Radiation-stimulated processes in Si surface layers

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ABSTRACT

Molecular dynamics computer simulations have been performed to study the character of disordering of atom configurations in Si surface layers. The relaxation of free Si surface was investigated. The main structural parameters were calculated, such as a distribution of angles between chemical bonds, the density of dangling bonds, structural peculiarities of Si surface layers and radiation effects. It was concluded that Si surface at real conditions is a disordered phase similar to a-Si [1].

Keywords: Si surface, molecular dynamics, relaxation processes, radiation effects

1. INTRODUCTION

Investigations of Si surface microstructure have shown the new atom configurations formation as a result of surface layers relaxation. One of the main features of Si surface relaxation is atom dimers appearing. At present two types of such dimers are established. For instance pseudopotential calculations predicted that the symmetric (2x1) and asymmetric c(4x2) tilted Si-dimers should be stable on (100) Si-surface [1,2]. The barrier between these configurations is only 0,09 eV per dimmer [3]. Reconstruction processes at Si surface and also the dimerization depend on many conditions.

It is known that low energy ion beams have application as Si surface cleaning and dry etching. That is why it is important to study surface structural changes following such ion bombardment. In theoretical and experimental works devoted to Si surface investigations the main attention is paid to features of several top layers without detailed discussing of their real structure as a result of the complete relaxation of the system. There are not calculations of relaxation processes of Si surface layers with taking into account structural defects and dangling bonds creation and making clear the specific role of each layer in equilibrium atom configurations arising. Such information cannot be got by ab initio methods. So we have applied molecular dynamics method and semi-empirical potentials to obtain the realistic picture of Si surface layers relaxation.

2. MODEL AND METHODS

The starting configuration was taken as a parallelepiped containing 864 atoms. There were 12 layers with 72 atoms in each one. Periodic boundary conditions were used in two dimensions. At first all atoms were in normal lattice positions. We investigated the relaxation of the Si surface which represents a shearing cut (001). MD method was applied in its standard form [4] i.e. the equations of motion were solved by using the central difference scheme. The time-step was 10^{-14}s.

Simulations were performed with Keating [5] and Stillinger-Weber [6] potentials. These potentials give a good description of Si for the study of small Si clusters and bulk Si. Comparison to density functional calculations with ab initio pseudopotentials [7] shows good agreement between these electronic structure methods and above mentioned semi-empirical potentials. We have chosen new routes to investigate relaxation processes in Si surface layers, the older one being unsatisfactory because only the partial relaxation was considered. In the case of a partial relaxation it is possible to use ab initio calculation methods [8]. But such calculations do not allow to obtain the detailed information about real Si surface layers structure with lattice and electronic defects. So in this work we have used the semi-empirical potentials [5,6] for investigations of full Si surface relaxation with structural defects and dangling bonds arising as it was done in [8] for amorphous Si modelling.

3. CALCULATIONS PROCEDURE AND RESULTS

The relaxation process is beginning when the cutting of a crystal occurred and a free surface arised. The primary crystal had a given temperature and after cutting of a crystal we had a corresponding temperature of crystal surface. Relaxation processes were observed at temperatures 100 and 290 K.

By analogy to [8] the model is based on the assumption that each atom during the relaxation creates chemical bonds with his four nearest neighbouring atoms. Thus, as a result of relaxation any atom may change his

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neighbouring atoms and it means that during the relaxation modelling rebuilding of chemical bonds and their re-hybridization take place. Such procedure leads to arising of non-usual polygons with n = 3 – 9 and nodes with 1 – 3 electrons which do not participate in chemical bonds creation. So we obtained nodes with more than one dangling bond. Computer programs allow us to get radial distribution function (RDF) and angle distribution functions (ADF) (The angles between chemical bonds are implied). The second part of the work is connected with investigations of bombardment effects on Si surface relaxation. It was interesting to see the influence of low energy particles bombardment on relaxation processes in Si surface layers. The following energies of bombarding particles were chosen: 10, 20, 30, 40 and 50 eV. The impulse irradiation was modeled so that one impulse corresponded to $2 \cdot 10^{12}$ particles/sm^2·s.

The main conclusion consists in arising of disordered phase as a result of Si free surface relaxation. The RDF are similar to those for a-Si (Fig. 1). We concluded that it is important to consider Si real surface layers as a disordered system (DS) as it was mentioned in [9, 10]. This DS has a number of peculiarities. It was established that only four layers belong to DS. The fifth layer does not differ practically from more deep layers. Each of mentioned four layers has his specific microstructural characteristics. In Fig. 2 it is shown the distribution of polygons with different number of sides. One can see that the third layer is the most perfect one. This layer has only 2,8% dangling bonds (n(3) = 2,8%) and what's more such nodes have only one non-paired electron. We see that n(3) = 8% in the first layer, n(3) = 6,9% in the second layer and n(3) = 11,1% in the fourth layer.

