

Phase Diagram and Commensurate-Incommensurate Transitions in the Phase Field Crystal Model with an External Pinning Potential

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We study the phase diagram and the commensurate-incommensurate transitions in a phase field model of a two-dimensional crystal lattice in the presence of an external pinning potential. The model allows for both elastic and plastic deformations and provides a continuum description of lattice systems, such as for adsorbed atomic layers or two-dimensional vortex lattices. Analytically, a mode expansion analysis is used to determine the ground states and the commensurate-incommensurate transitions in the model as a function of the strength of the pinning potential and the lattice mismatch parameter. Numerical minimization of the corresponding free energy shows good agreement with the analytical predictions and provides details on the topological defects in the transition region. We find that for small mismatch the transition is of first-order, and it remains so for the largest values of mismatch studied here. Our results are consistent with results of simulations for atomistic models of adsorbed overlayers.

PACS numbers: 64.60.Cn Order-disorder transformations; statistical mechanics of model systems, 64.70.Rh Commensurate-incommensurate transitions, 68.43.De Statistical mechanics of adsorbates, 05.40.-a Fluctuation phenomena, random processes, noise, and Brownian motion

I. INTRODUCTION

In nature there exist many modulated structures which possess two or more competing length scales. Such systems often exhibit commensurate-incommensurate (CI) phase transitions [1, 2], which are characterized by structural changes induced by competition between these different scales. Systems in this class that have received intense attention for many years include spin-density-waves [3, 4] in Cr and charge-density-wave systems [5] *e.g.* in "blue bronze". They are characterized by an order parameter (*e.g.*, charge or spin density) that is modulated in space with a given wave vector q . In these systems the transition from a commensurate (C) state to an incommensurate (I) state is controlled by temperature and interaction with defects of the lattice [6]. Other systems of interest are materials which exhibit magnetic phase with spiral-like structures [7, 8]. Finally, vortex lattices in superconducting films with pinning centers [9] and weakly adsorbed monolayers [10, 11] on a substrate comprise a 2D realization of systems exhibiting CI transitions. In these systems the interparticle interactions are minimized by a configuration with a lattice constant a , while the substrate-adsorbed monolayer interaction is minimized by a configuration with lattice constant b usually incommensurate with a .

The simplest theoretical model for a CI transition is the 1D Frenkel-Kontorova (FK) model [12, 13]. It consists of a chain of particles interconnected by springs, representing an adsorbate layer, and placed in a periodic potential describing the effects of a substrate. The potential energy of a such system is given by

$$U = \sum_n \left[\frac{\lambda}{2} (x_{n+1} - x_n - a)^2 + V(x_n) \right], \quad (1)$$

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