

Computer simulation and theory for the nucleation of crystal phases

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Nucleation is how crystal phases start to form, and if the barrier to it is too high, the crystal will never form. In my talk I want to do two things. The first is present the results of computer simulations aimed at achieving a molecular-level understanding of nucleation. We have results showing that the nucleation of crystal phases can be qualitatively different from that of liquids, and that predicted by classical nucleation theory. The second is to show how experimental studies of nucleation may be modeled quantitatively. Under common experimental conditions, the nucleation rate may not be in thermodynamic limit. This has profound consequences for how we use experimental data under one set of conditions to try and predict the behaviour if we change an experimental parameter.