Phase-field-crystal modelling of the $(2 \times 1)$–$(1 \times 1)$ phase transitions of Si(0 0 1) and Ge(0 0 1) surfaces

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Abstract

We propose a two-dimensional phase-field-crystal model for the $(2 \times 1)$–$(1 \times 1)$ phase transitions of Si(0 0 1) and Ge(0 0 1) surfaces. The dimerization in the $2 \times 1$ phase is described with a phase-field-crystal variable which is determined by solving an evolution equation derived from the free energy. Simulated periodic arrays of the dimerization variable are consistent with scanning tunnelling microscopy images of the two dimerized surfaces. The calculated temperature dependence of the dimerization parameter indicates that normal dimers and broken ones coexist between the temperatures describing the characteristic temperature width of the phase transition, $T_L$ and $T_H$, and a first-order phase transition takes place at a temperature between them. The dimerization over the whole temperature is determined. These results are in agreement with experiment. This phase-field-crystal approach is applicable to phase transitions of other reconstructed surface phases, especially semiconductor $n \times 1$ reconstructed surface phases.

1. Introduction

Semiconductor surfaces are of huge importance, especially in the modern era of nanoscience and nanotechnology. Usually, a bulk terminated surface ($1 \times 1$) is unstable, will undergo a surface reconstruction and become a stable reconstructed surface phase ($m \times n$) [1–3]. Most of the reconstructed surfaces transit to corresponding $1 \times 1$ structures at elevated temperatures. The Si(0 0 1) and Ge(0 0 1) reconstructed surfaces have been extensively studied because they are closely relevant to modern computer technology [4, 5]. For both of them, the reconstruction is realized through the forming of regular arrays of dimers in the top layer ($2 \times 1$ or dimerized phase), which has been confirmed by scanning tunnelling microscopy (STM) experiments [1, 4, 5]. It was shown experimentally [6, 7] that when heated to certain temperatures, the $2 \times 1$ reconstructed surfaces will transit to $1 \times 1$ structures. There were some first-principles calculations for the local atomic configurations of the $2 \times 1$ surfaces [8], but it is controversial even for the essence of the phase transitions [6, 7]. Considering that a structural phase means an averaging of local atomic structures over large enough scales, the reconstructed surface phases need further clarification and the essential physics of the phase transitions are still unknown. A theory that can elucidate the issues is highly desirable.

Phase-field method is a reliable approach to modelling and simulating structural phases and dynamical phase transitions [9, 10]. It has been applied to various fields such as spiral surface growth [11], dendritic growth [12], alloy solidification [13], crystal nucleation [14], step-flow growth [15, 16], epitaxial island growth [17–19] and surface phase transition dynamics [20]. Recently, a phase-field-crystal approach was proposed to model the internal spatial structures of a given phase [21], and periodic lattices were obtained by solving evolution equations derived from the free energies. This powerful approach has been successfully used for natural modelling of elastic interactions [22] and binary alloy solidification [23].

In this paper we propose a phase-field-crystal model for the Si(0 0 1) and Ge(0 0 1) dimerized surface phases and their phase transitions. We use a two-dimensional (2D) phase-field-crystal variable to describe the dimerization of atoms in the top layer and determine the variable by solving an
There are two kinds of (0 0 1) surfaces, type-S\textsubscript{A} and type-S\textsubscript{B}, for both Si and Ge. They appear alternately in the vertical direction, but do not coexist in the same layer in high-quality samples [2–5]. Because the dimerization takes place only in the horizontal direction because there are two top-layer nearest dimers with the same bond length, $\tilde{r}$, in the horizontal or $\bar{x}$ direction because there is no dimerization in the other direction [6, 7]. The phase-field-crystal variable $\phi(\tilde{x}, \tilde{y})$ is periodic in the $\bar{x}$ direction and uniform in the other direction. The key order parameter is the dimerization-induced change in the bond length, $\Delta b$, in the horizontal or $\bar{x}$ direction because there is no dimerization in the other direction [6, 7]. The phase-field-crystal variable $\phi(\tilde{x}, \tilde{y})$ is periodic in the $\bar{x}$ direction and uniform in the other direction. 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we express the free energy (1) and the CH equation as

\[ F = \mathcal{F}_0 \int \Omega \, d\vec{x} \left\{ \frac{\psi}{2} \left[ \varepsilon + \left( 1 + \frac{\partial^2}{\partial x^2} \right)^2 \right] \psi - \frac{u}{4} \psi^4 + \frac{1}{6} \psi^6 \right\} \]

(4)

and

\[ \frac{\partial \psi}{\partial \tau} = \nabla^2 \left\{ \left[ \varepsilon + \left( 1 + \frac{\partial^2}{\partial x^2} \right)^2 \right] \psi - u \psi^3 + \psi^5 \right\} + \zeta. \]

