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Two Approaches to Dislocation Nucleation in the Supported Heteroepitaxial Equilibrium Islanding Phenomenon

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Abstract. We study the dislocation formation in 2D nanoscopic islands with two methods, the Molecular Static method and the Phase Field Crystal method. It is found that both methods indicate the same qualitative stages of the nucleation process. The dislocations nucleate at the film-substrate contact point and the energy decreases monotonously when the dislocations are farther away from the island-wetting film contact points than the distance of the highest energy barrier.

1. Introduction

The shape and size of islands resulting from growth processes has been a subject of numerous recent experimental and theoretical studies [1, 2, 3, 4, 5, 6, 7, 8, 9, 11, 13, 14, 15]. In particular, when the growing islands are of nanoscopic size the central issue is the possible spontaneous self-organization of islands into arrays of islands with a narrow size distribution. Such cases offer immediate technological applications in modern nanotechnology. The details of such self-organization processes are poorly understood, however. In particular, there are still uncertainties as to whether the observed shapes and sizes of growing islands in heteroepitaxy correspond to thermodynamic equilibrium state of minimum free energy or they are limited by kinetic effects. In the earlier analytical and numerical studies, in addition to assuming predefined shapes for the islands, the role of dislocation nucleation has not been included.

In the present work we study the dislocation nucleation in two dimensional islands with two methods, the Molecular Static method and the Phase Field Crystal method (PFC) [10]. The appeal of the latter method is that we do not need to initialize the transition path by hand. The way in which the two models reach the timescale of the nucleation process is quite different and our focus is on the qualitative stages of the process and on the agreement between the two approaches.

In the first section on this paper we explain the methods. We use the first, atomistic, model to study the strain relief caused by dislocation formation by minimizing a transition path between

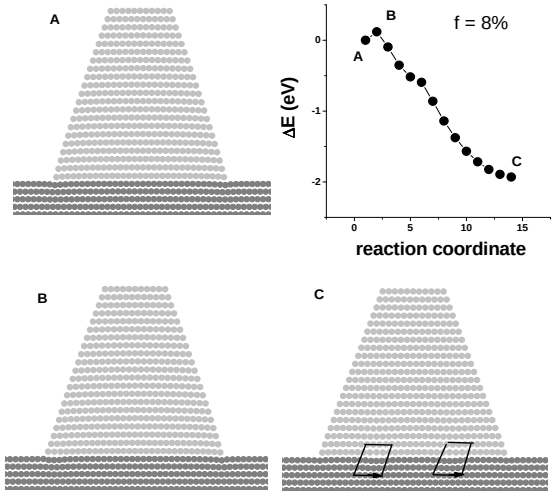


Figure 1. The minimum energy path between coherent and dislocated configurations is obtained with Nudged Elastic Band method in system with 411- atom island and 5 layers thick wetting film [19]. The dislocations are nucleated at the island-wetting film contact points. At a certain distance from the contact point the energy barrier is highest. After this point the energy is lowered monotonously as the dislocations move to the island centre.

the coherent and dislocated states with Nudged Elastic Band (NEB) Method [20]. Then we explore the same process with the PFC method in two dimensions. The nucleation is seen to be qualitatively similar with both approaches.

2. Models and Methods

2.1. Molecular Static Method

We adopt the 2D model used previously in Ref. [19], Interactions between all atoms in the system are described by a modified Lennard-Jones (LJ) pair potential [16] $V(r)$ with two parameters, namely the dissociation energy $\varepsilon_{\rm ab}$ and the atomic equilibrium distance $r_{\rm ab}$,

