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A new Si tetramer structure on Si (001)

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ABSTRACT

Interactions between Si ad-dimers on Si (001) have been studied by molecular dynamics simulations using the Stillinger–Weber potential. The interactions determine the formation of clusters from diffusing dimers. We show different pathways for the formation of multiple-dimer clusters and propose a new tetramer (T_{CC}) structure formation by two diffusing dimers interacting. This tetramer structure has been found to be energetically stable with respect to isolated ad-dimers. Moreover, their local bonding configuration is very similar to the B-type step edge which is known to be the favoured adsorption site for epitaxial growth. The proposed tetramer may play a crucial role as the nucleus of the new epitaxial layer on Si (001).

1. Introduction

It is extremely important to understand the initial processes in homoepitaxy growth on Si (001) surface, such as adatom diffusion, nucleation processes, and island formation mechanisms, because those processes critically determine the surface morphologies during growth and thus the quality of the thin-films. The properties of the dynamical interactions of isolated Si ad-dimer with this surface have been studied extensively theoretically and experimentally. A large amount of information about the statics and diffusion of adatoms and ad-dimers on Si (001) is well known.

Many reports predicted theoretically [1–3] and confirmed experimentally [4–6] the adatom mobility to be so high that scanning tunneling microscopy (STM) measurements cannot reveal isolated adatoms at room temperature. Highly mobile Si adatoms quickly combine to form dimers [7,8], since ad-dimer formation requires no energy barrier beyond that of adatoms diffusion. Since ad-dimers are relatively immobile, researchers can investigate the kinetic and dynamics behavior of ad-dimers by scanning tunneling microscopy (STM) at room temperature. Si ad-dimers also have recently been the subject of careful studies because of interesting phenomena, such as ad-dimer rotations [9–13], ad-dimer diffusions [14–21]. In spite of these researches on initial process of Si homoepitaxial growth on Si (001) surface, many fundamental questions remain not clear. Among them are how ad-dimers form bigger clusters and epitaxial layers.

Recently, Raj Ganesh S. Pala and Feng Liu [22] introduced a new concept of "critical epinucleation". By performing first-principle calculations, they proposed, for Si (001) homoepitaxy, the most stable "critical epinucleus" (CEN) consists of six adatoms (three ad-dimers) that have the correct epiconfiguration, whereas single ad-dimer is the critical classical nucleus (CCN). Then, how ad-dimers translate into the stable "critical epinucleus" (CEN). Do intermediate structures exist? In the process of formation of larger clusters from diffusing dimers, the dynamic behavior of ad-dimers and especially the interactions between them are crucial and play an important role. van Dam et al. [7] observed first interactions between ad-dimers using scanning tunneling microscopy (STM). They showed that the interaction of two dimers on top of two neighboring substrate dimer rows can yield two different tetramers. However, a little theoretical studies focus on this issue.

In this paper, using the Stillinger–Weber potential [23], we will study the interaction between two Si adsorbed dimers on the Si (001) by molecular dynamics simulations. If two ad-dimers happen to arrive next to each other, dimer–dimer interactions can cause the formation of a cluster. The formation of clusters from diffusing dimers cannot be observed directly using scanning tunneling microscopy (STM) at room temperature, because the dimer diffusion is negligible. Finite temperature molecular dynamics (MD) simulations are very helpful to study the interactions of diffusing dimers, as they allow following the ad-dimers on the surface. To facilitate the discussion, we first introduce the notations. Experimental and

