

Classical nucleation theory from a dynamical approach to nucleation

J.F. Lutsko; M.A. Durán Olivencia

Abstract-

It is shown that diffusion-limited classical nucleation theory (CNT) can be recovered as a simple limit of the recently proposed dynamical theory of nucleation based on fluctuating hydrodynamics [J. F. Lutsko, J. Chem. Phys. 136, 034509 (2012)] <https://doi.org/10.1063/1.3677191>. The same framework is also used to construct a more realistic theory in which clusters have finite interfacial width. When applied to the dilute solution/dense solution transition in globular proteins, it is found that the extension gives corrections to the nucleation rate even for the case of small supersaturations due to changes in the monomer distribution function and to the excess free energy. It is also found that the monomer attachment/detachment picture breaks down at high supersaturations corresponding to clusters smaller than about 100 molecules. The results also confirm the usual assumption that most important corrections to CNT can be achieved by means of improved estimates of the free energy barrier. The theory also illustrates two topics that have received considerable attention in the recent literature on nucleation: the importance of sub-dominant corrections to the capillary model for the free energy and of the correct choice of the reaction coordinate.

Index Terms-

Due to copyright restriction we cannot distribute this content on the web. However, clicking on the next link, authors will be able to distribute to you the full version of the paper:

[Request full paper to the authors](#)

If your institution has an electronic subscription to Journal of Chemical Physics, you can download the paper from the journal website:

[Access to the Journal website](#)

Citation:

Lutsko, J.F.; Durán-Olivencia, M.A. "Classical nucleation theory from a dynamical

approach to nucleation", Journal of Chemical Physics, vol.138, no.24, pp.244908-1-244908-15, June, 2013.