Extension of Mean-Field Nucleation Theory with Long-Range Interactions

JOHN A. VENABLES, JAMES DEGRAFFENREID, Dept. of Physics, Arizona State University, RAMON GRIMA, Institute for Mathematical Sciences, Imperial College, London, UK — Mean-field nucleation theory is an important tool in understanding various adsorbate-substrate systems, particularly in the context of epitaxial growth. Conventional mean-field theory does not take into account nonlocal interactions, but these can be important in the nucleation and growth of various nanostructures. An approach due to Ovesson [1] is based on the assumption that the change of saddle-point energy in a potential field equals the average changes at the neighboring binding sites, but this assumption is not generally satisfied. We reformulate the theory in a more general sense, as an extension of the work of Grima and Newman [2] and Venables et al. [3]. This leads to a continuum mean-field description in a general potential field, in which the transport coefficients are intrinsically connected with the interaction potential and with microscopic parameters. Computational examples are presented for Ge/Si(001) material parameters.

[1] S. Ovesson, PRL 88, 116102 (2002);