Energy of nuclei formation on curved active centers

Zdeněk Kožíšek, Robert Král, and Petra Zemenová

FZU - Institute of Physics of the Czech Academy of Sciences, Cukrovarnická 10, 16200 Praha 6, Czechia

Phase transition in a parent phase (supercooled melt or supersaturated solution) occurs via the formation of nuclei of a new crystalline phase by homogeneous or heterogeneous nucleation when clusters of a new phase appear due to fluctuations within the parent phase. The probability of nucleus formation is exponentially proportional to the nucleation barrier W^*, i.e. the work of formation of critical clusters plays an important role in model approaches to the nucleation process. Exact analytical solutions for $W^*$are well known for homogeneous and heterogeneous nucleation on a flat surface. This work focuses on heterogeneous nucleation on foreign surfaces, which serve as active centers, where the probability of nucleus formation is higher. On curved substrates, it is much more challenging to find an analytical solution for W^*, and using a more extended model is necessary. It is well known that the critical radius of the nucleus r^* is identical for homogeneous and heterogeneous nucleation unlike the number of monomers (atoms or molecules) i^* forming the critical nucleus. Nucleation kinetics suppose a step-by-step process, when the expression for formation energy of clusters W, as a function of the number of monomers I forming the cluster, is required. It is easy to express W(r) as a function of cluster radius r, and also W(i) as a function of cluster size i for homogeneous and heterogeneous nucleation on a flat surface. Generally, W(i) is difficult to express on curved surfaces. In this work, we summarize models for analytical approaches for W on concave and convex substrates as a function of cluster size [1, 2]. The analytical expression for W(i) is too difficult to find as even analytical r(i) dependency is not easy to find. It is shown that the probability of nucleus formation on a concave substrate is higher in comparison with a convex one. Moreover, in the case of crystallization of the small droplet, i. e. small encapsulated system, the depletion of the parent phase plays an important role [3]. The formation of crystalline nuclei can be even stopped due to an insufficient number of monomers within the parent phase.

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