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Physica E 32 (2006) 207–210
PHYSICA E
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Simulations of germanium epitaxial growth on the silicon (1 0 0) surface incorporating intermixing

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Available online 31 January 2006

Abstract

We present kinetic lattice Monte Carlo simulations of Ge deposition onto a reconstructed Si (1 0 0) surface. We account for the exchange of Ge with Si atoms in the substrate, considering two different exchange mechanisms: a dimer exchange mechanism whereby Ge–Ge dimers on the surface become intermixed with substrate Si atoms, and the exchange of Ge atoms below the surface to relieve misfit strain. We examine how Si–Ge exchange affects the interface between the materials when the growth simulations are done at different temperatures.

PACS: 68.35.Fx; 68.45.Da; 02.70.Lq

Keywords: Kinetic lattice Monte Carlo; Silicon; Germanium; Strain; Surface diffusion

Due to its importance for microelectronic and optoelectronic device applications, gaining a detailed understanding in the processes involved in the expitaxial growth of Ge films on the Si (1 0 0) surface has become a topic of great interest. Both experimental [1–3] and theoretical studies [4,5] have indicated that there is intermixing in the layers adjacent to the interface so that the Si–Ge interface is not generally abrupt. To aid in understanding this phenomenon, we present kinetic lattice Monte Carlo (KLMC) studies of Ge on Si growth that allow intermixing events to take place during the course of growth simulations, which are performed at different temperatures. Two intermixing mechanisms are implemented. The first involves dimer exchange events by which Ge atoms from Ge–Ge surface dimers exchange positions with substrate Si atoms, resulting in the creation of mixed Si–Ge surface dimmers [6–8]. The second involves the exchange of Si and Ge atoms below the surface to relieve misfit strain [5]. As we shall show, this latter mechanism dominates what occurs beyond one monolayer of coverage, and generates a highly non-uniform interface between Ge and Si regions, but with a tendency for Ge and Si atoms to be segregated depending on whether they are under a row or a trough, when they are several layers below the surface.

In the KLMC approach [9], one assumes that each adatom on the surface sits at a lattice site, coincident with a local potential minimum, as shown in Fig. 1(a). The right inset illustrates the potential energy landscape for two adjacent lattice sites, i and j, which are separated by an activation energy B_{ij}. When $B_{ij} \gg k_B T$ (k_B is Boltzmann's constant and T is temperature), the transition rate, r_{ij}^q, of going from site i to site j via a hopping process q is determined by an Arrhenius law:

$$r_{ij}^q = v_q \exp(-B_{ij}^q/k_B T). \quad (1)$$

The prefactor, v_q, represents the attempt frequency for hopping process q. Besides the intermixing events mentioned above, diffusion processes such as adatom and ad-dimer hopping are also included. Periodic boundary conditions are imposed, so any adatom or ad-dimer diffusing across a boundary is reinserted on the opposite end of the simulated domain as shown in Fig. 1(a). The computer program itself is implemented in FORTRAN 90 on a Windows XP workstation and was adapted from the publicly available AWL (Adams–Wang–Li) simulator

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doi:10.1016/j.physe.2005.12.037

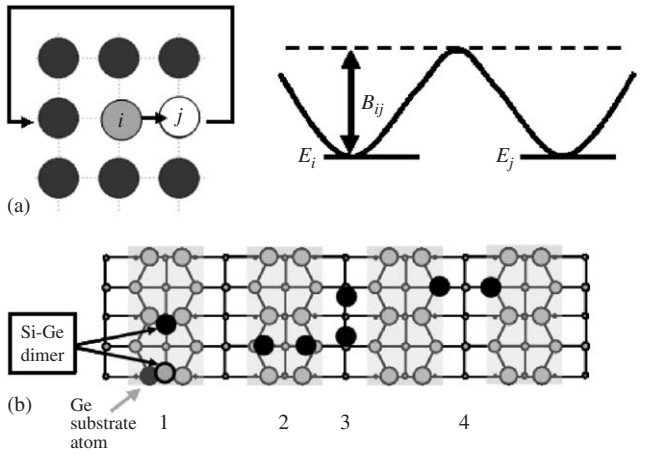

Fig. 1. (a) The energy barrier, B_{ij}, an adatom at site i must overcome in order to hop to site j as shown in the left inset. (b) The reconstructed Si (1 0 0) surface. Atoms closer to the surface are larger. The shaded bars indicate dimer rows, while unshaded regions are troughs. The four principle ad-dimer configurations on the Si (1 0 0) surface are indicated with one depicted as a mixed Si–Ge dimer, where a Ge atom has exchanged places.

(http://ceaspub.eas.asu.edu/cms/research/klmc.zip), originally developed to study growth of metallic films [10].

