A review of nucleation models in various systems

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Classical nucleation theory (CNT), which was originally derived for the formation of droplets, is often used to calculate the number of nuclei formed within a supersaturated or undercooled parent phase in various systems [1]. In some cases, however, the assumptions of CNT are not met, which is why the CNT approach is incorrect. Here, we summarize homogeneous and heterogeneous nucleation for vapor-liquid, vapor-solid, and liquid-solid phase transitions. In all cases, the formation of clusters plays an important role in the nucleation process. Nuclei of a new phase (supercritical clusters) form after overcoming the nucleation barrier W* at the critical size i*. In binary nucleation, W* corresponds to the saddle point when W reaches a minimum during the formation of nuclei. For heterogeneous nucleation on a foreign surface, W is influenced not only by interfacial energies but also by surface shape. A special case of heterogeneous nucleation is nucleation on active centers, where the nucleation barrier is lower, thus making active centers preferred for nucleation.

However, the formation of nuclei also depends on kinetics. In small encapsulated systems, the depletion of the parent phase, i. e., a decrease in supersaturation or a decrease in the number of atoms in the parent phase, influences the formation of nuclei. In very small systems, there is an insufficient number of monomers, so new nuclei cannot form. In the case of nucleation in a supersaturated vapor or solution within an encapsulated system, a decrease in supersaturation increases W, which influences the formation of nuclei.

For example, the polymorphic system L-glutamic acid (L-Glu) has two monotropic polymorphs: α-L-Glu (metastable) and β-L-Glu (stable). The numerical solution of the standard nucleation model [2] showed that the metastable α phase forms quickly. However, over time, the stable β phase forms and the metastable α phase disappears, which coincides with the Ostwald ripening mechanism.

Molecular dynamics (MD) simulations only allow us to simulate only limited time scales. However, the standard nucleation model overcomes this limitation, and the nucleation rates often coincide with MD simulations and experimental data [3].

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