Structure of the Si(100)-(2×2)In surface

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The question of whether the Si(100)-(2×2)In reconstruction consists of orthogonal or parallel In ad-dimers was answered by performing studies, using scanning tunneling microscopy and impact-collision ion-scattering spectrometry (ICISS), on low coverages of In adsorbed on a vicinal Si(100) surface. The formation of a predominantly single domain of the (2×2) phase on the vicinal surface allowed us to use the ICISS experiments to distinguish between the orthogonal and parallel ad-dimer geometries. Our results strongly support the model involving the parallel ad-dimer, in agreement with previous theoretical predictions.

Recent scanning-tunneling-microscopy (STM) experiments by Baski, Nogami, and Quate[1,2] on the adsorption of indium (In) on Si(100)-(2×1) surfaces have shown that for coverages at or below 0.5 monolayer (ML) and at a temperature of ~100 °C, a (2×2) reconstruction is formed. The structural model proposed by Baski, Nogami, and Quate[2] for the (2×2) geometry consists of an In ad-dimer located between the Si dimer rows, with the ad-dimer oriented orthogonally to the Si-Si dimer bond as shown in Fig. 1(a). They pointed out, however, that a parallel In ad-dimer configuration was also a possibility,

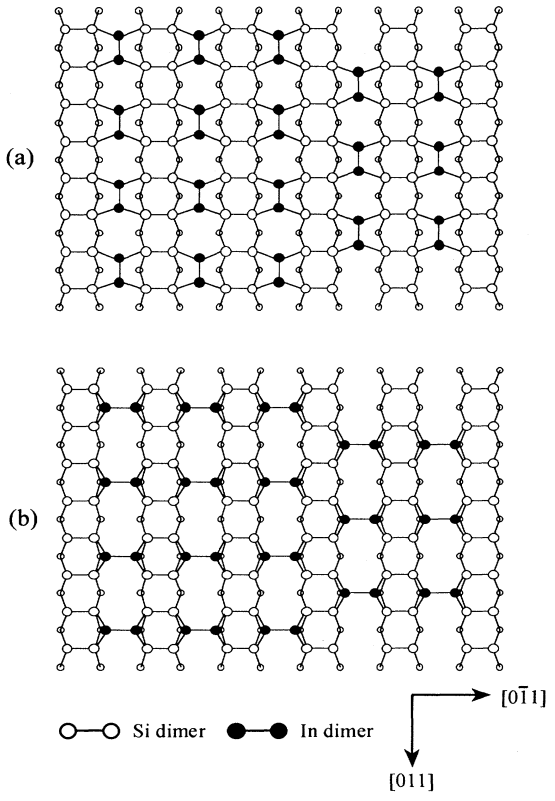

FIG. 1. Plan view of the Si(100)-(2×2)In structure with (a) orthogonal In ad-dimers and (b) parallel In ad-dimers. Antiphase domains are shown in both models.

consistent with a model they proposed in their work on the Si(100)-(2×2)Al reconstruction.[3] The parallel ad-dimer model is shown in Fig. 1(b). Inasmuch as the metal ad-dimers in the STM images are not atom resolved, it is uncertain which configuration represents the correct description of the (2×2) geometry. Recently, Northrup *et al.*[4] performed first-principles total-energy calculations on the two possible configurations for the (2×2) surface and the results strongly favor the parallel ad-dimer model. Moreover, they also found that the surface-state spectrum calculated on the basis of the parallel ad-dimer model was in good agreement with angle-resolved photoemission results for the Si(100)-(2×2)In surface. In this paper, we present results from STM and impact-collision ion-scattering spectrometry (ICISS) experiments to resolve the issue of whether the (2×2) surface consists of parallel or orthogonal In ad-dimers.