The reconstruction [11] that the Si (1 0 0) surface undergoes to attain a configuration, which minimizes the overall surface energy effects diffusion on the surface. In reconstruction, the surface atoms dimerize to reduce the number of dangling bonds while dimer buckling reduces surface stress. The resulting change in translational symmetry yields the well known 2×1 structure, which consists of rows of dimers separated by troughs, as illustrated in Fig. 1(b). It has been found that the diffusion across a reconstructed surface is anisotropic [12], with activation energies for adatoms depending on whether the diffusion is $\perp$ or $\parallel$ to the dimer rows and for ad-dimers on whether the dimers are moving over the surface dimer rows or in the troughs [13–16]. Fig. 1(b) also shows the main four configurations that ad-dimers are thought to occupy on the reconstructed Si (1 0 0) surface [13]. Ad-dimer's #1 and #2 are vertically and horizontally aligned, respectively, along dimer rows. Ad-dimer's #3 and #4 are in troughs. Besides hopping $\perp$ or $\parallel$ to the rows/troughs, the ad-dimers can also rotate, so that an ad-dimer in configuration #1 can make a transition to #2 and #3 can become #4. This kind of information regarding ad-dimer and adatom motion events must be included in any meaningful KLMC simulation of the Si (1 0 0) surface and is something we have incorporated in previous KLMC studies [17–19].

For Ge adatom motion parallel to the rows and troughs, we use $B_{\parallel}=0.62\,\text{eV}$ for the activation energy, a number computed in an ab initio study of Ge on Si by Ko et al. [4]. For perpendicular motion, we use $B_{\perp}=1.0\,\text{eV}$, a number suggested by the work of Mo et al. [12] on Si adatoms which we adopt for Ge. When adatoms meet, we allowed them to dimerize automatically, neglecting the energy required to form them, which are negligible compared to the activation energies of the other diffusion processes. Another type of event that is allowed to occur automatically is relaxation of adatoms from upper layer sites on a step edge to available sites on a lower layer.

In atom-tracking STM experiments [7] performed in situations where the Ge coverage was low, "rocking" ad-dimers were observed, which were determined to be a Si–Ge combination (the Ge atom sits further away from the substrate than the Si, making the rotation of mixed ad-dimers more observable). Ab initio calculations [20] have shown that mixed dimer formation, with the Si coming from the substrate, occurs with a very low activation energy, 0.1 eV, which is even lower than for Ge–Ge ad-dimer formation. A mixed dimer is illustrated in Fig. 1(b). In our KLMC simulations, the additional transition from Ge–Ge to a Si–Ge dimer via this exchange mechanism is made automatically, so that when two diffusing Ge adatoms meet each other on the Si (1 0 0) surface, the result is always a Si–Ge dimer.

Using the STM determined values [7] for the Ge–Si dimers, we fixed $B^{\text{d}}_{\text{rot}}=0.82\,\text{eV}$ for dimer rotation and $B^{\text{d}}_{\text{row}}=1.01\,\text{eV}$ for dimer hopping motion along a row (this is equivelant to ad-dimer #2 moving vertically in Fig. 1 (b)) with respective attempt frequencies $\nu_{\text{rot}}=7.94\times10^{12}\,\text{Hz}$ and $\nu_{\text{row}}=1\times10^{14}\,\text{Hz}$. We have used $B^{\text{d}}_{\text{trough}}=1.21\,\text{eV}$ for dimer hopping motion along a trough (ad-dimer #4 moving vertically), and $B^{\text{d}}_{\text{jump}}=1.36\,\text{eV}$ for dimer hops between the row and trough (dimers jumping back and forth from configurations #1 to #3 and from #2 to #4), with an attempt frequency $\nu=1.58\times10^{13}\,\text{Hz}$ used in both cases. The $B^{\text{d}}_{\text{trough}}$ and $B^{\text{d}}_{\text{jump}}$ numbers come from STM measurements made by Borovsky et al. [14] on Si–Si ad-dimers, which we apply to Si–Ge ad-dimers with the expectation that their behavior is not radically different.

The role of intermixing to relieve misfit strain at a Ge–Si interface has been studied by Nurminen et al. [5] using a periodic slab geometry. In that paper, values of the energy cost of substituting a Ge atom with Si atom in different sites near the Si (1 0 0) interface were tabulated. Regardless of the method of calculation, it was found that there was a dependence on whether the site was situated at a row or a trough. Also crucial was the number of layers away from the initial interface that the Ge atom was. For our simulations, the barriers we have adopted are $B_{\text{row}}(1)=0.314\,\text{eV}$, $B_{\text{row}}(2)=0.361\,\text{eV}$, $B_{\text{trough}}(2)=0.292\,\text{eV}$, $B_{\text{row}}(3)=0.344\,\text{eV}$ and $B_{\text{trough}}(3)=0.291\,\text{eV}$ (the numbers in brackets refer to the depth below the upper surface). Note the smaller barriers for the greater depths. These are from the LDA results in [5]. An important distinction between their simulations and ours is that they begin with three *complete* monolayers of Ge. In contrast, since we perform growth simulations, the height in monolayers can vary significantly at each position as a function of time and so which Si–Ge exchange barrier is