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Monte Carlo simulation of growth and recovery of silicon

Saulius Keršulis, Vladimir Mitin*

Department of Electrical and Computer Engineering, Wayne State University, Detroit, MI 48202, USA

Abstract

We report on the results of Monte Carlo (MC) simulation of epitaxial growth dynamics of Si(001). We propose an MC model which allows the formation of bulk vacancies and overhangs in the tetrahedral lattice structure of silicon. The surface relaxation (dimerization) as well as atom–atom interactions extending as far out as second-neighbor sites are included in the model. Our results demonstrate that the effect of the formation of vacant sites is pronounced only at low temperatures ($T = 500$–700 K) where there is no active hopping of atoms. At high temperatures ($T > 800$ K) this effect is washed out by intensive hopping of atoms. We found that in the temperature range 700–800 K growth mode changes from rough three-dimensional growth to smooth two-dimensional growth. Simulation of silicon recovery after interuption of growth showed that there are two different mechanisms of recovery. At low temperatures ($T = 500$–600 K) the recovery of the crystal surface is provided by the hopping of surface atoms residing in the vicinity of vacant sites. At high temperatures ($T > 700$ K) it is caused by the hopping of bulk atoms.

Keywords: Monte Carlo models; Molecular beam epitaxy; Silicon

1. Introduction

Two Monte Carlo (MC) models simulating the growth of silicon have been developed. The most popular is the solid-on-solid (SOS) model [1]. In this model an atom is accommodated on the lattice site only if there is already an atom underneath that site. In this way columns of atoms are grown where vacancies or overhangs are forbidden. However, vacancies and overhangs are present in real crystals, especially during growth at low temperatures. The other MC model which improves on the SOS approximation by allowing for bulk vacancies and overhangs was proposed by Marmorkos and Das Sarma (MS) [2,3]. Most papers published on silicon growth simulation have been based on the SOS model [4–9]. To our knowledge there are only two papers [2,3] devoted to MC simulation of crystal growth using the MS model.

In this work we extended the MS model including the possibility of the formation of bulk vacancies and overhangs in the real tetrahedral structure of silicon. Surface dimerization as well as atom–atom interactions out to second-nearest neighbors were taken into account. Applying our MC simulation technique we revealed the effect of allowing for the formation of bulk vacancies on the quality of growing silicon crystal.

2. The model

Fig. 1(a) shows a fragment of the tetrahedral lattice structure of silicon. In the SOS model, an impinging atom is accommodated at the lattice site A (Fig. 1(b)) only if both nearest neighbors (B and C) are present in the layer below.

In our model we allow an impinging atom to reside at the lattice site A if two conditions are satisfied. First, there is at least one nearest-neighbor atom (B or C) in the layer below (B in this particular case). Second, there is at least one undimerized second-nearest neighbor in the same layer (E or D). If these two conditions are satisfied the impinging atom resides at the lattice site A and forms a dimer with one of the second-nearest neighbors (E or D). If both lattice sites E and D are occupied, the "partner" for atom A to form a dimer is chosen randomly.

We simulated a monoatomic system where the atoms were deposited onto the (001) plane (taken to be the xy plane with the z direction as the growth direction in Fig. 1) of the tetrahedral structure. Incorporation of this structure and the surface reconstruction was very

*Corresponding author; Telephone (313)-993-7651; Fax (313)-577-1101; e-mail mitin@ece6.eng.wayne.edu.