(5)

Now we have only three independent parameters: \( \mathcal{F}_0, \varepsilon \) and \( u \). \( \mathcal{F}_0 \) has the dimension of energy and the other two are dimensionless. They can be expressed in terms of original parameters: \( \mathcal{F}_0 = \lambda q_0^2 / \sqrt{\mu_0}, \varepsilon = a(T - T_L)/q_0^2 = a(T / T_L - 1) \) and \( u = u_\lambda / (q_0^2 \sqrt{\mu_0}) \). The new random variable \( \zeta \) whose average value is also zero is subject to the two-point correlation function

\[ \langle \zeta(\vec{x}, \tau) \zeta(\vec{x}', \tau') \rangle = D \nabla^2 \delta(\vec{x} - \vec{x}') \delta(\tau - \tau') \]

(6)

with \( D = k_B T / \mathcal{F}_0 \). The average value of \( \psi(x, y) \), \( \bar{\psi} \), is conserved by equation (5) and therefore \( \bar{\psi} \) can be taken as an independent parameter.

### 3. Main simulated results and analysis

We solve the dimensionless evolution equation (5) by the difference method. The Laplace operator \( \nabla^2 \) and the second-order differential operator \( \partial^2 / \partial x^2 \) are discretized by the central difference formula as usual, and the time coordinate is discretized using the first-order finite differential approximation. The periodic boundary condition is adopted for all the simulations. The initial condition is subject to Gaussian random fluctuations. We find that resultant equilibrium patterns are independent of the random variable \( \zeta \). We keep \( \bar{\psi} = 0 \) because the high-temperature \( 1 \times 1 \) phase has \( \psi = 0 \). The parameter \( \mathcal{F}_0 \) is not directly relevant to our solving equation (5). We have tried various values for the system sizes and the parameters \( u \) and \( \varepsilon \). We choose approximately 40 periods or 80 surface lattice constants when doing the main simulations, but confirm our results using larger systems. We use \( \delta x = \pi / 16 \) and \( \delta \tau = 10^{-6} \) for space and time increments. The morphology presented in the following is only a part of the whole system.

In figure 2 the periodic morphology of phase-field-crystal variable \( \psi(x, y) \) is shown with the parameters \( u = 0.1 \), \( \varepsilon = -0.005 \) and \( \bar{\psi} = 0 \). The period is equivalent to \( 2\pi \) within an error of \( 10^{-5} \). The centre of the white stripe corresponds to the maximum \( \psi_{\text{max}} \) and that of the black stripe to the minimum \( \psi_{\text{min}} \). This phase-field-crystal simulated dimerization pattern is in agreement with experimental STM images of high-quality Si(0 0 1) and Ge(0 0 1) dimerized surfaces [2–5]. This stripe pattern is obtained for the parameter region 0.002 21 > \( \varepsilon \) > -0.01.

We use \( B = \psi_{\text{max}} - \psi_{\text{min}} \) as our order parameter and present its \( \varepsilon \) dependence for \( u = 1.0 \) and \( u = 0.1 \) in figure 3. It is clear that the phase transition is of first order. The \( B \), as a function of \( \varepsilon \), in the case of \( u = 0.1 \) is ten times smaller than in the case of \( u = 1.0 \). The \( \varepsilon \) width of the phase coexistence region, \( \varepsilon_{\text{HL}} - \varepsilon_{\text{L}} \), is proportional to \( u^2 \). Because \( \varepsilon \) is proportional to \( T - T_L \), the \( \varepsilon \) dependence implies the temperature dependence from zero temperature to \( T_L \) and finally beyond \( T_H \). It is proved using a series of simulated results that \( T_c \) is also proportional to \( u^2 \). Therefore, the parameter \( u \) describes the temperature width of the phase coexistence region. Systematic analysis of simulated results shows that \( \psi \) can be quantitatively described by the function

\[ \psi = \frac{B}{2} \sin \left( \frac{q_0 x}{q_0} \right), \]

(7)
especially in the neighbourhood of the maximum and the minimum. Here $B$ and $q$ are determined by the simulated results. $|q/q_0 - 1|$ can be very small as long as $u$ is small enough. Actually, $q$ is equivalent to $q_0$ within a tiny error less than $10^{-5}$ as long as $u$ is smaller than 0.1.

