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COMPUTER SIMULATION OF ADSORPTION OF C_{60} FULLERENE MOLECULE ON RECONSTRUCTED DEFECTIVE Si(100) SURFACE

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Abstract

In this work, based on the molecular dynamics (MD) method, the adsorption processes of C_{60} fullerene molecules on the reconstructed defective silicon Si(100) surface with different configurations were simulated in the LAMMPS open package program. Second-order Brenner interatomic potential was used to determine interactions between Si-Si, C-C and Si-C atoms. The interaction of various shaped defect areas with the C_{60} molecule on the surface of reconstructed silicon Si(100) was studied. As a result of calculations, stable adsorption states were determined by comparing the energy of C_{60} molecule adsorption to the defective silicon Si(100) surface and the Si-C bond lengths, energy and bond lengths that occur in this process.

Keywords: *Surface, fullerene molecule, defect, adsorption, silicon, modeling, Brenner potential, link length, atom, potential energy, interactions.*

Introduction

During the last few decades, as a result of the efforts to develop molecular devices compatible with existing semiconductor devices, the study of the adsorption of fullerene molecules on the surface of silicon with different cross-sections and different states has increased intensively [1,2]. The adsorption of fullerene molecules by semiconductor substrates differs from the adsorption of atoms or molecules due to the three-dimensionality of fullerenes [3,4]. The works in this field are carried out mainly in two directions, theoretically and experimentally. In experimental works, the processes of interaction of C_{60} molecule with Si(111) surface were studied using scanning tunneling microscope (STM) [5,6], scanning tunneling spectroscopy (STS) [7] and many other devices [8]. Also, experimental works on the base temperature of the interaction of the fullerene molecule with the Si(111) surface have been published [9]. Nevertheless, the importance of theoretical research in this research direction is also incomparable, especially as a result of studying the interactions of the C_{60} molecule with Si(100) and Si(111) surfaces using the density function theory (DFT) method [10] that the adsorption energy and the lengths of the resulting Si-C bonds on the silicon monocrystal surface of the fullerene molecule, as well as the stable or unstable adsorption depend on the state of the substrate surface (reconstructed or ideal), the configuration of the fullerene molecule, and whether it is adsorbed on dimer rows or trench was determined.

Nevertheless, the adsorption of fullerene molecules on the defective areas on the Si(100) surface has been studied very little. One of the theoretical works carried out in this direction, in the studies carried out by Jing Li et al. [1], the adsorption of C_{60} molecule on two different types of defective points formed on the reconstructed Si(100) surface was investigated by DFT method. According to it, it was determined that the Si-C bonds formed in the hexagonal configuration of the C_{60} molecule are stable compared to other configurations and are distinguished by the high adsorption energy corresponding to this state.

The most common dimer defects on the surface of the reconstructed silicon monocrystal are mainly three types, they are single dimer, side by side two dimers, and two dimers that are caused by the absence of silicon atoms [11]. Briefly, these defects are referred to as D1, D2 and D3 according to the above definition.

The aim of this research is to define the adsorption energy of C_{60} fullerene molecule in three most common different defective (D1, D2 and D3) areas on the reconstructed silicon Si(100) surface and to determine the average lengths of Si-C bonds by modeling the interaction process by using the molecular dynamics (MD) method, and to find out the stable states by comparing the obtained results.

1 Methodology

In this work, all MD simulations were performed using the open source MD simulator LAMMPS [12] package program and the Nanotube Modeler [13] computer program. The second-order Tersoff interatomic potential was used to determine the interactions between Si-Si, C-C and Si-C atoms [14]. In all simulations, a $34\times34\times15.2$ Å reconstructed defective silicon monocrystal with 1083 atoms and a fullerene molecule with 60 atoms were used based on periodic boundary conditions. The generated C_{60} molecule, the reconstructed silicon monocrystal, and the adsorbed states of the C_{60} molecule on the silicon monocrystal surface were visualized in the JMOL [15] computer program. Also, defects D1, D2 and D3 were formed on the reconstructed (100) silicon single crystal surface using the JMOL computer program. No size effects were observed when comparing the results obtained in the reconstructed defective silicon monocrystal of 1083 atoms with the results obtained in the reconstructed defective monocrystals of 1963 and 17670 atoms. A Nose-Hoover thermostat [16] was used to keep the selected temperature constant for the NVT ensemble. A Verle velocity-time plot was integrated with a time step of 1.0 fs. The center of mass of the system was chosen as fixed in order not to take into account the forward movements that may occur during the simulation. All simulations were performed in the time interval from 10 ns to 40 ns until reaching the equilibrium state.