Besides only third layer in surface DS has not nodes with n(2)≠0 (Fig. 2). But at the same time the third layer is strongly distorted. In the Table 1 it is shown the displacements upwards or downwards of atoms belonging to each layer. We see that atoms of the third layer are characterized by the largest displacement upwards relatively to the normal position of corresponding crystallographic plane (1.8712 Å). Only for the first layer atoms displacement is larger (0.1883 Å), but it is naturally. In the Table 2 we see also that the third layer on the whole has a largest displacement to the surface. As a result of relaxation the distance between the third and the fourth layers became 1.586 Å and between the third and the second layers 1.082 Å. Thus we concluded that the third layer in surface DS plays a special role. It is possible to say that this layer is transit one between the crystal volume and the surface DS and causes the certain configuration of surface layers.

Table 1

	Displacement (Å)			
Layers	Up		Down	
	Min	Max	Min	Max
1		0.1883	0.1010	2.7905
2	0.0040	1.4798	0.0461	1.6952
3	0.178	1.8712	0.0031	1.2565
4	0/0046	0.7731	0.0041	0.6137
5	0.0106	0.2653	0.0061	0.3874

Table 2

Distances between layers (Å)							
1,2	2,3	3,4	4,5	5,6	6,7	7,8	8,9
0.535	1.082	1.503	1.328	1.345	1.347	1.346	1.346

The next question is an arising of dimmer configurations in Si surface layers. In conditions of full relaxation dimerization effects have new features. First of all the disposition of dimers is not so well regulated as it come out if the system cannot to relax completely. We observed disordered disposition of dimers as it may be seen on Fig. 3 a,b. The case "a" corresponds to dimerization for not relaxed Si surface and "b" corresponds to complete relaxation which was obtained in our model. In the second case the chaotic disposition of dimers takes place. Another result consists in dimers arising not only in the first layer. Because of many destroyed bonds in lower layers the necessary conditions exist for dimers formation also in more deep layers (Fig. 4).

It is interesting to note that the bombardment effects on Si surface relaxation have a specific energy dependence. We compared the relation processes by using the value of time which was necessary for the system coming to the equilibrium state. Fig. 5 shows how this time depends on the energy of bombarding particles. As seen there are energy intervals in which the relaxation processes go more quickly. It is useful to take into account when ion beams are applied for Si surfaces treatment.

4. CONCLUSION

The microstructure of Si surface layers was studied by molecular dynamics method. As a result of the full relaxation of surface layers re-building and re-hybridization of chemical bonds are occured. We established that in relaxed Si surface layers there are dangling bonds and different types of atom polygons. New configurations of atom dimers at Si surface are also observed.

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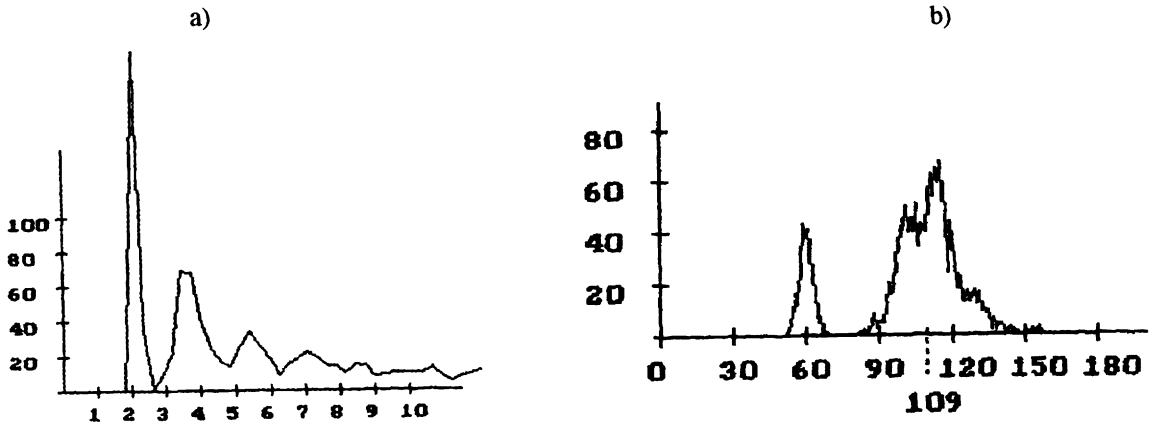