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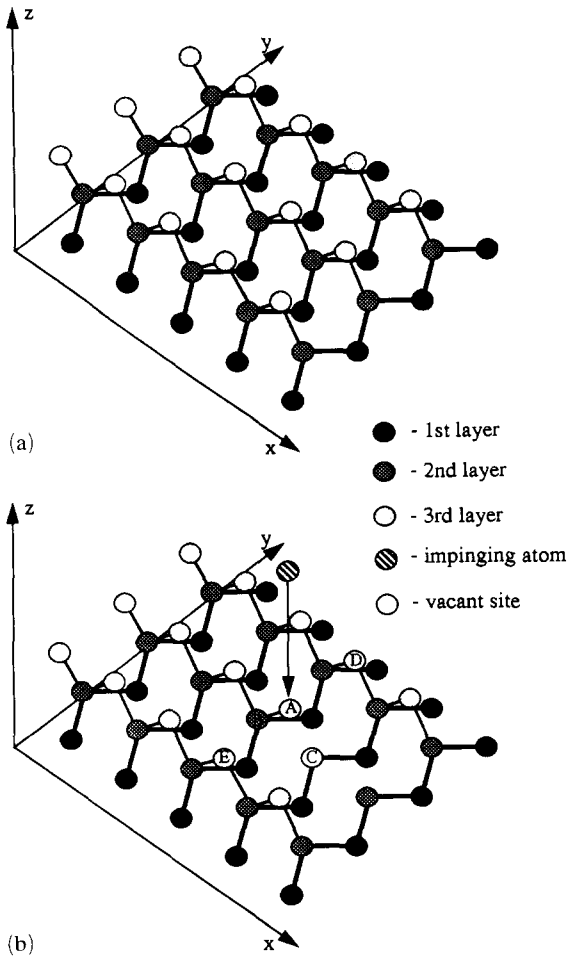

Fig. 1. (a) Fragment of the tetrahedral lattice structure of silicon; (b) process of deposition of an atom within the framework of our model allowing the formation of vacancies and overhangs. The impinging atom can be accommodated at site A even if there is no nearest neighbor at site C in the layer underneath site A.

similar to that proposed in [8]. Periodic-boundary conditions on the (001) plane were imposed and growth took place on a substrate of similar atoms with the same lattice structure.

The complexity of four kinetic processes taking part in the growth dynamics (deposition of the atom on the surface, migration of this atom on the surface, evaporation of deposited atoms from the surface, and surface relaxation) was simulated using the Arrhenius rate equation for each of these processes: $R = R_0 \exp[-(n_1 E_1 + n_2 E_2)/kT]$, where n_1 and n_2 are the number of first- and second-nearest neighbors, E_1 and E_2 are the first- and second-nearest neighbor interaction energies respectively. Numerical values used for simulation of the hopping event were chosen to be $E_1 = 0.6$ eV, $E_2 = 0.1$ eV, which are consistent with the experimental data [10,11]. Energy terms for the evaporation event were taken to be $E_1 = 1.1$ eV, $E_2 = 0.2$ eV. The pre-exponential hopping rate or hopping attempt frequency R_0 was assumed to be $R_0 = 10^{13}$ s^{-1}. The surface reconstruction process was simulated in a method analogous to that used in [8].

The MC algorithm used was similar to the fast molecular beam epitaxy growth algorithm of Maksym [12]. According to this algorithm the time, type, and site of each of the four events mentioned above are chosen randomly with a probability of occurrence that depends on the kinetic rates for the individual events at each lattice site.

3. Results

We applied our MC model presented in Section 2 to study the effect of vacancies and overhangs on the kinetics of the growth of silicon layers. Most of the results presented here are for a 80×80 lattice with typically ten layers grown on the substrate. Most of our results are means of ten simulations run using different random number sets. For a given deposition rate (impinging flux density) of 1 monolayer per second (i.e. deposition rate 6400 atoms per second for a 80×80 lattice) we changed the substrate temperature from 500 K to 900 K and compared the results obtained by our MC technique and the SOS model.

In Figs. 2 and 3 we show simulated dynamic growth profiles of layer coverages, number of vacant sites (i.e. lattice sites, which are forbidden in the SOS model, normalized to the number of deposited atoms) as well as surface roughness for substrate temperatures of 600 K and 800 K respectively. The surface roughness Δ was defined as the root mean square deviation in the surface height, $\Delta = \langle\langle h_i - \langle h \rangle\rangle^2\rangle^{1/2}$, where h_i is the height of the ith column of the system and averaging was done over all lattice sites i.