Figure 1 shows defects D1, D2, and D2 on the surface of a silicon substrate, and figure a depicts dimer raws with and without defects D1. In this case, the absence of one dimer bond among the dimers given in green colors caused the D1 defect. Figure b shows silicon (100) surfaces with defects D2, which lacks two adjacent dimers, and Figure c shows silicon (100) surfaces with defects D3, which causes the absence of two adjacent atoms involved in dimer bonding. In figure c, the missing silicon atoms

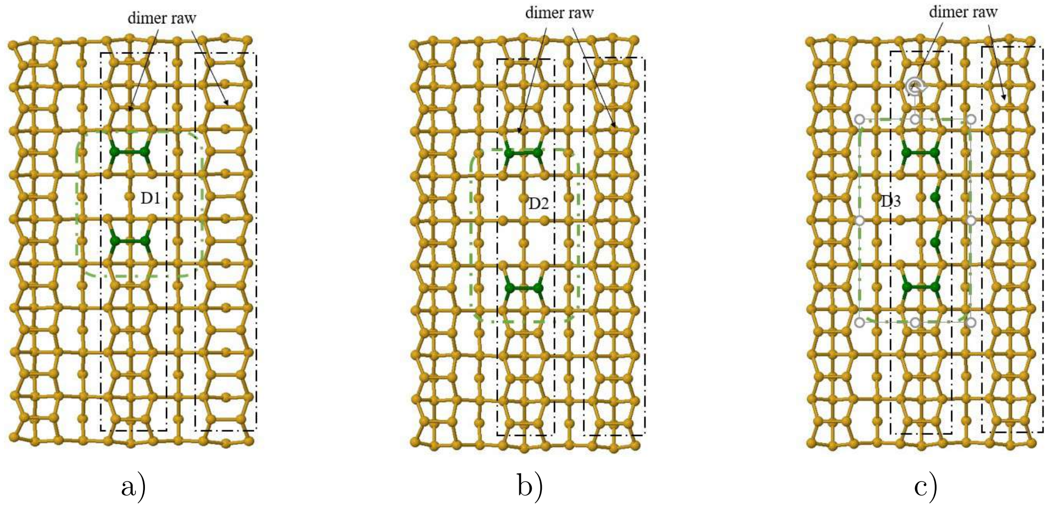

Figure 1: Defects on the surface of the silicon substrate and areas where fullerene C_{60} molecule adsorption is observed (light green dashed lines): a -D1 defect, b - D2 defect, and c - D3 defect.

should have formed a dimer bond (Si-Si bond forming dimers on the reconstructed silicon surface) with silicon atoms in green among the dimer bonds given in green. On the silicon surface, these two atoms (the two non-bonded atoms shown in green in figure c) can in some cases cross-link to form a dimer with perpendicular bonds to the dimer line [17]. Adsorption of the C_{60} molecule was observed in the area delineated by the green dashed line contour.

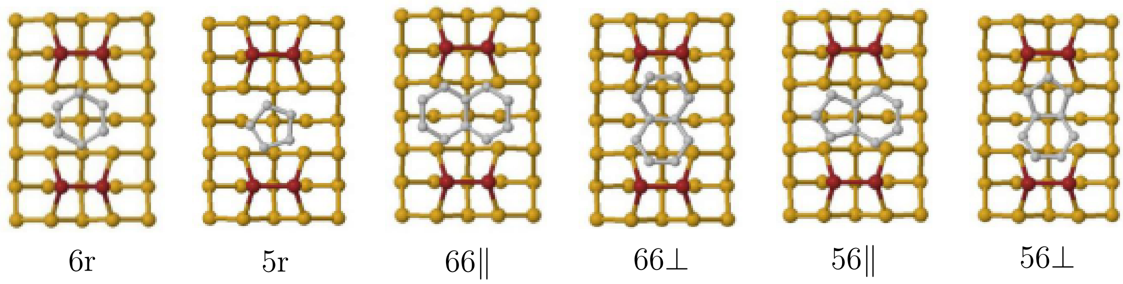

Figure 2: Six different locations of the C_{60} molecule on the surface of the D1 defective silicon substrate, corresponding to cases a, b, and c in Figure 1.

Figure 2 shows six different positions, which are relative to the dimer bonds, of C_{60} molecule on the D1 defective surface of silicon substrate which corresponds to the states shown a, b and c, as in figure 1. 6r (or 5r) expresses that C_{60} molecule in the D1 defective area with hexagon (or pentagon) and 66$\|$ and 66$\perp$ (or 56$\|$ and 56$\perp$) express that C_{60} molecule takes the position in the D1 defective area with hexagon+hexagon (pentagon+hexagon) conficurations relative to the Si-Si dimer bonds parallel or perpendicular respectively. Therefore, these configurations are appropriately abbreviated as 6r, 5r, 66$\|$, 66$\perp$, 56$\|$ and 56$\perp$.

