PHYSICAL REVIEW B VOLUME 53, NUMBER 3 15 JANUARY 1996-I

Structural study of the Si(100)2×2-In surface

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(Received 24 August 1995)

The structure of Si(100)2×2-In was analyzed using tensor low-energy electron diffraction. The parallel dimer model agrees with the experimental results. The features of atomic arrangement are discussed in terms of the size and chemical nature of In atoms.

Extensive works have been performed on column-III-atom-adsorbed Si(100) surfaces.[1] Up to now, the parallel dimer models have been widely accepted as the structures of the 2×2 phases.[2] The similarity of the atomic arrangements for Al-, Ga-, and In-induced 2×2 phases has been emphasized on the basis of the similar chemical nature of these species.[3–6] Indeed, we found similar tendencies of atomic displacements for Al 2×2 and Ga 2×2.[7,8] However, the effect of atomic size is essential in some cases. For example, As induces the 1×1 phase, whereas Sb and Bi induce the $\sqrt{3}\times\sqrt{3}$ phases on Si(111).[9–11]

In this paper, we carried out the analysis of the Si(100) 2×2-In structure, using tensor low-energy electron diffraction (LEED). The parallel dimer model was favored over the orthogonal dimer model, similar to Al 2×2 and Ga 2×2. However, the directions of the atomic displacements were the opposite of those in Al 2×2 and Ga 2×2, which is associated with the atomic size and chemical nature of In.

In atoms were evaporated from a Knudsen cell made of tantalum. Intensity vs voltage curves (*I-V* curves) of LEED were measured from the 2×2 structure formed at 100 °C with the coverage of 0.5 ML (1 ML $=9.6\times10^{14}$ atoms/cm^2), where the clearest 2×2 patterns were observed. The tensor LEED calculations were performed for the parallel dimer model and the orthogonal dimer model.[7] The calculated *I-V* curves were compared with the experimental ones to find the actual atomic arrangements. Other detailed experimental and theoretical procedures were described in previous papers.[7,8]

Figure 1 shows the atomic arrangements of the parallel dimer model and four geometrical parameters, which uniquely define the positions of atoms in the two topmost surface layers. In Fig. 2, the calculated *I-V* curves for the optimized geometries of the parallel dimer model and the orthogonal dimer model are compared with the experimental ones. Pendry's *R* factors for the optimized geometries of the parallel and orthogonal dimer models are 0.20 and 0.29, respectively. From these results, it can be concluded that the In-induced 2×2 structure is described by the parallel dimer model.

Four geometrical parameters for the optimized parallel dimer model are given in Table I, together with those obtained by total-energy calculations.[6] In dimers are contracted from the ideal covalent bond length (2.88 Å = double the Pauling covalent radius of In). The length of Si dimer bond is almost equivalent to the bulk bond length (2.35 Å), which is consistent with a single bond of Si dimer. Δz for the optimized geometry ($=1.22$ Å) is decreased from that for the ideal geometry, where all bond lengths are the sum of Pauling covalent radii ($=1.29$ Å). These findings are in clear contrast with the 2×2 structures of Al and Ga, where both adsorbate dimer and Si dimer are expanded from the ideal covalent bond lengths, and Δz is increased from that for the ideal geometry.[7,8] All these movements in Al 2×2 and Ga 2×2 are understood in terms of the recovery of bond angles of Al-Si and Ga-Si measured from the plane parallel to the surface (φ defined in Fig. 1), due to the small atomic sizes of Al and Ga. However, the In atom has a large atomic size, and

