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A GENERALIZED FRENKEL-KONTOROVA MODEL OF THE Ga/Si(112) DIMERIZED OVERLAYER SYSTEM WITH VACANCIES*

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We develop a Frenkel-Kontorova model to analyze the microscopic origins of vacancy-line interactions in a pseudomorphic adsorbate system. The atomic positions in the ground states are obtained by use of the gradient method. Our numerical results can explain the $2 \times N$ reconstruction observed in Ga/Si(112).

Keywords: Frenkel-Kontorova model, vacancy bond, gradient method
PACC: 6470, 6855, 6835

I. INTRODUCTION

Semiconductor surfaces exhibit a wealth of complex reconstructions which serve to reduce the number of dangling bonds, but at the cost of large structural distortions. When a material is grown pseudomorphically on a lattice-mismatched substrate, the resulting strain field can lead to self-organized structures with a length scale many times the atomic spacing. One well known example is the Ga/Si(112) dimerized overlayer system.[1] When Ga is deposited on Si and annealed, a small compressive strain can transform the 2×1 dimer structure to a more $2 \times N$ structure. Simply removing a dimer creates two extra dangling bonds which raise the energy. Pandey[2] proposed that the system lowers its energy by creating dimer vacancies in the surface layer; at the vacancy sites, the exposed atoms in the second layer rebond to eliminate their dangling bonds. These reconstructions are observed by scanning tunneling microscopy (STM).[3]

As usual in theoretical physics, one way to study these systems is to construct mathematical models which are sufficiently complex to mimic the phenomena of interest while also sufficiently simple to allow an exact analysis or a well defined series of approximations. The Frenkel-Kontorova (FK) model has been widely used to study complex static and dynamical phenomena arising from purely local interactions in many condensed-matter systems. The FK-type models are defined by the following Hamiltonian

$$H = \sum_{n=-\infty}^{\infty} [W(x_{n+1} - x_n) + V(x_n)], \qquad (1)$$

where $W(x_{n+1}-x_n)$ is the interatomic interaction and $V(x_n)$ is the local potential experienced by the n-th atom as a result of the interaction with a background of rigid atoms. Recently, Erwin *et al.*[4] have presented an exactly solvable FK model on Ga/Si(112), which contains only a single vacancy per unit cell. This model contains only nearest-neighbor harmonic interactions and the bonding of each atom to the substrate is also taken to be harmonic. The model reproduces the first-principles results quite accurately, and thus allows for a particularly simple analysis of the dominant interactions. In order to gain a better simulation to the real physical system, we present in this paper a generalized FK model in which the bonding of each atom to the substrate is a sinusoidal potential. The restoring force equations of the model are nonlinear, so the analytic solutions do not exist. We use the gradient method to determine the atomic positions in the ground state. If we ignore atomic displacements in transverse directions and allow the atoms to move only along the direction of the chain, this turns a two-dimensional surface problem into an effective one-dimensional system. Then the dimerized overlayer system can be mapped onto a one-dimensional diatomic chain of harmonic springs.[5,6] This is a variant of the FK model [7].

II. THE MODEL

To construct the microscopic model, we assume this one-dimensional diatomic chain to be periodic with a single vacancy per unit cell, that is, the length of a unit cell is Na, where a is the surface lattice

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constant and N is an positive integer. We now map this Ga-Si chain (with vacancy period N) onto a one-dimensional chain of harmonic springs connecting N Si atoms and $N-1$ Ga atoms in a unit cell. The bonding of each atom to the substrate is taken to be sinusoidal potential, with potential minima at the ideal substrate positions. Within the FK model, the potential energy used in this paper is

$$U = \frac{1}{2}K_{\rm Si}(b_1 - b_{\rm Si})^2 + \sum_{i=2}^{2N-1}\frac{1}{2}K(b_i - b^{\rm eq})^2 + \sum_{j=2m-1}^{2N-1} k_{\rm Si}(1-\cos(2\pi u_j/a)) + \sum_{j=2m}^{2N-2} k_{\rm Ga}(1-\cos(2\pi u_j/a)). \quad (2)$$

Here the one-dimensional atomic displacements u_j are defined with respect to the ideal positions $(a/2)j$ of the substrate atoms. This FK model has six parameters: $K_{\rm Si}$ and $b_{\rm Si}$ represent spring constant and equilibrium length of the Si-Si bonds at the vacancy respectively; K and $b^{\rm eq}$ represent spring constant and equilibrium length of the Si-Ga bonds in the bulk (away from the vacancy) respectively; $k_{\rm Si}$ and $k_{\rm Ga}$ represent the strengths of the rigid substrate potential for Si and Ga atoms in the chain respectively.