On the other hand, $B$ and $q$ can be analytically determined by minimizing the free energy (4) in terms of a variational expression $\psi = C \sin(px)$ similar to equation (7). In this way, we derive $p = 1$ and

$$C = \frac{1}{\sqrt{3}} \sqrt{3u + \sqrt{9u^2 - 40\alpha(T/T_L - 1)}}.$$  

This means $q = q_0$. Expression (8) is reasonable only when $T$ is not larger than $T_H$, which implies that $u$ can be expressed as

$$u = \frac{2}{3} \sqrt{10\alpha(T_H - T)/T_L}.$$  

We can obtain an analytical expression of the order parameter $B = 2C$ for $u \leq 0.1$ by requiring that $C$ given by equation (8) is equivalent to $B/2$ obtained by numerically solving equation (5). The phase-transition temperature $T_c$ is given by

$$T_c = \frac{1}{2}T_H + \frac{1}{2}T_L.$$  

Using the relation $\phi = q_0\psi$ (due to $u_b = 1$) and equation (9), we obtain $B = \Delta b/c$ and

$$\Delta b = 2c \sqrt{\frac{8\alpha(T_H - T_L)}{5T_L}} \sqrt{1 + \frac{T_H - T}{T_H - T_L}}.$$  

for $T \leq T_H$ and $B = \Delta b = 0$ for $T > T_H$. This expression determines the temperature dependence of the dimerization-induced change in the bond length, $\Delta b$.

4. Applied to the $(2 \times 1) - (1 \times 1)$ phase transitions of Si(001) and Ge(001)

For the Si(001) and Ge(001) dimerized surfaces, it is relatively easy to measure $T_L$, $T_H$, $c_0$ (zero temperature) and $\Delta b_{RT}$ (room temperature, 300 K). It should be noted that $q = 2\pi/c$, where $c = 2c_0 (c_0 = 2c_{py})$. We use these parameters as input. The parameter $\alpha$ can be determined by substituting $300 \text{K}$ and $\Delta b_{RT}$ for $T$ and $\Delta b$ in equation (11) and then calculating $u$ and $T_c$ in terms of equations (9) and (10). We calculate $u_b$ using the definition $u_b = u_0 q_0^2$ (due to $u_b = 1$). The input and calculated results are summarized in table 1. In figure 4 we present the dimerization parameter $\Delta b$ as a function of temperature for both the Si(001) and the Ge(001) surfaces. It is clear that $\Delta b$ is still finite at $T_c$ and jumps to zero once $T$ is larger than $T_H$.

It should be pointed out that our phase-field-crystal equilibrium patterns, as shown in figure 2, consist of regular arrays of infinitely long dimer chains. These are in agreement with large-scale experimental STM images of the parallel perfect dimer chains in high-quality Si(001) and Ge(001) surfaces [4, 5]. Generally speaking, such a dimer chain can be broken into several segments, but these segments are still completely in the same line [2–7] and can be considered to be an infinitely long dimer chain in the sense of averaging along the line. Actually, there is either type-$S_A$ or type-$S_B$ dimerized phases in high-quality (001) surfaces [4, 5]. Therefore, our phase-field-crystal theory can describe well the experimental regular arrays of dimer chains.

In addition, our simulated results are in agreement with the experimental observation that the dimers still exist above $T_c$ [6], as shown in figure 4. Some of the dimers begin to break at $T_c$ and all of them finally disappear at $T_H$. Between $T_L$ and $T_H$, there is a phase coexistence of the normal dimers and the broken ones, but there is no coexistence of the type-$S_A$ and type-$S_B$ discussed in earlier [25]. This is a clear sign of the first-order phase transition and thus there must be some dimers above the phase transition temperature $T_c$. Naturally, $T_H - T_c$ varies in different samples and can be so small that $T_H$ is equivalent to $T_c$ within the measurement error, which leads to some conclusions that there are no dimers above $T_c$ [7]. Essentially, a structural phase can be judged only when it has a large enough spatial size. Therefore, our modelling and simulated results are not only reasonable but also in agreement with the experiment [6, 7].

5. Conclusion

In summary, we have proposed a two-dimensional phase-field-crystal model for the Si(001) and Ge(001) dimerized systems.
surface phases and their phase transitions to corresponding $1 \times 1$ phases at elevated temperatures. We use a phase-field-crystal variable to describe the dimerization of atoms in the top layer and determine it by solving the evolution equation derived from the free energy. The simulated periodic arrays of dimer chains are consistent with STM images of the Si(0 0 1) and Ge(0 0 1) dimerized surfaces. The calculated temperature dependence of the dimerization parameter shows that normal dimers and broken ones coexist between $T_L$ and $T_H$ and the first-order structural phase transition takes place at $T_c$ in between. These results are in agreement with the experiments. This phase-field-crystal approach can be directly applied to phase transitions of semiconductor $n \times 1$ reconstructed surface phases and should be suitable for other semiconductor reconstructed surfaces and their phase transitions.

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