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Unification of classical nucleation theories via a unified Itô-Stratonovich stochastic equation

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Abstract-

Classical nucleation theory (CNT) is the most widely used framework to describe the early stage of first-order phase transitions. Unfortunately, the different points of view adopted to derive it yield different kinetic equations for the probability density function, e.g., Zeldovich-Frenkel or Becker-Döring-Tunitskii equations. Starting from a phenomenological stochastic differential equation, a unified equation is obtained in this work. In other words, CNT expressions are recovered by selecting one or another stochastic calculus. Moreover, it is shown that the unified CNT thus obtained produces the same Fokker-Planck equation as that from a recent update of CNT [J. F. Lutsko and M. A. Durán-Olivencia, J. Chem. Phys. 138, 244908 (2013)] when mass transport is governed by diffusion. Finally, we derive a general induction-time expression along with specific approximations of it to be used under different scenarios, in particular, when the mass-transport mechanism is governed by direct impingement, volume diffusion, surface diffusion, or interface transfer.

Index Terms-

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