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The behavior of commensurate-incommensurate transitions using the phase field crystal model

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A B S T R A C T

We study the behavior of the commensurate-incommensurate (CI) transitions by using a phase field crystal model. The model is capable of modeling both elastic and plastic deformation and can simulate the evolution of the microstructure of the material at the atomic scale and the diffusive time scale, such as for adsorbed monolayer. Specifically, we study the behavior of the CI transitions as a function of lattice mismatch and the amplitude of substrate pinning potential. The behavior of CI phase transitions is revealed with the increase of the amplitude of pinning potential in some certain lattice mismatches. We find that for the negative lattice mismatch absorbed monolayer undergoes division, reorganization and displacement as increasing the amplitude of substrate pinning potential. In addition, for the positive mismatch absorbed monolayer undergoes a progress of phase transformation after a complete grain is split. Our results accord with simulations for atomic models of absorbed monolayer on a substrate surface.

1. Introduction

Commensurate-Incommensurate (CI) transitions occur in many systems of nature which often possess one or more competing length scales. All of these systems are distinguished by a parameter ψ (e.g. averaged atomic density in this work) coordinated with a periodicity a. The periodicity a is often incommensurate with the substrate lattice which possesses a periodicity b. The simplest model of the CI transition is the 1D Frenkel-Kontorova (FK) model, which describes the dynamics of the particle chains interacting with the nearest neighbor in the presence of external periodic potentials [1–3]. The two dimensional model [4–6] of CI transition has recently attracted a large amount of attentions since it can be used in many actual systems, such as at the interface between two crystals or at the interface between the crystal and the surface monolayer. The 2-D model of this transition has been studied experimentally and theoretically for many years.

Experimentally, CI transitions exist in many materials. The most attraction is the rare gas monolayer absorbed on graphite or other carbides [7–18]. Some experimental work in the literature committed to analysis of the krypton molecular layer on the graphite surface combined extended x-ray-absorption fine structure [7], high-resolution x-ray scattering measurements [12,14], low-energy electron-diffraction(LEED),neutron scattering studies [15] and synchrotron X-ray diffraction studies [17]. Recently, Yang and her colleagues [19] have found that a transition from high-order commensurate phase to a weak incommensurate phase (HC-WI) in rubrene films grew on Bi (0001) surface. Woods and his co-workers [10] have studied the CI transition for graphene on top of hexagonal boron nitride(hBN). According to the rotation angle between the lattices of the two crystals, the graphene can be stretched to accommodate a slightly different hBN periodicity (for a small angle, resulting in a commensurate state) or almost no adjustment (incommensurate state). In an incommensurate state, the region having the matching lattice constant is separated by the domain walls of the accumulated strain.

Theoretically, the CI transition has been studied mainly with Monte Carlo methods [20–24], molecular dynamics [25] and phase field crystal model [26–32]. There are a large number of Monte Carlo models modeling CI transitions in krypton monolayer on graphite. Recently, Maiga et al. [24] model the adsorption of noble gases such as argon, krypton and xenon on a graphene sheet, using Grand Canonical Monte Carlo (GCMC) simulations. They calculated the two-dimensional gas-liquid critical temperature for each adsorbate, resulting in fair agreement with theoretical predictions and experimental values of gases on graphite. They determined the different phases of the monolayers and constructed the phase diagrams. They found two-dimensional incommensurate solid phases for krypton, argon and xenon, and a two-dimensional commensurate solid phase for krypton. Also phase field crystal model have been used to model CI transitions. Achim and his workers [29,30] studied the phase diagram of the CI transitions in a phase field model coupled with two dimensional crystal