A normal Si(100) surface contains an almost equal distribution of (2×1) and (1×2), or type *A* and type *B* in Chadi's notation,[5] terraces because of the slight vicinality that generally persists. This creates a problem for ICISS experiments, because to the incident ion beam a parallel In ad-dimer of the (2×2) reconstruction on the type-*A* terrace is equivalent to an orthogonal ad-dimer on the type-*B* terrace. ICISS will be of no use in distinguishing between the two models under such experimental conditions. To overcome this problem, we used a vicinal Si(100) surface with a misorientation of 4° towards the [011] direction. Such a surface is found to consist predominantly of type-*B* terraces, i.e., with dimer rows perpendicular to the step edge, separated by double steps,[6] as predicted by Chadi.[5]

Figure 2 shows an STM image of the Si(100) vicinal surface with type-*B* terrace widths of ~45 Å. An analysis of five STM images similar to Fig. 2, taken on different regions of the Si(100) vicinal surface, indicates that the surface comprises 85% type-*B* terraces and 15% type-*A* terraces. Indium was deposited onto the Si(100)-(2×1) vicinal surface at temperatures of ~100 °C. The (2×2) reconstruction was observed at coverages from 0.25 to 0.5 ML, as shown in Fig. 3, in the form of In dimer rows. Individual atoms in the In ad-dimers cannot be resolved, and the (2×2)In structure can be represented by either the orthogonal or the parallel ad-dimer model

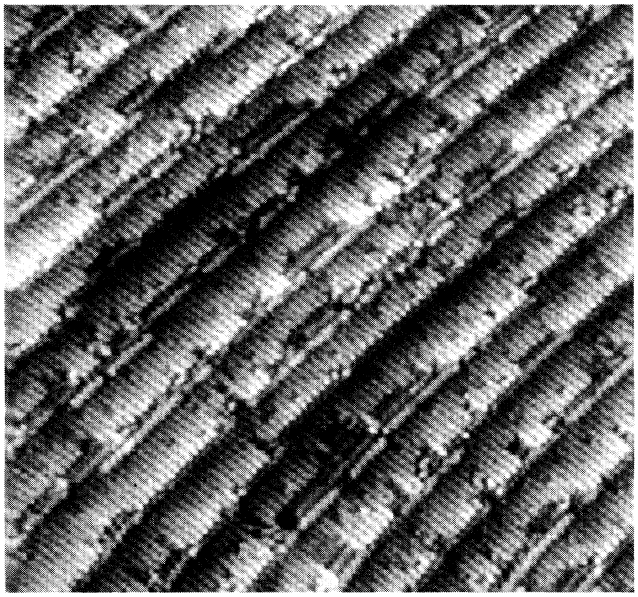

FIG. 2. A 500×500-Å^2 STM image of a clean vicinal Si(100) surface tilted 4° towards [011], comprising mostly type-B terraces ~45-Å in width. The Si dimer rows are clearly visible. The terraces step down from upper left to lower right.

shown in Fig. 1. The existence of antiphase domains found in all (2×2)In STM images such as those in Fig. 3 is reflected in our two models shown in Fig. 1. Most of the (2×2)In dimer rows lie along the step edges of the Si(100) vicinal surface, presumably adsorbed on the type-*B* terraces, while a smaller number are found to lie perpendicular to the step edges, presumably on type-*A* terraces. Interestingly, however, the ratio of these two domains of In ad-dimers changes with coverage. As the In coverage increased from 0.25 to 0.5 ML, the proportion of In dimer rows parallel to the step edges was found to decrease from almost 90% to about 75% from an analysis of a series of STM images. Such a change implies that In adsorption has caused movement of the step edges and hence changes in terrace widths of the vicinal surface. The phenomenon of metal-adsorbate-induced motion of step edges has been reported previously by Nogami, Baski, and Quate[7] on Ga adsorption on vicinal Si(100) surfaces. As a result of our STM investigations, we performed the ICISS experiments with coverages between 0.3 and 0.4 ML where ~85% of the (2×2)In reconstruction was expected to consist of a single domain, i.e., with the In dimer rows parallel to the step edge.

The ICISS experiments were carried out in a separate ultrahigh vacuum chamber described previously.[8] The Si(100) vicinal surface was flashed to 1200 °C for several seconds and cooled to room temperature where the low-energy electron-diffraction (LEED) pattern indicated a predominately single-domain (2×1) surface. The [0$\bar{1}$1] step edge direction was confirmed by the splitting of spots in the (2×1) pattern. Indium was deposited via a heated tungsten basket onto the Si(100) vicinal surface, at ~100 °C, with the coverage measured by a quartz crystal monitor. After deposition of 0.3–0.4 ML of In, a (2×2) LEED pattern was obtained. Polar angle scans for 2-keV Li^+ ions backscattered (scattering angle 163°) from the In adatoms were taken along the two main azimuths [011] and [0$\bar{1}$1] directions, i.e., perpendicular and parallel to the step edges, respectively. Typical polar angle scans taken along the two azimuths are shown in Fig. 4. Repeated scans produced essentially the same results, with the major shadowing peak occurring at a 9° polar angle for the [011] azimuth and at 12° for [0$\bar{1}$1]. The solid curves in Fig. 4 are fits to the scans produced from a computer-simulation procedure of the ICISS process in which the backscattered ion intensity was represented by

