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1994 J. Phys.: Condens. Matter 6 1083

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The two-dimensional pair correlation function for the Si(001) surface: computer simulation results

Jia Zhengming, Yang Genqing, Cheng Zhaonian, Liu Xianghui and Zou Shichang

Ion Beam Laboratory, Shanghai Institute of Metallurgy, Chinese Academy of Sciences, Shanghai 200050, People's Republic of China

Received 26 July 1993

Abstract. A two-dimensional pair correlation function (TPCF) has been introduced into the study of the surface structure of materials. A molecular dynamics simulation was then performed to obtain the TPCFs for the Si(001) surface and deeper layers. The atoms interact via a potential developed by Stillinger and Weber, which includes both two-body and three-body contributions. The analysis of TPCFs shows that the atoms in deeper layers of Si(001) do not derive from their original (001) atomic plane lattice sites, but just thermally vibrate in the vicinity of their equilibrium sites, and the nearer to the surface layer the atoms are, the more violent the vibration is. The analysis also indicates that a rearrangement of atoms has occurred in the Si(001) surface and, while the majority of these atoms form bonds, a minority still exists as non-bonding atoms.

1. Introduction

The study of the surface structure of materials is one of the most important and productive areas of research in condensed matter, statistical and solid state physics. Because many devices are grown on the surfaces of materials, it is important to understand the structure of the surface and the defects that are likely to occur.

The pair correlation function, $g(r)$, which is proportional to the local number density of particles at a given distance, r , from a fixed reference particle, is very useful because it provides an insight into the structure of the material [1]. $g(r)$ is a statistical function and the structure of the material may conveniently be described by it. In most cases, $g(r)$ is used to describe the structure of a three-dimensional (3D) system and can be obtained both from scattering experiments [2] and computer simulations [3]. In the two-dimensional case, $g(r)$ can be obtained from computer simulations and, recently, was used to study the structure of the two-dimensional Lennard-Jones fluid [4]. As to the application of $g(r)$ to the study of the surface structure of materials, to our knowledge, little research has been carried out.

The surface of a solid material, especially the surface of crystalline material, can be treated as a two-dimensional system. In order to describe the arrangement of the surface atoms, we introduce a two-dimensional pair correlation function (TPCF) into such a system. A TPCF is defined as

$$g_{\alpha\beta}(r) = \frac{1}{\rho} \left\langle \frac{N_{\beta}(r, \delta)}{2\pi r \delta} \right\rangle$$

where $N_{\beta}(r, \delta)$ is the average number particle of species β at a distance between $r - (1/2)\delta$ and $r + (1/2)\delta$ from the central particle α . ρ is the plane density of particles. $\langle \rangle$ infers a

statistical average over a typical number of instantaneous atom configurations produced by simulation.

The (001) surface of Si has been the subject of a large number of both experimental and theoretical investigations [5]. The ideal Si(001) surface has two dangling bonds per surface atom. There is now ample theoretical [6–7] and experimental [8–11] evidence to suggest that surface atoms having two dangling bonds form a dimer, to lower their energy, and collectively lead to a 2×1 reconstructed surface. However, there is still some controversy over the structural details.

Recently, although several molecular dynamics (MD) simulations [12–15] have been made on the Si(001) surface, we have not seen a simulation which utilizes the TPCF to discuss the behaviour and the bonding of atoms of the Si(001) surface and deeper layers. Most of the simulations carried out give the result of a reconstructed Si(001) surface just from an instantaneous MD configurational image.

In this paper, we will perform a MD simulation to obtain the TPCFs for Si(001) and, from a statistical role, we will study the arrangements of atoms of the Si(001) surface and deeper layers. We will especially discuss the effect of the reconstructed surface layer on the behaviour of atoms in deeper layers. Some characteristic values for the structure will be given such as the nearest-neighbour distance, the coordination number, etc, which are important for understanding the microscopic details of the structure of materials and are difficult to obtain from this experiment.

