The Temperature of Small Nucleating Droplets

David Reguera [C, S] and Jan Wedekind
Departament de Fisica Fonamental, Universitat de Barcelona, Barcelona, Spain

Nucleation is the first step in many phase transformations, and it is probably the most characteristic example of a non-equilibrium process where fluctuations play a crucial role. There have been many discussions of the role of cluster temperatures and the influence of their inevitable fluctuations on the nucleation rate. We have investigated the temperature of nucleating and growing droplets using molecular dynamics simulations. We find that, due to the latent heat released in the phase transition, cluster temperatures can be several degrees different from the bath temperature. In particular the most probable value of the temperature of sub-critically sized clusters tends to be colder than the bath temperature, while sub-critically sized clusters are warmer. However, the average temperature of all clusters is found to be always higher than the bath temperature. Even though nucleation is highly sensitive to temperature, the results surprisingly show that the deviation of the cluster temperature from the bath temperature does not have a significant influence on the nucleation rate. We show how these results can be understood and quantified in the framework of nonequilibrium thermodynamics. Finally, we also analyze the role and efficiency of the carrier gas in thermalizing the nucleating clusters and its potential influence on the rate at which nucleation proceeds.