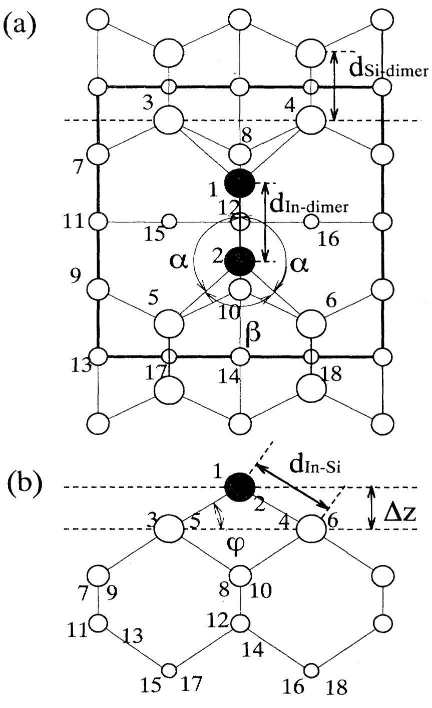

FIG. 1. A schematic illustration of the parallel dimer model. (a) top view, (b) side view. Open and filled circles denote Si and In atoms, respectively. Four structural parameters ($d_{\text{In-dimer}}$, $d_{\text{Si-dimer}}$, $d_{\text{In-Si}}$, Δz) are indicated by arrows.

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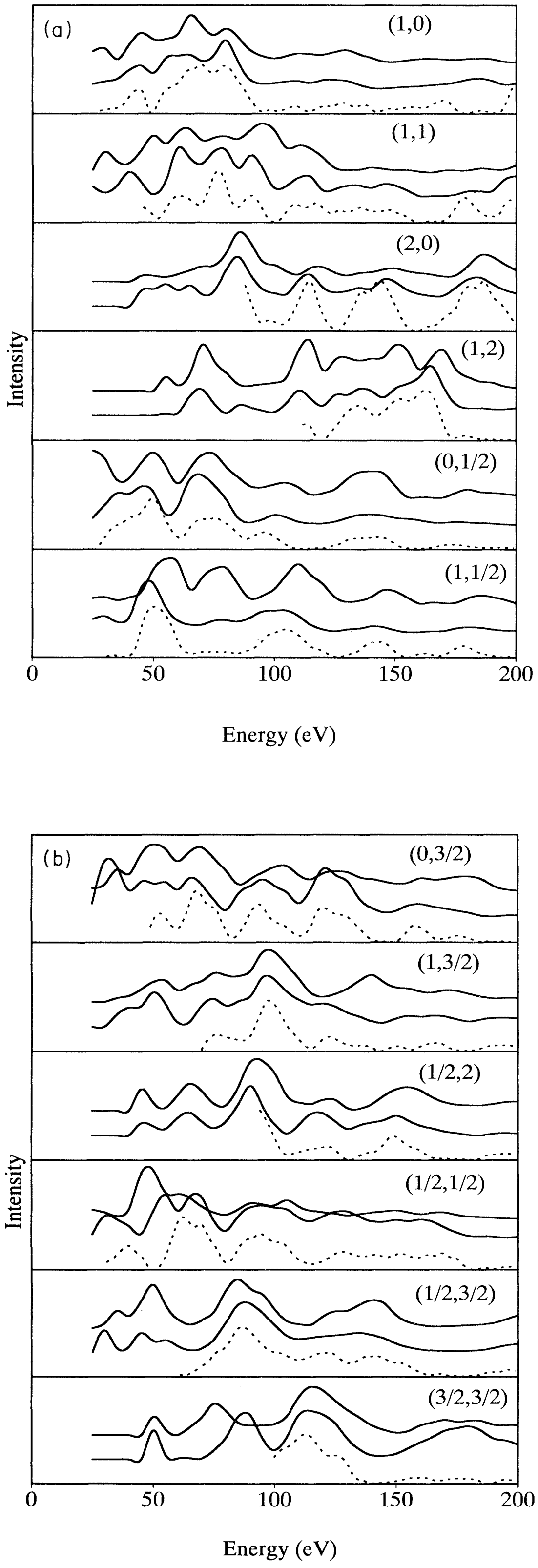

FIG. 2. Experimental (dashed lines) and theoretical *I-V* curves optimized for the orthogonal (upper solid lines) and parallel (lower solid lines) dimer models.