Let the atoms be located at x_j for $j = 1, 2, ..., 2N-1$. Define the displacement by $u_j = x_j - (a/2)j$. The bond lengths are defined as

$$b_i = x_{i+1} - x_i = u_{i+1} - u_i + \frac{1}{2}a, \quad (i = 2, 3, ..., 2N-1). \quad (3)$$

$$b_1 = x_1 - x_{-1} = u_1 - u_{-1} + a, \ (i = 1). \quad (4)$$

To solve for the displacement field that minimizes the energy, we consider the force equations for atoms in equilibrium. In the bulk, the force experienced by an atom is

$$F_j = 0 = K(2u_j - u_{j-1} - u_{j+1}) + \frac{2\pi k_j}{a}\sin(2\pi u_j/a), \quad (5)$$

where $k_j = k_{\rm Si}$ for odd j and $k_j = k_{\rm Ga}$ for even j. At the vacancy, the force on the first Si atom is

$$F_1 = 0 = K_{\rm Si}(u_1 - u_{-1} + a - b_{\rm Si}) - K(u_2 - u_1 + \frac{a}{2} - b^{\rm eq}) + \frac{2\pi k_{\rm Si}}{a}\sin(2\pi u_1/a). \quad (6)$$

Assuming periodicity, the chain is reflection symmetric about $j = 0$ and $j = N$, so that

$$u_j = -u_{2N-j}, \quad (7)$$

$$u_1 = -u_{2N-1} = -u_{-1}. \quad (8)$$

Clearly we need only consider one end of the chain. Equation (6) then reduces to

$$0 = (2K_{\rm Si} + K)u_1 + \frac{2\pi k_{\rm Si}}{a}\sin(2\pi u_1/a) - Ku_2 + (2K_{\rm Si} - K)\frac{a}{2} + (Kb^{\rm eq} - K_{\rm Si}b_{\rm Si}). \quad (9)$$

To apply this general solution to Ga/Si(112) we must determine numerical values for the six FK parameters appearing in Eq.(2). We do this either analytically from the Stillinger-Weber potential or numerically from first-principles total-energy calculations.[4,10] The six parameters are $K_{\rm Si} = 5.5$ eV/10^{-2}nm^2, $b_{\rm Si}$=0.225 nm $K = 9.8$ eV/10^{-2}nm^2, $b^{\rm eq}$=0.20 nm, $k_{\rm Si} = 2.0$ eV/10^{-2}nm^2, $k_{\rm Ga} = -0.7$ eV/10^{-2}nm^2, respectively. Basically this says that an inverted substrate potential can, in principle, cause the system to become unstable. If we assume $k_j \ll K$, which is true for our system, then the system is stable as long as $k_{\rm Si} + k_{\rm Ga} > 0$. The surface lattice constant a is 0.384 nm for Si(112).

Ⅲ. GRADIENT METHOD AND GROUND STATES

Since the interatomic interaction is a convex function, we can use the gradient method to determine the periodic ground states.

The gradient method[8,9] is part of Aubry's monumental contribution to nonintegrable dynamics. Considering a commensurate state with winding number $\omega = p/q$, the initial positions of the q atoms are set up in an equal spacing array

$$x_i(0) = i\frac{p}{q}a + \alpha, \quad (i = 1, 2, ..., q), \quad (10)$$

where a is the period of the external potential and the phase α is a constant throughout the system which satisfies

$$m_i \le 2(i\omega a + \alpha) \le m_i + 1. \quad (11)$$

Here m_i is the integral part of $2x_i$,

$$m_i = [2x_i]. \quad (12)$$

Let the system evolve in time according to the q differential equations

$$\frac{\mathrm{d}x_i}{\mathrm{d}t} = -\frac{\partial H}{\partial x_i}, \qquad (i = 1, 2, ..., q). \tag{13}$$

A periodic condition

$$x_0 = x_q - pa, \qquad x_{q+1} = x_1 + pa, \tag{14}$$

is imposed. This evolution relaxes the system towards the ground state under the influence of restoring forces. It has been shown that the resulting configuration is always a ground state if the initial configuration is given by Eq. (10). Equations (13) and (14) can be solved by the standard fourth-order Runge-Kutta method. When the ground state is reached, the force on each atom should vanish. In practice, the ground state can be considered found if all $\mathrm{d}x_i/\mathrm{d}t$ become less than a given prescribed value.

