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Full Length Article

Kinetic Monte Carlo study on the evolution of silicon surface roughness under hydrogen thermal treatment

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ABSTRACT

The evolution of a two-dimensional silicon surface under hydrogen thermal treatment is studied by kinetic Monte Carlo simulations, focusing on the dependence of the migration behaviors of surface atoms on both the temperature and hydrogen pressure. We adopt different activation energies to analyze the influence of hydrogen pressure on the evolution of surface morphology at high temperatures. The reduction in surface roughness is divided into two stages, both exhibiting exponential dependence on the equilibrium time. Our results indicate that a high hydrogen pressure is conducive to obtaining optimized surfaces, as a strategy in the applications of three-dimensional devices.

Silicon Fin field-effect transistors (FinFETs) and gate-all-around (GAA) FETs have attracted great interest in integrated circuit industry because they offer continuous scaling. In the device fabrication process, however, the rough surfaces of channels generated by plasma dry etching or chemical wet etching severely degrade carrier transport performance [1–4]. Therefore, many efforts have been made to reduce surface roughness [5,6]. Notably, hydrogen thermal treatment is highly useful for reducing sidewall roughness [7] and improving carrier mobility and reliability because surface roughness scattering limits the transport of FinFETs and GAAFETs [8,9]. It was reported that the saturation current for n-type FinFETs was increased by about 30%, and the low-frequency noise level was decreased in the drain current range, by the smoothing of sidewall surfaces during hydrogen thermal treatment [10]. It has also been found that the gate leakage current of FinFETs was reduced by about four-orders of magnitude after hydrogen thermal treatment [11,12]. All of these results are attributable to the surface diffusion mechanism during the hydrogen thermal treatment process [13,14], which substantially improves the surface morphology of FinFET channels. Various studies have shown that the surface atom migration and roughness reduction are governed substantially by the interactions between silicon and hydrogen, which depend on the thermal treatment conditions, such as temperature, hydrogen pressure, and initial surface roughness. Evidently, a deep understanding of the surface diffusion process of silicon atoms under hydrogen thermal treatment is crucial for device applications.

In addition to experimental work on the evolution of surface morphology [15,16], various theoretical methods have been developed to investigate the migration of surface atoms at the molecular or atomic level. For example, the continuous theory of surface diffusion has been applied to describe the evolution of periodic surface structures [17]. The kinetic Monte Carlo (KMC) method has been used to analyze the migration behavior of surface atoms without considering the crystal orientation, as well as the evolution of surface morphology [18]. In this letter, the KMC method is adopted to investigate the evolution of surface morphology for crystalline silicon under hydrogen thermal treatment, focusing on the dependence of the migration behaviors of surface atoms on both the temperature and hydrogen pressure. The surface roughness can be reduced, yielding atomically smooth surfaces, by optimizing the process of hydrogen thermal treatment.

A two-dimensional triangular lattice is used to model the atomic arrangement of crystalline silicon (Fig. 1a). The two-dimensional model in this work is taken as the corresponding equivalent simplified model for crystalline silicon. The highest and lowest rows on the vertical axis are the boundaries of the two-dimensional system, and atoms are forbidden to migrate to these sites. The sites of the triangular lattice have two possible states: a site may be empty (no atom present), or it may be occupied by an atom. Each site has from zero to six neighboring sites. For crystalline silicon, each surface atom in a column *j* occupies the highest site in that column. Therefore, the silicon surface is morphologically characterized by the

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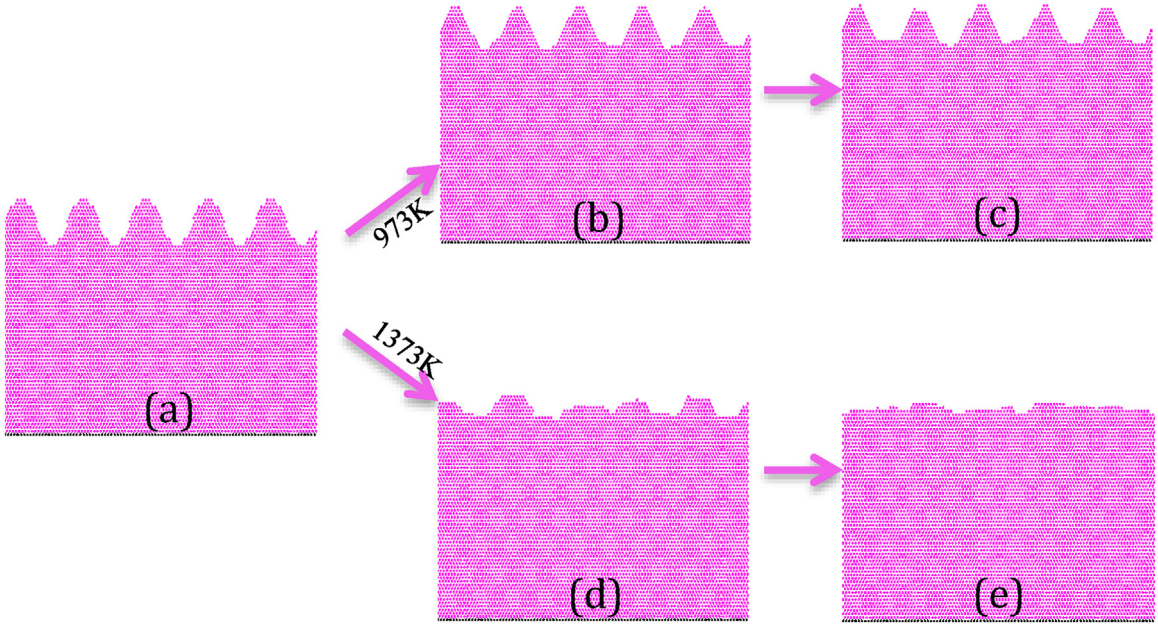