It follows from Fig. 2 that growth at $T = 600$ K is rough as indicated by the roughness Δ which increases with time (Fig. 2(b)) according to both our and the SOS model. The reason for this rough growth of silicon is that the temperature is low enough to "keep" deposited atoms in the very first lattice site reached during the deposition process. The difference in Δ obtained by the two different models is caused by the presence of vacant sites in growing silicon (Fig. 2(a)) which are allowed by our MC technique but forbidden in the SOS model. The temporal evolution of layer coverages depicted in Fig. 2(c) also indicates rough growth with many (5–6) layers growing together at the same time and the effect of allowing the formation of vacant sites.

The results of the simulations at $T = 700$ K were close to those at $T = 600$ K.

Growth at $T = 800$ K, as can be seen from Fig. 3, is intermediate between the rough three-dimensional

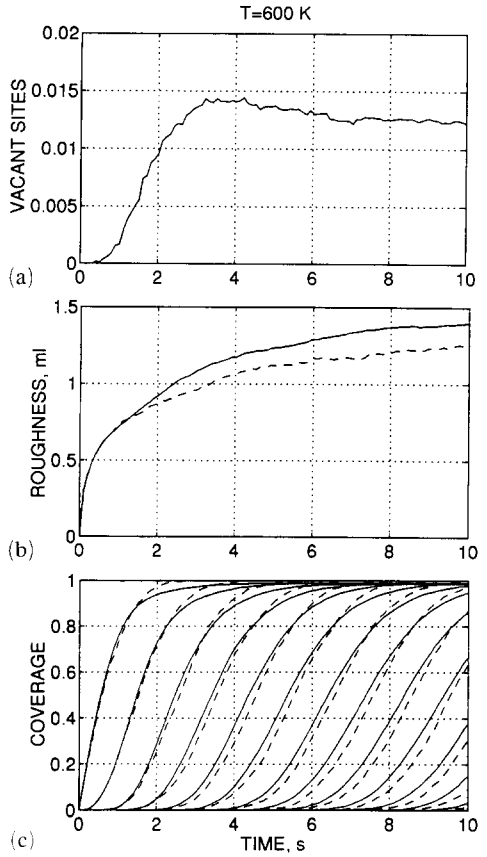

Fig. 2. The temporal evolution of the number of vacant sites (a), surface roughness (b), and coverage (c) during deposition of 10 monolayers of Si at $R_d = 1$ monolayer per second and $T = 600$ K. Solid lines in (b) and (c) represent the results of calculations using our model allowing for vacancies; the dashed lines are the results of simulations using the SOS model.

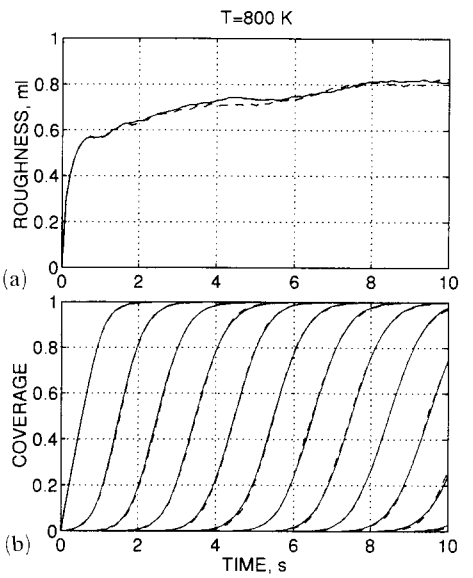

Fig. 3. The temporal evolution of the surface roughness (a) and coverage (b) during deposition of 10 monolayers of Si at $R_d = 1$ monolayer per second and $T = 800$ K. Solid lines represent the results of calculations using our model allowing for vacancies; the dashed lines are the results of simulations using the SOS model.