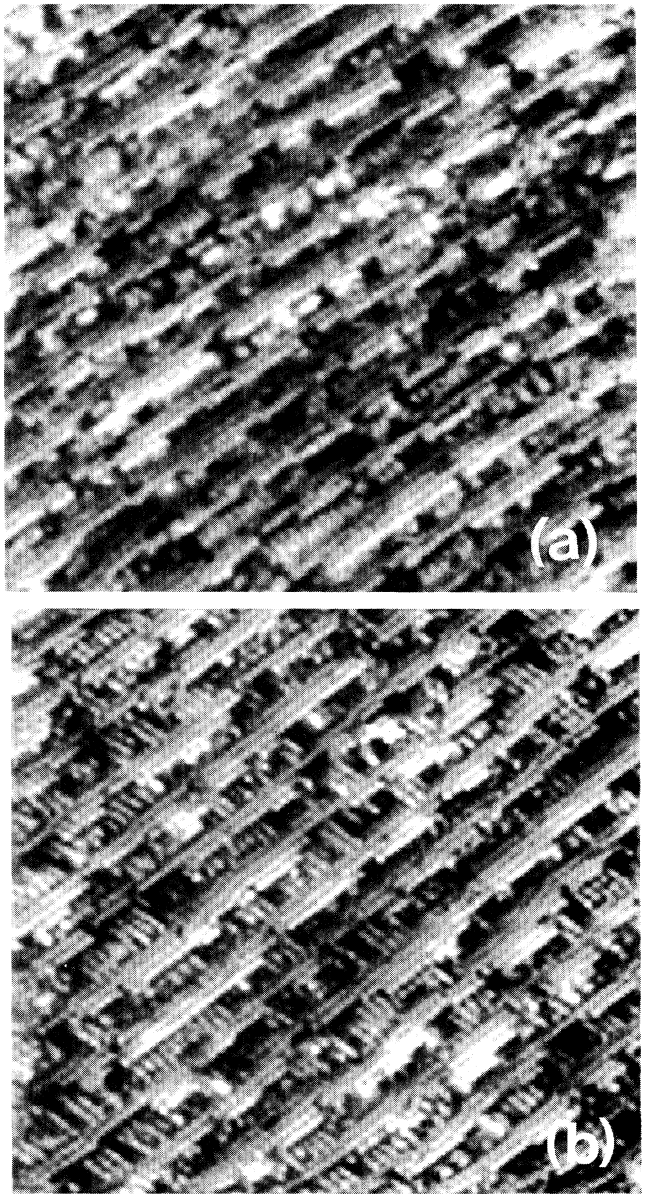

FIG. 3. Vicinal Si(100) surfaces after deposition of In at coverages (a) 0.25 ML and (b) 0.5 ML. The In ad-dimer rows of the (2×2) structure are clearly visible. Scan area is 500×500 Å^2.