2 Calculation of adsorption energy

The adsorption energy of E_{ads} for a molecule or atom on the surface of the substrate is equal to the difference between the potential energy $E^{tot}_{ads/sub}$ of the substrate and molecule on the substrate and the total potential energy E^{tot}_{sub} of the substrate atoms and potential energy E^{tot}_{ads}t of molecule when they do not interact each other [18,19]:

$$E_{ads} = E^{tot}_{ads/sub} - (E^{tot}_{sub} + E^{tot}_{ads}).$$

Initially, the interaction potential energy E^{tot}_{sub} of the atoms forming a silicon single crystal with a known defect was determined at 0K temperature, and in the same way, the interaction potential energy E^{tot}_{ads} of the atoms of the C_{60} molecule was obtained. At the next stage, the potential energy of the entire system $E^{tot}_{ads/sub}$t was determined for the case where the C_{60} molecule is adsorbed on the defective silicon substrate. All calculations were performed in the LAMMPS package program.

3 Results

The considered configurations (Fig. 1 and 2) are 6 different, and table 1 shows the adsorption energies of the C_{60} molecule in all configurations corresponding to each defect. Analysis of the results and comparisons shows that the energies of adsorption to the D2 defective area with 66‖, 66⊥, 56‖ and 56⊥ configurations are significantly different from their adsorption energies in the other two defective areas and have sufficiently large values. The following conclusion can be drawn from this: in these configurations, the adsorption of the C_{60} molecule on the surface is stable enough, and the reason for this is the absence of two side-by-side dimers in the dimer rows, the fullerene molecule with the silicon atoms in the lower layer (according to the arrangement of the silicon atoms, in the second layer) allows for the formation of a larger number of bonds, and as a result, these resulting bonds are shorter than the Si-C bonds formed with atoms in the primary layer. By comparing the bond lengths and bond energies related only to these bonds, it was shown that the bonds between carbon atoms and silicon atoms in the secondary layer are short and strong.

Figures 3, 4, and 5 show the adsorption of C_{60} molecules on the defective Si(100) surface with the configurations shown in Figure 2, in which the top and side views of the state of adsorption of C_{60} molecule with the 6r, 66‖, 66⊥, 5r, 56‖ and 56⊥ configurations on the D1, D2 and D3 defective silicon surface with respect to the silicon substrate. In the images, carbon atoms forming Si-C bonds with silicon atoms are in green color, located in the first layer of the silicon substrate surface, and silicon atoms that formed Si-C bonds are in brown color and silicon atoms locate in the lower layer (secondary layer) compared to the substrate surface and take part in the Si-C bonding are shown in red color.

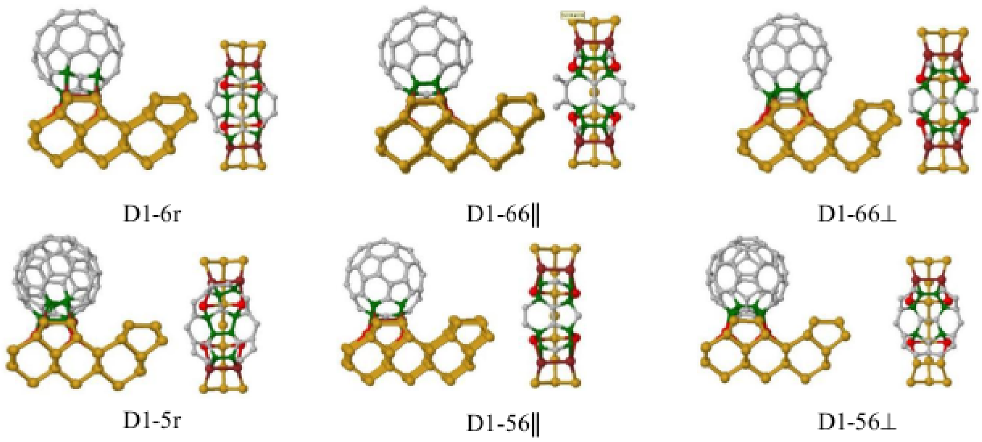

Figure 3: Side and top views of the states and configurations of C_{60} molecule adsorbed on D1 defect silicon surface.