2. The model

In the calculation presented here the atoms interact via a potential developed by Stillinger and Weber [16] (SW) to simulate the properties of liquid and solid silicon. The potential comprises both two-body and three-body contributions, v_2 and v_3 , scaled by the energy and length scales ϵ and σ :

$$v_2 = \epsilon f_2(r_{ij}/\sigma)$$

$$v_3 = \epsilon f_3(r_i/\sigma, r_j/\sigma, r_k/\sigma)$$

where

$$f_2(r) = \begin{cases} A(Br^{-4} - 1) \exp[(r - a)^{-1}] & r < a \\ 0 & r \geq a \end{cases}$$

and

$$f_3(r_i, r_j, r_k) = h(r_{ij}, r_{ik}, \theta_i) + h(r_{ji}, r_{jk}, \theta_j) + h(r_{ki}, r_{kj}, \theta_k)$$

$$h(r_{ij}, r_{ik}, \theta_i) = \lambda \exp[\gamma(r_{ij} - a)^{-1} + \gamma(r_{ik} - a)^{-1}](\cos \theta_i + \frac{1}{3})^2$$

$r_{ij}, r_{ik} < a$; otherwise

$$h(r_{ij}, r_{ik}, \theta_i) = 0$$

where θ_i is the angle between atoms j and k subtended at vertex i , etc. The SW parameter set is $A = 7.049\ 556\ 277$, $B = 0.602\ 224\ 5584$, $a = 1.8$, $\lambda = 21.0$ and $\gamma = 1.20$.

Our MD model consists of a truncated Si(001) surface with eight atomic planes. The first layer is the topmost (surface) layer in a bulk silicon configuration with the [001] direction pointing in the positive z direction. Each layer consists of 32 silicon atoms and hence the original system contains 256 particles. In order to decrease the size effects, periodic boundary conditions were applied in the x and y directions, whereas the topmost layer has free boundary conditions. The atoms in the bottom two layers (the seventh and eighth layer) are fixed at their ideal lattice sites.

The equations of motion are solved numerically with an integration step $\Delta t = 7.66 \times 10^{-16}$ s. The total time-step number of running is 6000 and the TPCF is calculated over the last 1000 steps. The temperature of the system is 300 K.

3. Results and discussion

Figure 1 shows the TPCFs of the Si(001) first (surface) layer to the sixth layer, averaging over 1000 instantaneous atom configurations. Table 1 gives the characteristic values for each TPCF first peak and second peak, specifically the peak's position, height, width, and the area under each peak.

On examining figure 1 we see that the TPCFs of layer 2 to layer 6 have the same number of peaks and their corresponding peak positions are almost equal. But in the second layer the TPCF peak height is lower and the width is broader than for the other layers. Characteristic values in table 1 show that the TPCF first peaks from layer 2 to layer 6 are all at 3.81 Å and the area under each peak is equal to 4. The second peak, in layer 3 to layer 5, is at 5.43 Å, whereas in layer 2 and layer 6 it is at 5.38 Å. The second peak area is equal to 4 in each case.

Table 1. Characteristic values for each TPCF.

	First peak				Second peak			
	Position (Å)	Height	Width (Å)	Area	Position (Å)	Height	Width (Å)	Area
1st layer	2.40	3.001	0.57	0.813	3.87	5.594	0.68	2.116
2nd layer	3.81	6.972	0.94	4.000	5.38	4.474	0.94	4.000
3rd layer	3.81	12.087	0.73	4.000	5.43	6.934	0.73	4.000
4th layer	3.81	12.760	0.73	4.000	5.43	8.139	0.68	4.000
5th layer	3.81	14.459	0.63	4.000	5.43	8.674	0.63	4.000
6th layer	3.81	13.488	0.57	4.000	5.38	8.860	0.63	4.000

The first- and second-peak positions correspond to the first- and second-nearest-neighbour distances between atoms in the layer, and the area under each peak is the corresponding nearest-neighbour coordination number of the central atom. We know that the first- and second-nearest-neighbour distances between atoms in crystalline Si(001) atomic planes are 3.84 Å and 5.43 Å, respectively, and the corresponding coordination numbers are all 4. These indicate that the atoms in deeper layers under the topmost Si(001) surface do not derive from their original lattice sites, but just thermally vibrate in the vicinity of their equilibrium sites. However, the amplitudes of vibration are different for the different layers of atoms.

From Abraham and Batra's simulation result [12], that the surface layer is reconstructed (our simulation shows the same reconstructed patterns), this reconstructed surface may have