Fig. 1 RDF (a) and ADF (b) for four layers

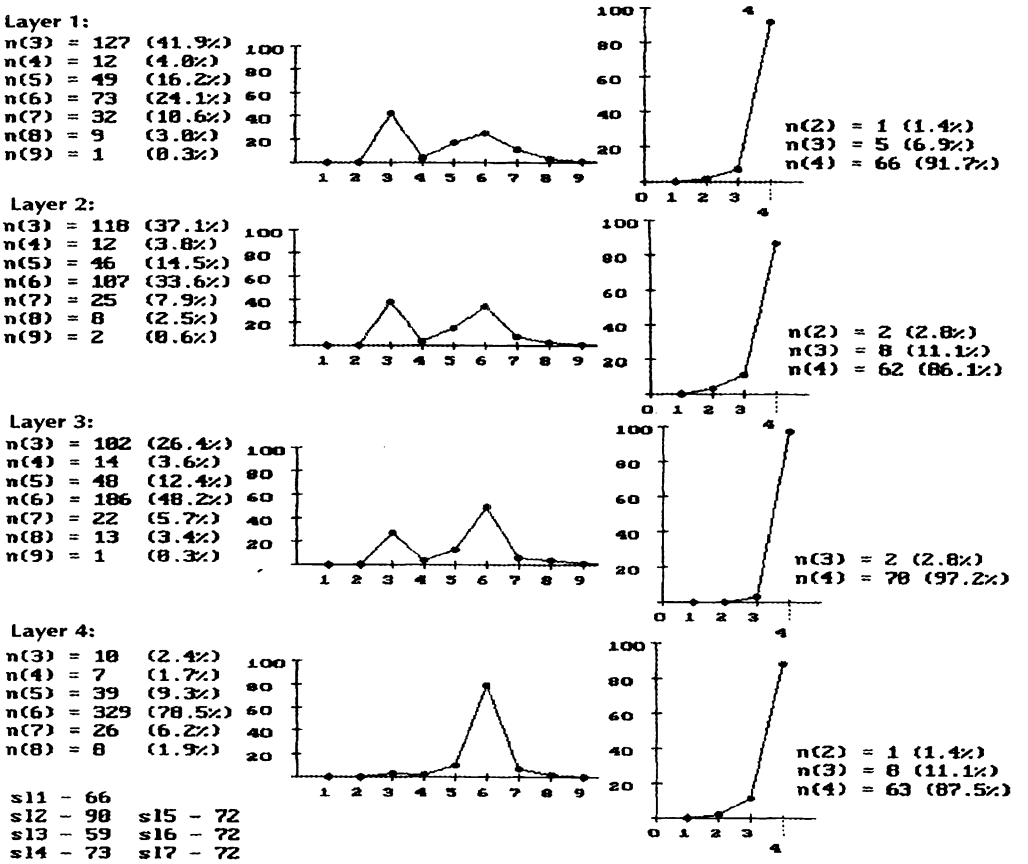
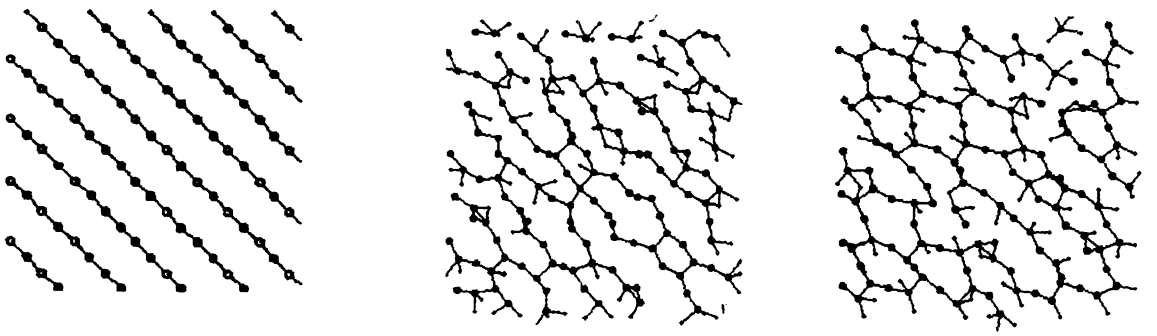


Fig. 2 Distribution of polygons (left) and non-saturated bonds in different layers



T=100 K

a) b)

