SIMULATING NUCLEATION AND GROWTH PROCESSES

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Under suitable conditions, first order phase transitions such as the freezing of a liquid or the structural transformation of a solid occur via a nucleation and growth mechanism, in which a nucleus of the stable phase is formed in the metastable phase. Due to the high free energy barrier related to the creation of a nucleus of critical size, nucleation is typically a rare event complicating the simulation of such processes with molecular dynamics simulations. Here, I will present various computer simulation methods to simulate and analyze rare nucleation events. As illustrative examples I will discuss the crystallization of a supercooled liquid and cavitation in water at negative pressures.

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