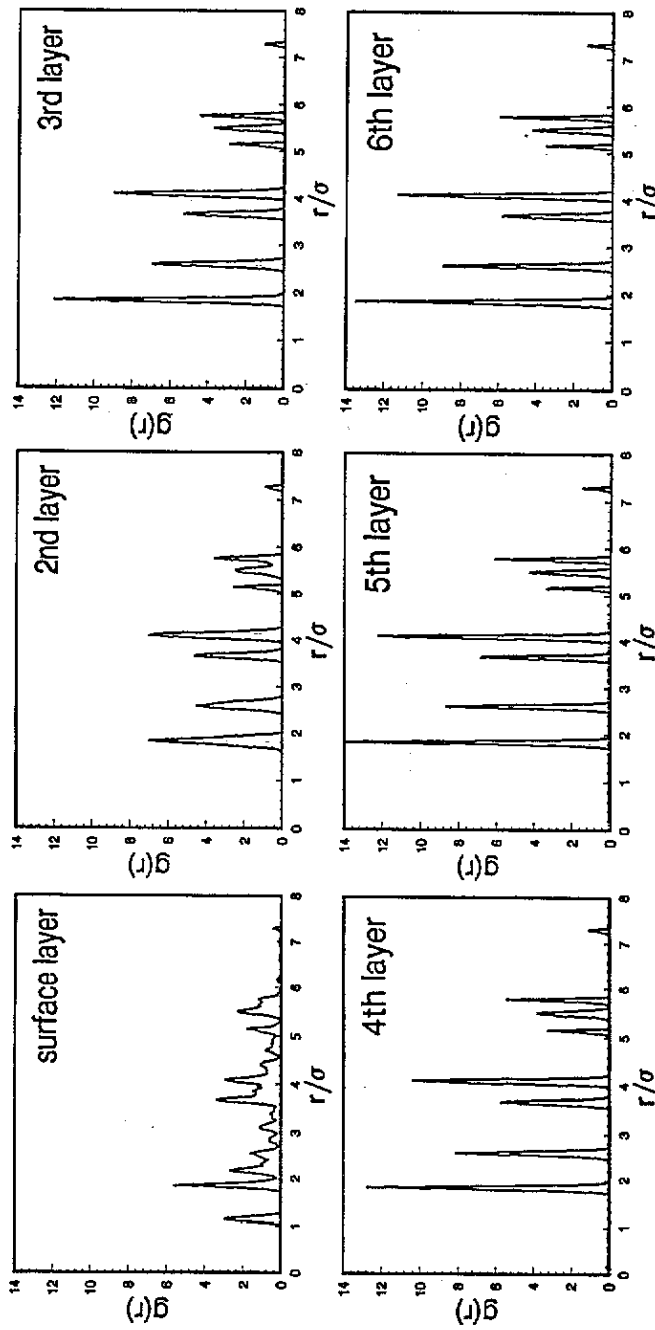


Figure 1. The two-dimensional pair correlation functions (PCRFs) for the Si(001) surface and deeper layers.

effects on deeper layers. The second layer is adjacent to the surface layer, so atomic vibration in this layer is relatively violent. This makes its TPCF peak height lower, and width broader, and even makes the second peak shift forward, the sixth and seventh peaks becoming continuous instead of separated. The effect of the reconstructed surface on layers 3, 4, and 5 gradually decreases, and, therefore, their TPCFs become more and more similar. The sixth layer's TPCF is much more similar to the fifth's, and the difference between their second-peak positions probably results from either the error of statistical calculation or the closeness of the bottom fixed double layers.

As we can see from figure 1, the surface layer's TPCF is apparently different from those of the deeper layers. Its first peak appears at 2.40 Å, rather than 3.81 Å. The following peaks are almost continuous. Besides, the peak's height is obviously lower than for deeper layers. This evidence shows that a rearrangement of the surface layer atoms has occurred. Because the first-peak position corresponds to the first-nearest-neighbour distance, and noticing that the experimental value for the bond length of an atom in crystal silicon is 2.35 Å [17], it is easy to conclude that bonding of two neighbouring atoms in the surface layer has occurred, and the bond length is 2.40 Å. This result is consistent with the experimental observation that atoms in the Si(001) surface form bonds and lead to a reconstructed surface. Furthermore, the first-nearest-neighbour coordination number is 0.813, rather than 1.0, suggesting that while the majority of atoms in the Si(001) surface layer form bonds, the minority still exist as non-bonding atoms.

4. Conclusions

In this paper we have introduced a two-dimensional pair correlation function into the study of the surface structure of materials. We performed a MD simulation to obtain the TPCFs for the Si(001) system and, from a statistical viewpoint, discussed the arrangement of the atoms of the Si(001) surface and deeper layers. The analysis of TPCFs shows that the atoms in deeper layers of Si(001) do not derive from their original (001) atomic plane lattice sites, but just thermally vibrate in the vicinity of their equilibrium sites and, the nearer to the surface layer the atoms are, the more violent the vibration is. The analysis also indicates that a rearrangement of atoms has occurred in the Si(001) surface and, while the majority of these atoms form bonds, the minority still exist as non-bonding atoms. Our simulation result is qualitatively consistent with experimental observation and, furthermore, provides an insight into experimental studies of the surface structure of Si(001).

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