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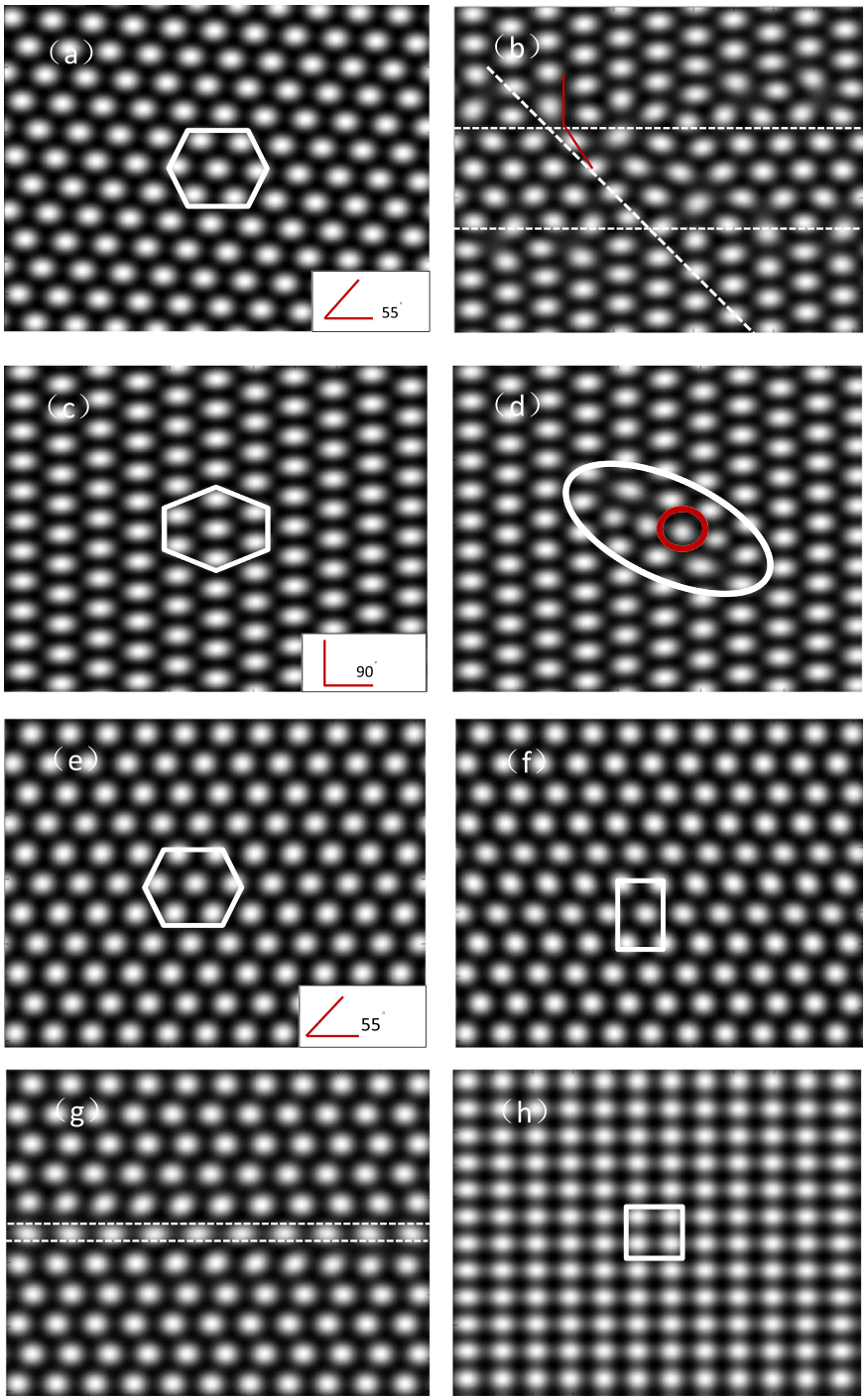

Fig. 1. The evolution of CI phase. transitions. (a) V_0 = 0. (b) V_0 = 0.003. (c) V_0 = 0.004. (d) V_0 = 0.005. (e) V_0 = 0.006. (f) V_0 = 0.012. (g) V_0 = 0.017. (h) V_0 = 0.040.

lattice in the presence of external pinning potential.

Even though the previous studies have attained fruitful achievements, some defects still existed in their theories. First, one more interesting problem is some microscopic models (such as Monte Carlo Model) cannot simulate the evolution of the microstructure of the material at the atomic scale and the diffusive time scale. But phase field crystal model can completely overcome the problem. Also recent works using phase field crystal model which coupled with an external pinning potential just revealed the phase diagram [29,30] of the CI transitions but did not study the behavior in the process of CI transitions. Therefore, the main aim of this paper is the behavior of CI transitions with increase of the amplitude of pinning potential in some certain lattice mismatches by using phase field crystal model. Also, we discuss the behaviors of CI transitions from the perspective of free energy.

2. Model and simulation

2.1. PFC model

In the phase field crystal model [33,34], the free energy function is:

$$f = \int d\vec{r}^2 \left(\frac{a\Delta T}{2}\Psi^2 + u\frac{\Psi^4}{4} + \frac{\Psi}{2}G(\nabla^2)\Psi \right) \quad (1)$$

In this case $G(\nabla^2) = \lambda(q_0^2 + \nabla^2)^2$ and the experimental structure factor relate to its eigenvalues [35]. We use Eq. (1) to describe a crystal