T=290 K

Fig. 3 The first layer before (a) and after (b) relaxation

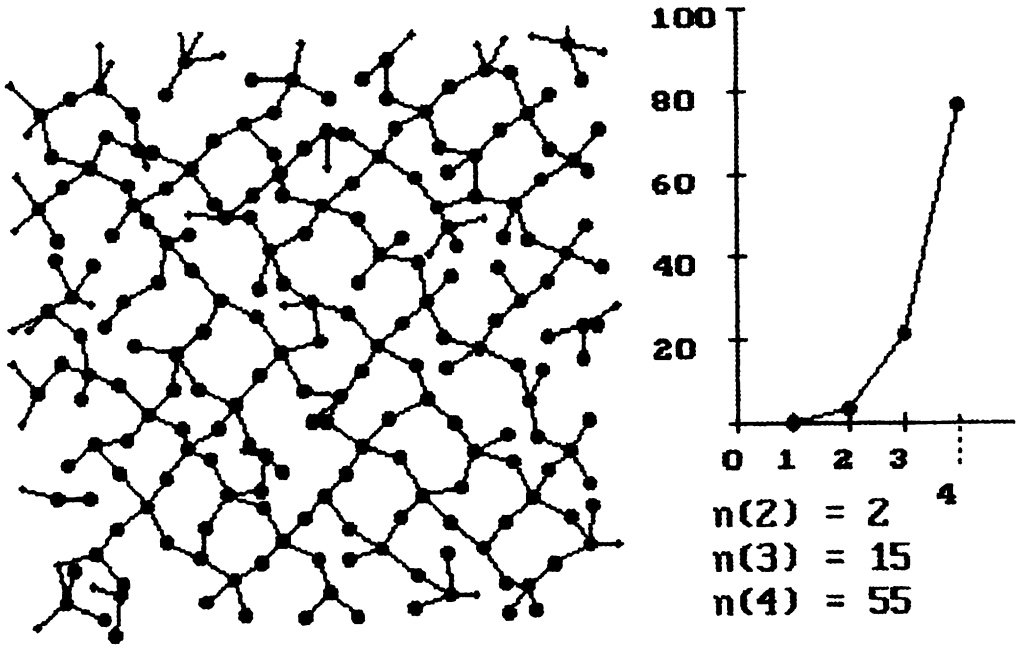


Fig. 4 The microstructure of the second layer

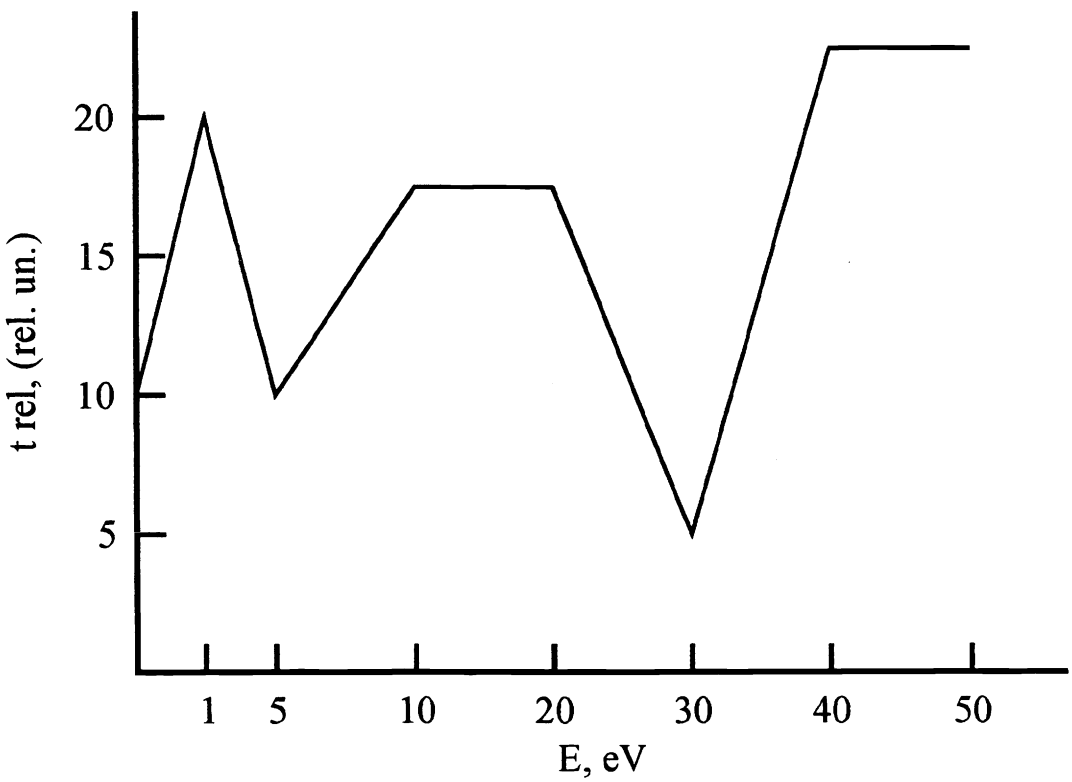


Fig. 5 The energy dependerce of the relaxation time (t_{rel})