Two Step Nucleation

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Two step nucleation is the process by which a bulk metastable phase undergoes a phase transition to a stable phase via the formation of a local fluctuation of an intermediate phase of sufficient size to be able to grow spontaneously to macroscopic scale. In the case of "two-step nucleation" (TSN), the first step in the phase transformation process consists of the appearance in the bulk metastable phase of a local fluctuation that resembles an intermediate phase distinct from the stable phase. In the second step of TSN, this intermediate fluctuation undergoes a transition in which the stable phase emerges from within the intermediate phase. Evidence for TSN has been observed experimentally in a wide range of molecular and colloidal systems, including important cases relevant to understanding protein crystallization and biomineralization. In recent work, James et al. (2019) evaluated the free energy surface (FES) describing TSN as it occurs in a simple 2D model of a metamagnet, and Iwamatsu (2011) proposed an equation modelling the FES of TSN. In both cases, the FES shows there is a well-defined size for the growing nucleus at which the stable phase becomes more stable than the intermediate phase, providing a thermodynamic prediction for the nucleus size at which the second step of TSN begins. We analyze the FES presented in James et al. in terms of Iwamatsu's model and show that it is in excellent agreement with the numerical data. We also identify conditions at which the spontaneous transition within the nucleus occurs at much larger size than predicted by thermodynamics, demonstrating that the system dynamics can have a dramatic impact on how TSN is observed in practice.