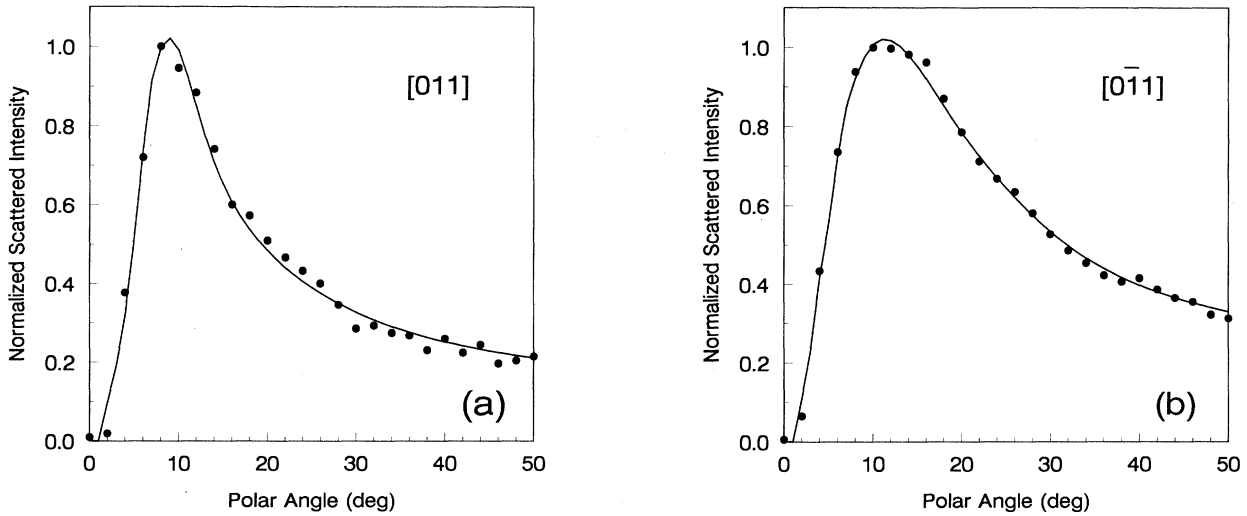

FIG. 4. ICISS polar angle scans for 2-keV Li^+ ions backscattered from In atoms along (a) the [011] azimuth and (b) the [0$\bar{1}$1] azimuth. The solid curves are computer-simulated fits based on the parallel ad-dimer model shown in Fig. 1(b).

the hitting probability in a two-atom model proposed by Tromp and van der Veen.[9] Thermal vibrations of the In adatoms, 0.26 Å, were incorporated in the simulation. A scaling factor of 0.65 was used in calculating the Fermi screening radius in the Moliere potential for the 2-keV Li^+ ions.[10]

The curve fits to the ICISS polar angle scans in Fig. 4 are based on the parallel ad-dimer model in Fig. 1(b). The main shadowing peak at 9° for scattering along the [011] azimuth, i.e., perpendicular to the step edges, in Fig. 4(a) is due to the In-In shadowing distance of 7.7 Å. This is the only shadowing condition for the parallel ad-dimer configuration along the [011] azimuth and the polar angle scan shows a sharp peak at 9° with a rapid falloff towards both lower and higher angles. The computer simulation (solid curve) shows good agreement with experiment. Along the [0$\bar{1}$1] azimuth, i.e., parallel to the step edges, the polar angle scan in Fig. 4(b) shows a broad peak around 12° with a gradual falloff at higher angles. This is caused by the blending of two shadowing conditions: (a) an In atom shadowing another In atom within the In ad-dimer, with a shadowing distance equal to the ad-dimer bond length of 2.8 Å; and (b) an In atom of an ad-dimer shadowing the nearest In atom of a neighboring ad-dimer, with a shadowing distance of 4.9 Å. No other shadowing conditions exist. Once again, the computer-simulated curve shows good agreement with experiment. The bond lengths used in the computer simulations were taken from the calculations of Northrup *et al.*[4] To obtain the best fit with experiment we have assumed that 17% of the (2×2)In surface consists of the second domain, i.e., with In dimer rows perpendicular to the step edges. This is in agreement with our STM observations that the ratio of the two (2×2)In domains on the Si(100) vicinal surface is around 80:20 at the coverage range of 0.3–0.4 ML.

If the (2×2)In surface consists of orthogonal dimers instead of parallel dimers, the computer simulations will be exactly reversed for the two azimuths because of the symmetry of the two configurations, i.e., the narrow peak at 9° would occur along the [0$\bar{1}$1] azimuth, and the broad peak at 12° would occur along the [011] azimuth. It would be highly desirable to perform ICISS polar angle scans along azimuths other than [011] and [0$\bar{1}$1] to further confirm our findings. Unfortunately, however, because of the existence of antiphase domains in the (2×2) reconstruction as evident in the STM images, scattering along azimuths between the [011] and [0$\bar{1}$1] directions tends to produce near-identical shadowing conditions for both orthogonal and parallel ad-dimer models. So the polar angle scans along the [011] and [0$\bar{1}$1] azimuths are the only ones useful for distinguishing between the two ad-dimer configurations. Our results strongly favor the parallel ad-dimer model, in agreement with the total-energy calculations of Northrup *et al.*[4]