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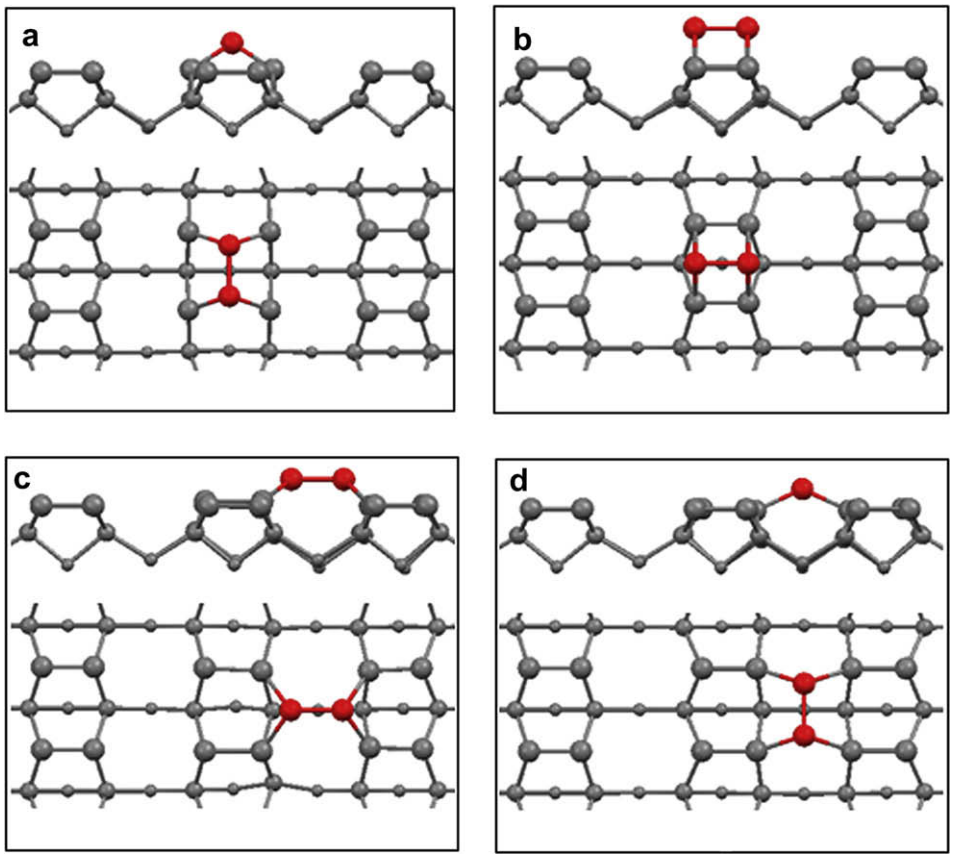

Fig. 1. Four different Si adsorbed dimer configurations on Si (001). The top of each of picture is the side view and the bottom is the top view. Black circles represent the substrate atoms and red circles represent ad-atoms. The following figures are presented in the same way. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.).

theoretical evidences suggest that four principal dimer configurations on Si (001). As shown in Fig. 1, a dimer can sit on top of a dimer row (A and B) or in the trench between two dimer rows (C and D), with its axis oriented either parallel or perpendicular to the dimer row direction. Next, we will describe the interactions between these adsorbed dimers on Si (001). It will turn out that these elementary interactions of ad-dimers are useful to understand the more complex transitions in multiple-dimer clusters. It enables us not only to determine the structures, it also gives insight about how they are formed. It is shown that the interactions of two ad-dimers on Si (001) can yield different tetramers.

2. Theoretical details

Simulations were performed using Stillinger–Weber semi-empirical potential [23]. Although the potential is semiempirical, it can give out better results about some properties of bulk silicon and Si (001) surface [1,9,23,24]. The Si (001)-(2×1) surface was modeled with a slab containing 1664 atoms, 13 layers of 128 atoms each. We have determined that the finite cluster size does not affect the relative energies. We chose the x-axis to be along the [110] direction, the y-axis along the [−110] direction, and z-axis along the [001] direction. Periodic boundary conditions were imposed on the x and y directions. In order to eliminate the interaction between the upmost surface and the downmost one, a vacuum space corresponding to twenty silicon layers, which is about 22 Å, had been used to separate them. To control the system temperature to be isothermal, the velocity scale constant temperature scheme was applied. For the numerical integration, the Verlet algorithm was applied to integrate Newton's 3N equations with a timestep of 0.5 fs. Before starting the MD simulations, the geometry of the Si (001) surface applied by the simulations were optimized, in order to start from the ordered (2×1) reconstructed surface. The simulations were done at several temperatures ranging from 300 to 1300 K, below the melting point of Si (001).

3. Geometry and energetics of adsorbed dimers

We have first calculated the geometry and energetics of the four adsorbed dimers. The results are summarized in Table 1. In this table, Ad-dimers A, B, C, D configurations are the same as shown in Fig. 1.

Among the four ad-dimers, the most stable configuration is "A" (the ad-dimer bond length is 2.41 Å), when the ad-dimer axis lies parallel to the dimer rows. In this configuration, the two dimers underneath the ad-dimer open. The height of the ad-dimer is 1.34 Å

Table 1
Atomic geometry and energetics of four optimized structures of Si ad-dimers on the Si (001) as shown in Fig. 1. ΔE is the energy in eV relative to the most stable configuration A, d_1 and d_2 are the bond lengths of ad-dimer and that of between the adatom and the corresponding substrate atom in Å, respectively. z represents the average height of the ad-dimer from the Si (001) surface.

Ad-dimers	ΔE(eV)/dimer	d_1(Å)	d_2(Å)	z(Å)
A	0	2.41	2.37	1.34
B	0.82	2.41	2.53	1.84
C	0.63	2.52	2.50	1.21
D	0.12	2.40	2.52	0.93