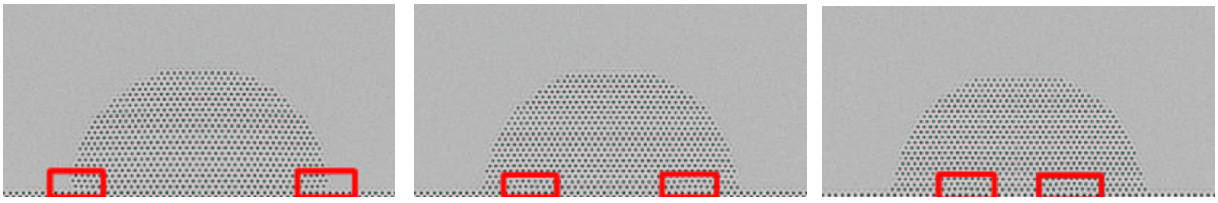
$$V_{ab}(r) = \varepsilon_{\rm ab}\left[\frac{5}{3}\left(\frac{r_{\rm ab}}{r}\right)^8 - \frac{8}{3}\left(\frac{r_{\rm ab}}{r}\right)^5\right] \tag{1}$$

with a smooth cut-off as in [16]. The indices ab of the equilibrium distance are ss, ff and fs for the substrate-substrate, adsorbate-adsorbate and adsorbate-substrate interactions, respectively. We model the attraction and lattice mismatch between the two materials by changing potential depth $\varepsilon_{\rm ab}$ and the equilibrium interatomic distance $r_{\rm ab}$ between the substrate and the film. The substrate-substrate interaction parameters were set to $\varepsilon_{\rm ss} = 3410.1$ K and $r_{ab} = 2.5478$ Å corresponding to a Cu substrate [16]. In terms of the lattice mismatch $r_{\rm ff} = (1+f)r_{\rm ss}$ and $r_{\rm fs} = (r_{\rm ff} + r_{\rm ss})/2$. A positive mismatch $f > 0$ corresponds to compressive strain and negative $f < 0$ to tensile strain when the adsorbate island is coherent with the substrate. Analogously we define an interaction parameter $\kappa = (\varepsilon_{ss} - \varepsilon_{sf})/\varepsilon_{ss}$ which describes the relative difference between the potential minimum depths in the substrate-adsorbate and absorbate-adsorbate interactions. A negative value of $\kappa < 0$ corresponds to an effectively attractive and positive $\kappa > 0$ to a repulsive substrate. The potential depths can be written as $\varepsilon_{\rm ff} = \varepsilon_{\rm ss}$, $\varepsilon_{\rm fs} = (1+\kappa)\varepsilon_{\rm ss}$ in the adsorbate-adsorbate and substrate-adsorbate interactions, respectively. We used periodic boundary conditions in the horizontal direction. Two bottom layers of the substrate were held fixed to simulate a semi-infinite substrate while all other layers were free to relax.

2.2. Phase Field Crystal Method

The phase field crystal method (PFC) has been applied in a variety of problems related to unideal crystal structures [10]. The method finds the ground state of a given truncated free energy functional without any reference to the instantaneous position of individual atoms. This enables us to find the dislocated ground states even if they were behind kinetic barriers, which would be insurmountable for atomistic simulations. The free energy is

$$F = \int d\vec{r}\left\{\frac{1}{2}\varrho\left[\vartheta + \left(q^2 + \nabla^2\right)^2\right]\varrho + \frac{1}{4}\varrho^4 + h\varrho\right\} \tag{2}$$



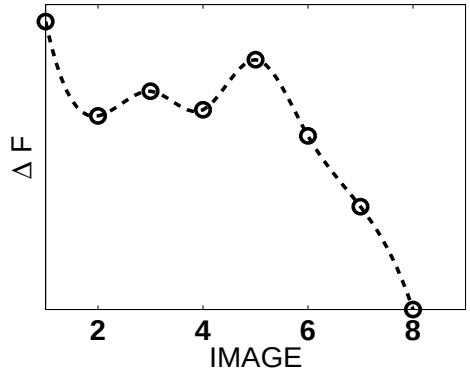


Figure 2. The figures in the upper row are PFC configurations at different stages of dislocation formation. The figure in the left shows the free energy landscape as a function of the image number in arbitrary units. The figures in the upper row correspond to images 1, 5 and 8. The misfit $f = -7.8\%$ and the pinning potential depth is half of the amplitude in the periodic phase. The line in the energy landscape is drawn to guide the eye. The dislocations positions are indicated by the square loops.