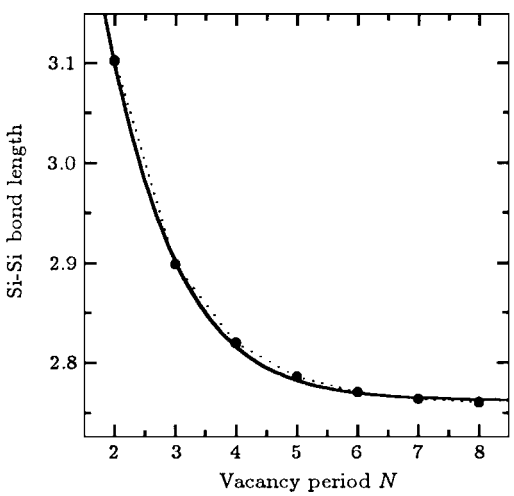


Fig.1. Si-Si vacancy bond length vs. vacancy period, where the black circles denote the results from the FK model, the dot broken lines link directly the black circles and the solid line denotes the curve fit of the results.

The ground states of the generalized FK model can be determined by the gradient method. Equilibrium bond lengths from the FK model are shown in Figs.1 and 2. Figure 1 shows Si-Si vacancy bond length vs. vacancy period, where the black circles denote the results from the FK model, the dotted broken lines link directly the black circles and the solid line denotes the curve fit of the results. In Fig.1, the vacancy bonds with vacancy periodicities from $N = 2$ to 8 are completely relaxed. Figure 2 shows Ga-Si bond length vs. bond number, where the black circles denote the results from the FK model and the broken lines link directly the black circles. In Fig.2, relative to the equilibrium Si-Ga bond length of 2.00 Å, bonds far from the vacancy (numbered 5–7) are compressively strained, bonds near the vacancy (3–4) are essentially unstrained, but bonds very close to the vacancy (1–2) are tensilely strained. This result indicates that part of Si-Ga bonding chain experiences tensile strain when the vacancy period N becomes small.

The agreement between our results and that of Erwin's model is remarkably good. Note the oscillatory behavior of the Ga-Si bond lengths which results from the unequal Ga- and Si-substrate binding strengths is strikingly confirmed by the local-density approximation results.[10]

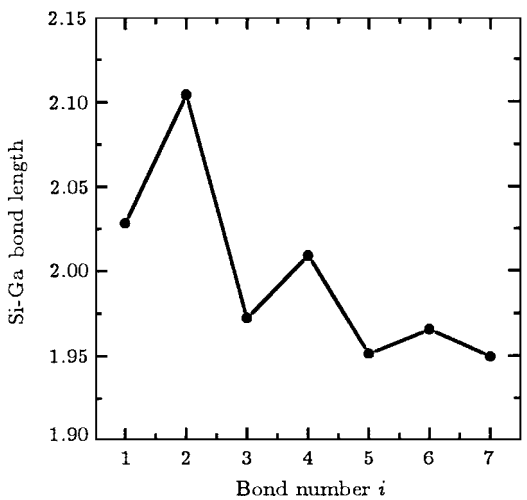


Fig.2. Ga-Si bond length vs. bond number, where the black circles denote the results from the FK model and the broken lines link directly the black circles.

IV. CONCLUSION

In this paper, we have developed a Frenkel-Kontorova model to analyze the microscopic origins of the reconstruction on the Ga/Si(112) dimerized overlayer system. The model is applied to Ga/Si(112) by extracting values for the microscopic parameters from total-energy calculations. The atomic displacements in the ground state are obtained. Our calculations explain the $2 \times N$ reconstruction observed in Ga/Si(112). The reconstruction represents the first unambiguous confirmation of energy lowering by Pandey's mechanism of rebonding at a missing dimer.[2] We hope to report elsewhere on the results of another exactly solvable FK model which contains an arbitrary number of vacancies per unit cell and the bonding of each atom to the substrate is also taken to be harmonic. In general, we expect the future analysis of similar strain-induced

self-organized adsorbate systems to benefit from these types of simple but accurate models.

A number of interesting questions remain unanswered about the model. We have restricted our attention to the convex interaction, nonconvex interactions are very common in solid state physics. For the FK-type models with nonconvex interactions, the equilibrium configuration $\frac{\partial H}{\partial u_n} = 0$ holds for metastable and unstable states, so the traditional approaches to find the ground states are no longer valid. The effective potential method can solve the nonconvex interactions, but it request an infinite system. The atomic chain with vacancy period N restricts, in some sense, the method to be applied to the Ga/Si(112) dimerized overlayer system. How to determine the ground states of the models with nonconvex interactions requires further studies.

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