TABLE I. Four geometrical parameters for the optimized geometry of the parallel dimer model. Values obtained by total-energy calculation are also shown.

	This work	Northrup *et al.* (Ref. 6)
$d_{\text{In dimer}}$	2.78	2.82
$d_{\text{Si dimer}}$	2.35	2.40
$d_{\text{In-Si}}$	2.61	2.60
Δz	1.22	1.38

$\varphi=29.6°$ for the ideal geometry is close to $\varphi=35.3°$ for the Si(100) 2×1 surface. Thus, the recovery of bond angle φ is not a driving force for reconstruction in the In-2×2 structure. Indeed, $\varphi=28.0°$ for the optimized geometry is rather decreased from 29.6°.

The definitive factor for the In-2×2 structure may be angles among one In-In and two In-Si bonds (α and β defined in Fig. 1). Meade and Vanderbilt demonstrated that the energy of column-III-atom-adsorbed Si(111) surface is lowered by sp^2 bond hybridization of column-III atoms.[12] Since $\alpha=119.2°$ and $\beta=94.7°$, α is almost 120°. The decrease of Δz contributes to the increase of α and β. However, this induces a compressive stress on In and Si dimers, which results in the contractions of In and Si dimers.

Subsurface layer reconstructions are shown in Fig. 3. Upward displacements of atoms 8, 10, 12, and 14 (where the number of each atom is given in Fig. 1) and downward displacements of atoms, 7, 9, 11, and 13 are observed, although the magnitudes of them are small in comparison with those in Al 2×2 and Ga 2×2. Here, again, the directions of these displacements are the opposite of those in Al 2×2 and Ga 2×2. All Si bond lengths among the second layer (including atoms 3–6) and the fifth layer (including atoms 15–18) are within 2% from the bulk bond length. The displacements of atoms along the z axis in Al 2×2 and Ga 2×2 are caused by the movement of Si dimer toward Al and Ga dimers. The displacements shown in Fig. 3 should be understood as a re-

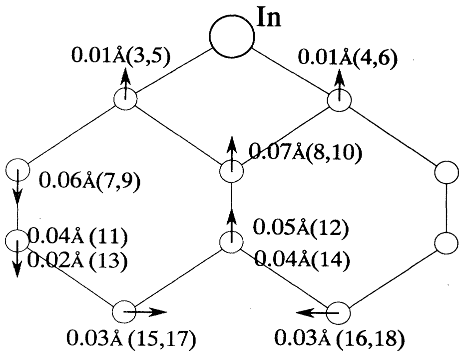

FIG. 3. Side view of the optimized geometry of the parallel dimer model. Arrows denote the direction of the displacements of atoms from bulk positions. The magnitudes of the displacements are given in Å.

sult of the movement of the Si dimer away from the In dimer. Such a movement of the Si dimer was not detected in the present analysis, due to a small magnitude of movements; however, if that is the case, this movement also results from a compressive stress on the Si dimer.

The elongation of Si dimer backbonds (bond between atoms 3 and 7 or atoms 3 and 8) was observed in Al-2×2 and Ga-2×2 structures.[7,8] However, the length of Si dimer backbonds is almost the same as the bulk bond length in In 2×2. This difference in two cases can also be explained by the mechanism of the reconstructions discussed above. The elongation of Si dimer backbonds contributes to the recovery of bond angle φ in Al 2×2 and Ga 2×2. However, the elongation of Si dimer backbonds is unnecessary for In 2×2, where the recovery of φ is not a driving force for reconstructions.

In summary, the structure of Si(100) 2×2 In is determined using tensor LEED. The result favors the parallel dimer model over the orthogonal dimer model. Slight contractions of In and Si dimers, the decrease of Δz, and subsurface layer reconstructions are observed. The directions of the displacement of atoms are the opposite of those in Al-2×2 and Ga-2×2 structures, which is associated with a large atomic size of In.

We would like to thank Mr. N. Akiyama for providing substrates. This work was supported by a Grant-in-Aid for Science Research from the Ministry of Education, Science and Culture.

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