and the parameters $\vartheta = 1/2$ and $q = k(1 + f/100)$, k is the period of the pinning potential to be defined later. The components of the vector $\vec{r} = (x, z)$. This agrees with 2D model of [10]. We use periodic boundary conditions in the horizontal and mirror boundary conditions in the vertical direction. The function h is a pinning potential, which zero, if $2z > 3\sqrt{3}\pi/k$ and otherwise

$$h(\vec{r}) = \bar{h}\left[\cos(kx)\cos(kz/\sqrt{3}) - \cos(2kz/\sqrt{3})/2\right], \tag{3}$$

where $k = b\sqrt{3}/2$. The factor $b \sim 1$ ensures that the potential is continuous in the horizontal direction. The amplitude $\bar{h}$ is the pinning potential depth and it plays the same role as the interaction parameter in the Molecular Static method. The difference of the pinning potential and triangular phase periods k and q is adjusted to give the wanted lattice mismatch. The time step $\Delta t = 0.005$ and the grid size $\Delta x = 0.7854$. The simulation was done on $1024\Delta x \times 512\Delta x$ grid. The average density $\bar{\varrho} = 0.37$. This corresponds to a point in the middle of the constant phase-triangular phase coexistence in the one mode approximation of the phase diagram of Eq. 2. The initial state has an island of half-disc shaped region of triangular phase on the bottom edge of the simulation cell, see Fig.2. This island is surrounded by constant phase. The initial state is evolved according to

$$\frac{\partial \varrho}{\partial t} = \nabla^2 \frac{\delta F}{\delta \varrho} + \zeta, \tag{4}$$

where ζ is Gaussian distributed conserved noise [10].

3. Results and Discussion

The Fig. 1 shows an energy path between coherent and dislocated configurations [19]. The misfit $f = 8\%$ and $\kappa = 0$. The initial chain of states is obtained by simple linear interpolation. This chain is minimized with NEB method [20]. The results show an energy barrier for the initial detachment of the dislocation from the island-wetting film contact point. When the distance to the contact is larger than the distance of the highest energy peak, the energy decreases monotonously as the dislocations approach the island center. Finally the defects stop at a finite distance from each other.

We use PFC model to make a similar calculation. We use mismatches $\pm 7.8\%$ and pinning potential depth 0.5 times the amplitude of the triangular phase. The initial state is the upper

half of a disk standing on the simulation cell edge where the pinning potential is effective. For compressive mismatch, the island does not form dislocations but adopts a concave shape with reduced size of the island-wetting film contact area.

In the tensile case dislocations are nucleated symmetrically from both sides of the island base. This is shown in Fig. 2. The defects move towards the island centre. The free energy landscape is given in arbitrary units as a function of the image number. It shows the combined effect of dislocation nucleation and facet formation. These effects could be studied separately by starting from dislocated or faceted initial configuration. The general shape of the curve in Fig. 2 is similar to that of Fig. 1.

The island shape is almost rounded in the compressive and strongly faceted in the tensile case. The asymmetry of tensile and compressive has been studied also in [17, 18]. This asymmetry is clearly visible in the PFC model, because it does not nucleate dislocations in the latter case. This suggests, that the difference of energy barriers between the compressive and tensile cases in this model is larger than in the atomistic model.

4. Conclusions

We studied the dislocation nucleation in 2D strained heteroepitaxial nanoislands. We employed both an atomistic model and phase field crystal method. We saw, that the results are qualitatively consistent with each other. The dislocations were nucleated near the island-wetting film contact under tensile strain. After an initial energy barrier the dislocation detached from the contact point and moves to the middle of the island. During the move the energy was lowered gradually. The island shape in the tensile case were observed to be more strongly faceted than in the compressive case. The PFC model was found to have stronger asymmetry between compressive and tensile strains than the atomistic model.

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