surface or at the droplet's edge depending on how we tune the substrate

Invited Talk SKM-SYMF 1.4 Thu 16:00 TRE Ma
Polymer Crystallization: Ordered Structures in Complex Systems — •Jens-Uwe Sommer — Leibniz-Institut für Polymerforschung Dresden, Hohe Straße 6, 01069 Dresden — Insitut für Theoretische Physik, Technische Universität Dresden, Zellescher Weg 17, 01069 Dresden

The crystallization of long chain molecules requires two ordering processes which take place simultaneously: Transition of each chain from the randomly coiled state into the partially folded and extended state, and the growth of a regular crystalline structure which involves the attachment of many chains. This leads to complex crystallization and nucleation pathways which usually result in non-equilibrium meta-stable states. I will first discuss some issues of possible equilibrium states of chain crystals [1]. Then, coarse grained models which describe the growth and melting behavior of polymer crystals in thin films are presented [2]. Here, I indicate the essential role of the internal transition of chain conformations for the growth of polymer crystals. Finally, large scale molecular dynamics simulations are presented which allow to investigate molecular details of single lamellar growth out of an entangled polymer melt [3]. Spatial-temporal measures of the state of order are introduced to detect precursor states of crystallizing chains during the crystallization pathway.

[1] J.-U. Sommer, Eur. Phys. J. E 19, 413 (2006)
[2] J.-U. Sommer and G. Reiter, J. Chem. Phys. 112, 4384 (2000)
[3] C.-F. Luo and J.-U. Sommer, Phys. Rev. Lett. 102, 147801 (2009)

Invited Talk SKM-SYMF 1.5 Thu 16:30 TRE Ma
Phase formation and microstructure development in multicomponent alloys — •Jürgen Eckert — IFW Dresden, Institut für Komplexe Materialien and TU Dresden, Institut für Werkstoffwissenschaft

The talk will report on the phase formation and the microstructure development in (often multicomponent) metallic liquids that tend to form glasses upon solidification at sufficiently high cooling rate. Upon slower cooling typically very fine-scale eutectic-like structures can be achieved. The resulting structure depends on both the actual alloy composition and the employed quenching conditions. The existence of quenched-in short- and medium-range order structures for triggering the phase formation will be assessed, and the role of decomposition and heterogeneous nucleation for establishing nanoscale microstructures will be explored. Examples how tuned-in microstructures can be achieved for optimizing the mechanical properties of such alloys will also be given.