

Effects of nearest and next-nearest-neighbor (NNN) interactions in epitaxial growth on vicinal surfaces studied by kinetic-Monte-Carlo simulations

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Abstract:

In the dynamic scaling theory of surface roughening, one of the successful approaches to studying the scaling of growing surfaces is by formulating continuum Langevin-type equations which are assumed to incorporate the physics of growth processes and then applying analytical or numerical analysis to the growth equations so as to determine their scaling properties, which are called universality class of the molecular-beam epitaxy (MBE). Each growth universality class can be characterized by the specific values of the two scaling exponents: the roughness exponent α and the growth exponent β [1]. Indeed, theoretical as well as experimental studies have confirmed the existence of scaling laws during the epitaxial growth [2-3 and ref. therein]. This work is motivated by a calculation based on nearest-neighbor interactions that underestimates many features of the surface morphology. Our kinetic Monte-Carlo (kMC) simulation results enhance this idea for several materials. Besides, we present some ideas to explain the discrepancy between theory and experiments.

In this study, we are interested to the meandering instability that is induced by an Ehrlich-Schowebel (ES) effect. We used a model for kinetic growth that mimics the physics of MBE and where we introduced the diffusion into nearest and also next-nearest neighbor (NN & NNN) sites on crystal surface and the next-nearest-neighbor (NNN) interactions [4] and discuss their effect on the surface morphology and the roughening exponent. In the first part, we make a comparison study between different materials. Indeed, we found that there had two sets of materials. The first set, such as (Cu,Co,Ni,Fe), are similar to the results of hamouda et al.[1] in the case of Si (001), where two specific phenomenon have been distinguished : super-roughness and anomalous scaling. But in a second set, such as (Ga,Ge,Si), we found different surface morphologies, as well as a wide variation of critical exponents with temperature. In the second part, we focused to only two materials (Co,Si) where we tried to explain the effect of (NN & NNN) interactions and the direction of diffusion on the critical exponents.

Keywords: Growth, Molecular-beam-epitaxy, kMC simulation, Meandering instability, Roughness, Nearest and Next- nearest-neighbor interactions.

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