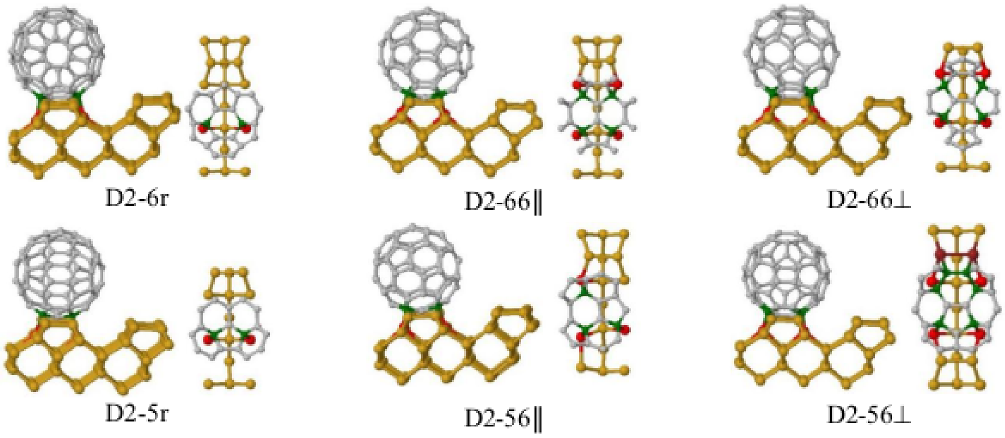

Figure 4: Side and top views of the states and configurations of C_{60} molecule adsorbed on D2 defect silicon surface.

Table 1: Adsorption energies of C60 molecule in defect areas D1, D2 and D3 and the lengths of resulting bonds are given in this table.

D1	6r	66‖	66⊥	5r	56‖	56⊥
E_{ads} (eV)	-3.4860	-3.8998	-3.4079	-2.7208	-4.0118	-3.7722
λ (nm)	1.95-2.07	2.00-2.01	2.01-2.04	2.00-2.21	1.99-2.06	1.97-2.02
D2	6r	66‖	66⊥	5r	56‖	56⊥
E_{ads} (eV)	-3.2413	-5.2265	-5.1973	-3.3550	-5.0402	-5.4575
λ (nm)	1.94-1.95	1.92-1.98	1.92-1.99	1.95	1.93-1.97	1.92-1.98
D3	6r	66‖	66⊥	5r	56‖	56⊥
E_{ads} (eV)	-3.3051	-2.3324	-0.1101	-3.3819	-3.3039	-0.5583
λ (nm)	1.93-1.94	2.00-2.01	1.96-2.10	1.94	1.94	1.89-2.21

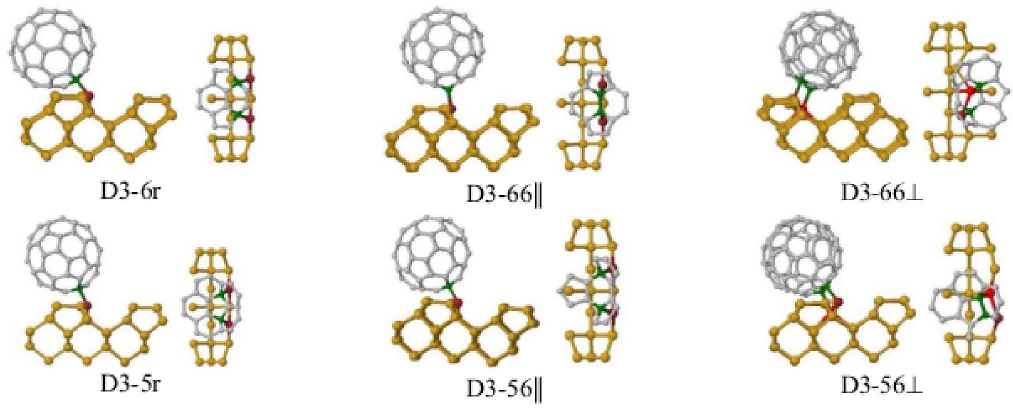

Figure 5: Side and top views of the states and configurations of C_{60} molecule adsorbed on D2 defect silicon surface.

The following conclusions can be drawn from the conducted research:a) The adsorption energy of C_{60} molecule on the reconstructed defective Si(100) surface, the bond lengths and the number of formed bonds depend on the adsorption geometry, that is, on which point of the substrate surface the molecules are adsorbed and in what configuration; b) it was found that the states of adsorption observed in the D2 defect area of the silicon substrate surface are more stable than in the other defect areas; c) adsorption energy depends on the number of bonds, and as the number of bonds increases, the adsorption energy also increases; d) it was observed that bond lengths are relatively shorter in bonds with high adsorption energy.

4 Conclusion

The following conclusions can be drawn from the conducted research:a) The adsorption energy of C_{60} molecule on the reconstructed defective Si(100) surface, the bond lengths and the number of formed bonds depend on the adsorption geometry, that is, on which point of the substrate surface the molecules are adsorbed and in what configuration; b) it was found that the states of adsorption observed in the D2 defect area of the silicon substrate surface are more stable than in the other defect areas; c) adsorption energy depends on the number of bonds, and as the number of bonds increases, the adsorption energy also increases; d) it was observed that bond lengths are relatively shorter in bonds with high adsorption energy.

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