

CPP 37: Poster: Heterogeneous Nucleation and Microstructure Formation (related to SYMF)

Time: Wednesday 17:00–19:00

Location: P2

CPP 37.1 Wed 17:00 P2

Crystallization of charged macromolecules — ●KAI KRATZER and AXEL ARNOLD — Institut für Computerphysik, Universität Stuttgart

The crystallization of charged macromolecules has a number of important applications in many fields, such as biology, pharmacology or materials design. For example, proteins are crystallized for purification or structure determination and colloidal crystals are promising candidates for photonic crystals. However, the crystallization of proteins or colloids is still more an art rather than a technique due to the poor understanding of the underlying physical mechanisms. To create defect-free crystals (or to prevent their growth), it is necessary to know the microscopic details of the onset of crystal growth, namely the nucleation. This process is described by the classical nucleation theory (CNT) as a balance of surface tension between liquid and crystal and the crystal's lower chemical potential. We performed computer simulations of the nucleation process to gain a better understanding of how charges carried by the macromolecules and the presence of neutralizing salt and precipitation agents influence nucleation. Since nucleation is a rare event, it is inaccessible to brute force computer simulations. We succeeded in this challenge by using the Forward Flux Sampling (FFS) method, which has only recently become available. We present first FFS results on systems of charged macromolecules in the presence of an explicit salt. This will help in developing a closed theory of protein and colloidal crystallization and thereby making targeted crystallization possible.

CPP 37.2 Wed 17:00 P2

Heterogeneous nucleation at a flat wall in a colloidal model system of charged spheres — ●ANDREAS ENGELBRECHT, RAFAELLA MENESES, and HANS JOACHIM SCHÖPE — Staudingerweg 7, 55099 Mainz

The physical and chemical properties of solidified crystalline materials depend in a crucial way from the conditions of crystal nucleation. In order to improve the conditions of production processes and even to develop novel materials with extraordinary properties a detailed

knowledge of the nucleation process is most desired.

We studied the kinetics of wall induced heterogeneous nucleation in colloidal model systems of charged spheres as function of undercooling determining nucleation rate densities, crystal growth velocities and the resulting micro structure. Applying classical concepts we extract key parameters of the nucleation process giving us the possibility to characterize the competition homogeneous and wall induced heterogeneous nucleation.

Classical theories of heterogeneous nucleation predict a reduction of the nucleation barrier height, which only depends on the contact angle of the crystal nucleus. We investigated the nucleation barrier height and its dependency on the undercooling in the system. Those results were compared with microscopic investigations of the contact angle.

CPP 37.3 Wed 17:00 P2

Gauging the Phase Field Crystal Model on Simple Systems: Hard Spheres — MARCO BERGHOFF¹, BRITTA NESTLER¹, ●MARTIN OETTEL^{2,3}, and TANJA SCHILLING⁴ — ¹Institute of Materials and Processes, Karlsruhe University of Applied Sciences and Institute of Reliability of Components and Systems, Karlsruhe Institute of Technology — ²Institut für Physik, Universität Mainz — ³Material- und Prozesssimulation, Universität Bayreuth — ⁴Theory of Soft Condensed Matter, Université du Luxembourg

The Phase Field Crystal (PFC) Model is a simple Landau-type free energy model for a density-like order parameter which exhibits a phase diagram with spatially constant liquid phases and crystal phases in which the order parameter periodically varies. Supplemented with diffusive dynamics, a wealth of time-dependent processes involving crystal-liquid interfaces are describable. However, precise matching of the PFC model parameters to an actual material is difficult. Here we discuss the gauging of the model to the soft matter system of hard spheres (HS) for which both reliable simulation and density functional results exist. It is found that the HS density functionals cannot be straightforwardly mapped to the PFC free energy. As a result, crystal-liquid interface tensions and growth properties can be compared only qualitatively.