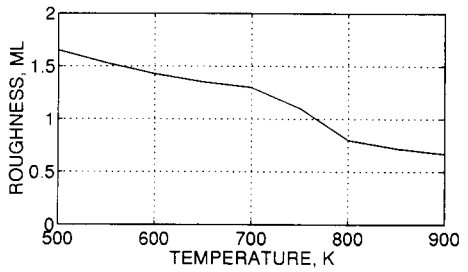

Fig. 4. The dependence of surface roughness on temperature after deposition of 10 monolayers.

growth and epitaxial layer-by-layer growth. From Fig. 3(a) we can see that the surface roughness Δ tends to saturation with time, reaching value $\Delta = 0.8$ at $t = 10$ s. However, at the very beginning of growth ($t = 1$ s) at least one temporal oscillation in Δ can be detected which indicates the tendency to two-dimensional layer-by-layer growth. It should be pointed out also that there is no difference between the results obtained by our model and the SOS model at this temperature. The temporal evolutions of Δ and surface coverage (Figs. 3(a) and 3(b)) coincide for both models at $T = 800$ K. The reason for this is the absence of vacant sites in the growing material simulated within the framework of our model, because the temperature ($T = 800$ K) is high enough to provide intensive hopping of atoms from one site to another. Owing to the fact that atoms accommodated in the vicinity of vacant sites have fewer first- or second-nearest neighbors, their hopping kinetic rate is higher, so they are the most "active"; they leave their sites and occupy vacant sites very quickly.

The simulation of growth at $T = 900$ K gave results close to those at $T = 800$ K.

The dependence of surface roughness on the temperature is shown in Fig. 4. It is clearly seen from this figure that in the temperature range from $T = 700$ K to $T = 800$ K the growth mode changes from rough three-dimensional growth to smooth two-dimensional growth, which is in good agreement with experimental data [13,14].

As a second set of investigations the effect of recovery after the interrruption of growth on the quality of growing silicon crystal was studied. The growth was interrupted at time $t = 10$ s and the system was allowed to recover during the next 10 s.

The results of simulations in the range of temperatures $T = 500$–900 K are presented in Fig. 5. Fig. 5(a)

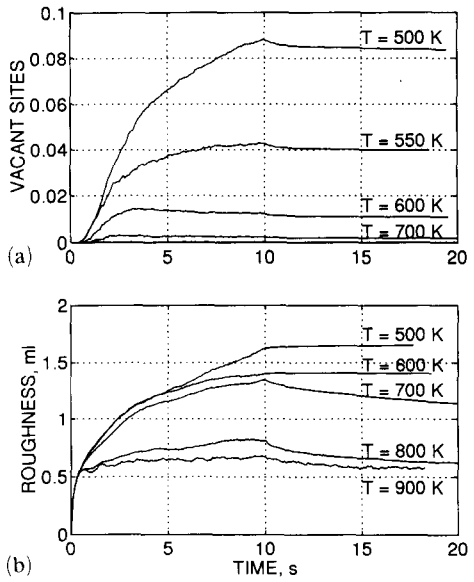

Fig. 5. The temporal evolution of the number of vacant sites (a) and roughness (b) during growth ($t < 10$ s) and recovery ($t > 10$ s) at different substrate temperatures.

shows the evolution of the number of vacant sites at different temperatures. It can be seen from this picture that the temperature $T = 700$ K is the critical temperature for the formation of vacant sites in the crystal. Above this temperature the possibility of the formation of vacant sites is eliminated by the intensive hopping of atoms. The interesting feature of the evolution of the number of vacant sites after interruption of growth is that it occurs in two stages. The first is the regime of fast recovery of vacant sites during approximately 1 s provided by the hopping of surface atoms having the smallest number of neighbors in the vicinity of vacant site. The second stage of evolution is a slow relaxation due to the rare hopping of bulk atoms.

The temporal evolution of surface roughness at different temperatures is depicted in Fig. 5(b). It can be seen from this figure that the growth during the first 10 s before growth interruption is the same in the whole range $T = 500$–700 K. After growth interruption the roughness does not change at temperatures $T = 500$ and $T = 600$ K while at $T = 700$ K there is a clear manifestation of decreasing Δ. That means that $T = 700$ K is critical for the mechanism which provides the recovery of the crystal surface. At $T = 700$ K and higher the recovery of the surface is caused by hopping of bulk atoms while at $T = 500$ and $T = 600$ K the recovery is the result of hopping of surface atoms with the smallest number of neighbors.

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