Kinetic Monte Carlo Simulations of Germanium Epitaxial Growth on Silicon

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Due to its importance for microelectronic and optoelectronic device applications, there is great interest in gaining a detailed understanding in the processes involved in the epitaxial growth of Ge films and structures such as quantum dots and wires on the Si surface. Experimentally, a technique known as "atom tracking" has been employed using scanning tunneling microscopes to study the diffusion of Ge adatoms and ad-dimers [1-3]. The information about the surface kinetics extracted from these measurements provide a starting point for meaningful Kinetic Lattice Monte Carlo (KLMC) simulations, which we have implemented. As shown in Fig. 1, in this approach, atoms sit at discrete lattice sites in potential wells. The rate of hopping from site to site via a mechanism q is governed by an Arrhenius law, $r_q = \nu_q \exp(-B_{ij}/k_bT)$, where ν_q is the attempt frequency. In our simulations, we also take into account the effects of surface reconstruction on the Si (100) surface. As shown in Fig. 2, this leads to the formation of rows and troughs which lead to anisotropy in the barriers for adatom and ad-dimer motion.

Importantly, 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. We have used two inter-mixing mechanisms to account for this in our simulator. The first, illustrated in Fig. 3, is the dimer exchange mechanism, whereby Ge-Ge ad-dimers become Si-Ge ad-dimers when Si atoms are promoted from the substrate. The second involves the exchange of Si and Ge atoms below the surface to relieve misfit strain [5], which 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.

One method of controlling what structures result from the growth process is to use a pre-patterned substrate (see, for example, Ref. [7]). We shall present the results of simulations on patterned substrates. An example is shown in Fig. 4, where the starting surface features a grid pattern. Here, the indentation is only 3 atomic layers deep with step edges. As shown in Figs. 5 and 6, our KLMC simulations in this case yield growth upon the surface, rather than in the pits. This gives Ge-Si stripes, that result largely from the anisotropy generated from the surface reconstruction. Some growth in the pits also occurs, but the major effect is on the surface.

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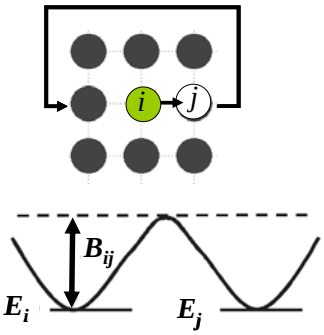

Fig. 1 In the KLMC approach, each adatom on the surface sits at a lattice site, coincident with a local potential minimum, as shown above. The bottom inset illustrates the potential energy landscape for two adjacent lattice sites, i and j, which are separated by an activation energy B_{ij}. When $B_{ij} >> k_BT$ (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 process q is determined by an Arrhenius law.

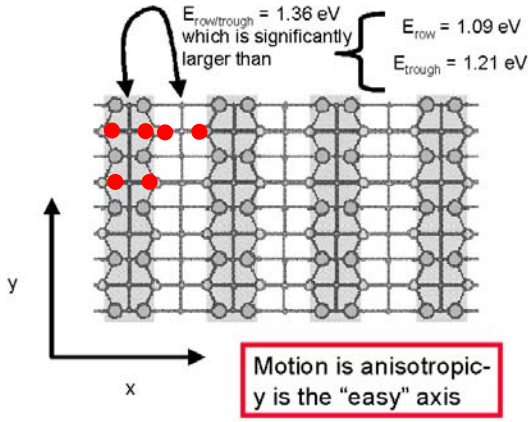

Fig. 2 The A top view of the reconstructed Si (100) surface. The diffusion of adatoms and ad-dimers across the reconstructed surface is anisotropic, with activation energies depending on whether the diffusion is ⊥ or ∥ to the dimer rows.

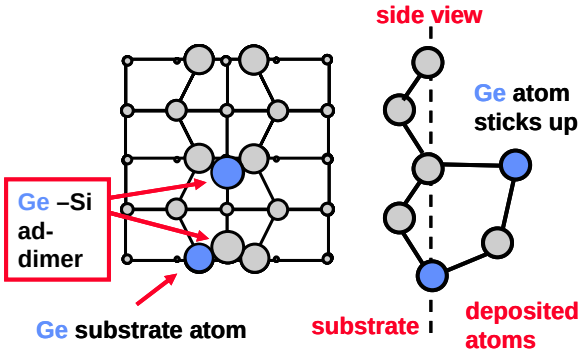

Fig. 3 Illustration of the surface dimer exchange mechanism. When two Ge adatoms meet on the surface, they form a dimer. However, it then becomes energetically favorable for one Ge atom to exchange places with a Si atom in the the substrate, resulting in a mixed dimer on the surface.

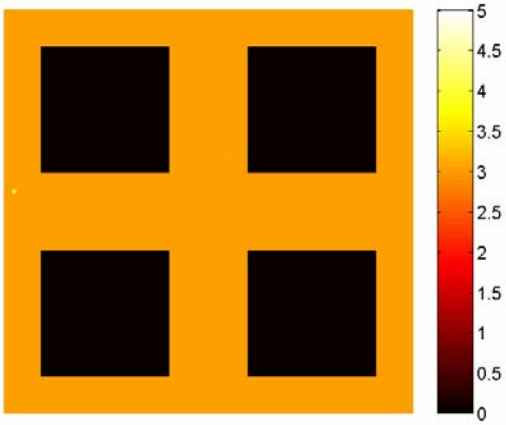

Fig. 4 The Si surface after a single Ge adatom has been deposited. Color indicates the number of atomic layers. The initial substrate has been patterned so that there is a Si grid, three atomic layers high and square voids.

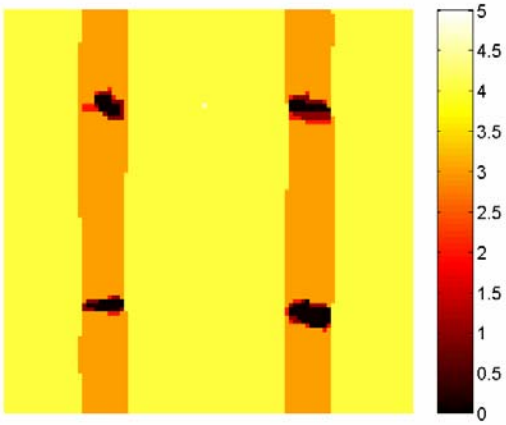

Fig. 5 As above, but after after two monolayers of Ge have been deposited at 470 K. The initial grid combined with the anistropic hopping barriers have led to the formation of Ge/Si stripes on the surface.

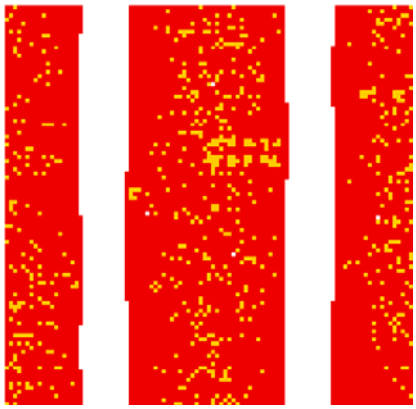

Fig. 6 The fourth atomic layer after deposition, with red corresponding to where there are Ge atoms and orange to Si. The Si atoms have been promoted from the substrate mainly via the exchange mechanism illustrated in Fig. 3.