Fig. 1. Schematic views of surface structures in KMC simulation. (a) Initial surface configuration of crystalline silicon. (b) and (c) surface shapes after 1000 and 5000 MCS, respectively, during kinetic evolution at a temperature of 973 K. (d) and (e) surface shapes after 1000 and 5000 MCS, respectively, during kinetic evolution at a temperature of 1373 K.

surface roughness R_q, expressed as the root-mean-square roughness,

$$R_q = \sqrt{\frac{1}{N}\sum_{i=1}^{N}\left[h_i(t) - \bar{h}(t)\right]^2} \quad (1)$$

where $\bar{h}(t) = 1/N\sum_{i=1}^{N} h_i(t)$, $h_i(t)$ is the highest site in column j on the specific surface structure, and the surface roughness is represented by a lattice constant (a), i.e., a unit of length.

In the present simulation, an atom in the j^{th} vertical and k^{th} horizontal axis can jump to a neighboring site, assuming that it is empty. An atom with six neighboring sites cannot jump because the sites have all been occupied. Surface diffusion is the main mechanism driving the evolution of the surface morphology during thermal treatment. Therefore, only surface atoms can migrate in the present KMC model. The initial surface structure can evolve continuously because of the surface diffusion currents. The jump probability J for a surface atom with n_i neighbors is given by

$$J = \nu exp(-n_i E_{act}/k_b T) \quad (2)$$

where we take $\nu = 8.4 \times 10^{13}$ Hz for the Debye frequency, k_b is the Boltzmann constant, T is the thermal treatment temperature, and $n_i E_{act}$ is the activation energy of neighboring site n_i. The jump probability from the surface site to its empty neighbors is first calculated by Eq. (2) in the present KMC model. Then, a randomly chosen jump event is either executed or not according to its calculated jump probability. The surface system will be updated if the jump event has occurred. The iteration of the main loop starts again if the convergence criteria are not satisfied. The surface structure continues to evolve owing to the migration behavior of surface atoms. The simulation ends when the surface roughness reaches a steady state in the system.

The effective activation energy E_{act} in Eq. (2) is a critical parameter to describe the surface evolution process. It determines the jump probability of surface atoms in a diffusion event. In fact, the surface species are not only silicon atoms but SiH_x radicals, including surface monohydride, dihydride, and trihydride species [19]. The activation energy for SiH_3 radicals has been estimated in the range from 0.18 to 0.89 eV on hydrogenated amorphous silicon surfaces according to density functional theory calculations [20], and as 0.4 eV for nearest neighbors by pseudopotential calculations [21]. The effective activation energy for a hydrogen-covered surface is generally higher than that for a bare silicon surface, because hydrogen atoms saturate the silicon dangling bonds and transfer easily to the bond-center sites [22]. Given that the hydrogen pressure affects the jump probability of surface species in thermal treatment experiments, and taking into account previous density functional theory and molecular dynamics simulation results, we adopt three activation energies in our numerical calculations. These three energies represent relatively low, intermediate, and high pressures of ambient hydrogen, respectively.

Fig. 1 shows the evolution of the surface morphologies at the temperatures of 973 and 1373 K with the corresponding number of Monte Carlo steps (MCS). Here, the initial silicon surface is described by a sinusoidal function as shown in Fig. 1(a). The effective energy is set to 0.6 eV, corresponding to a hydrogen pressure range of 10–100 Torr. At 973 K, Fig. 1(b) shows that the surface structure has a local triangular shape and the average number of neighbors is almost four, except at edges and angular points on the surface, for all numbers of MCS (i.e., throughout the simulations). Furthermore, the presence of triangular structures makes it difficult to transfer silicon atoms from high-index planes (the sides of the triangle) to low-index planes (the bottom of the surface valley). Clearly, the local triangular shape on the silicon surface can be sustained for a long time at a low temperature, as shown in Fig. 1(c). As shown in Fig. 1(d), as the temperature increases to 1373 K, the initial surface morphology rapidly changes. This indicates that the surface atoms have a relatively high mobility, enabling them to rearrange the triangular structure and obtain a smooth surface.

Fig. 2 shows the relationship between the surface roughness and the number of MCS at different thermal treatment temperatures. The surface roughness decreases slowly at the temperatures of 973 and 1073 K, indicating that the surface structure is still rough. At the temperature of 1273 and 1373 K, the surface almost reaches equilibrium and can be approximated to an atomically smooth