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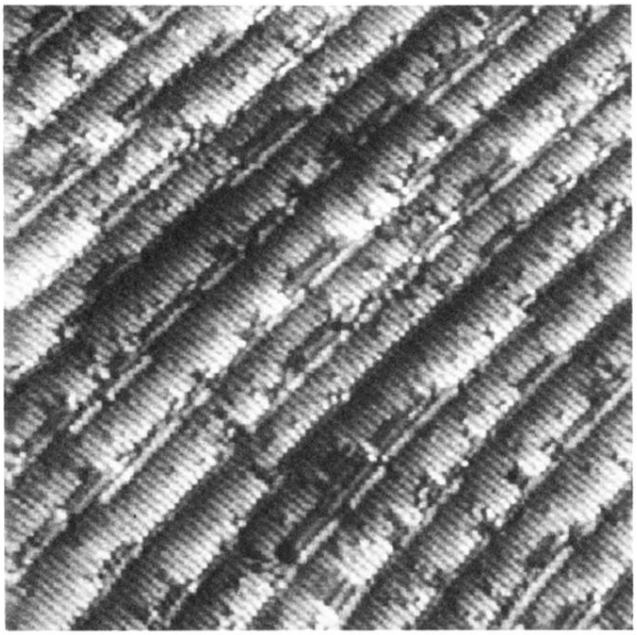

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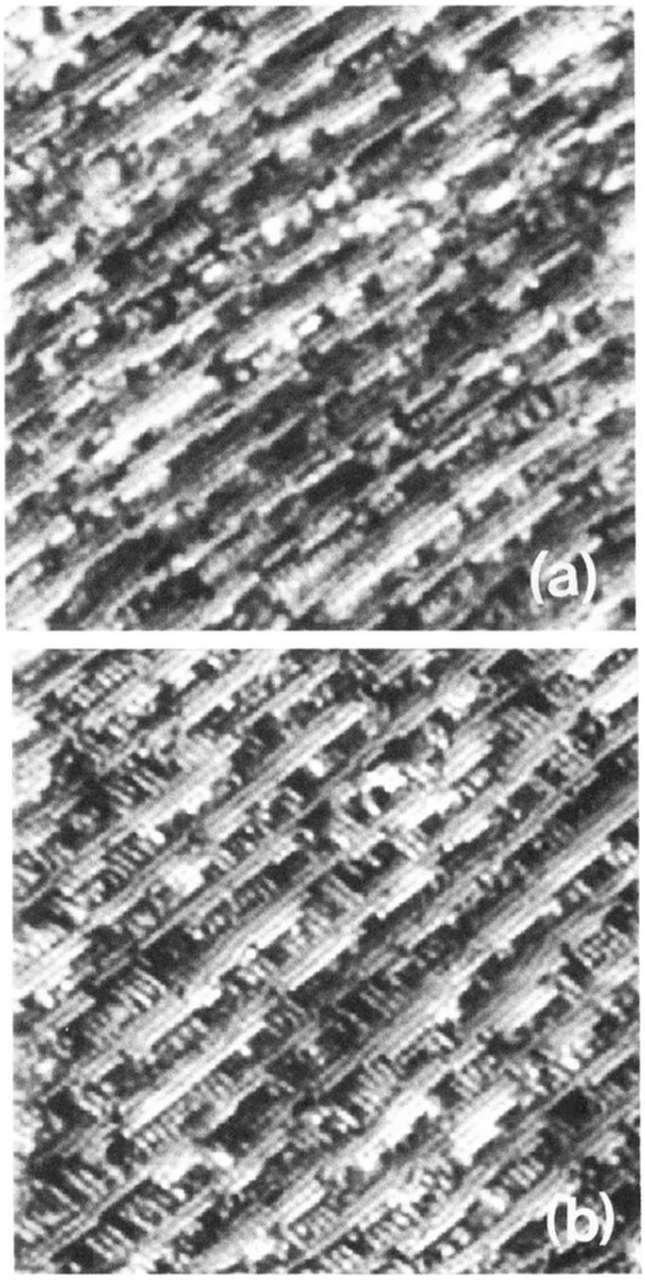

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