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Atomic configuration of hydrogenated and clean Si(110) surfaces

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Step structure models for hydrogenated and clean Si(110) surfaces are proposed by kinematical analysis of low-energy electron diffraction patterns. The step structures are described as periodically up and down sequence of terraces with $[\bar{1}\bar{1}2]$ step boundaries and the step height is within ±5% of the bulk Si(110) layer spacing. The number of Si atoms on each terrace along a [110] direction is 8±1.

I. INTRODUCTION

In the past, for clean Si(110) surfaces neither the unit cell nor the atomic configuration had been clarified. Some workers[1-6] reported the various unit cells at room temperature. Recently, we have determined that the unit cell of the clean surface is a "16×2" structure suggested by Yamamoto and Ino[6] and that the other unit cells, i.e., 4×5, 2×1, and 5×1 structures are induced by a small amount of nickel.[7]

In the present paper, we report on our study of atomic configuration of the surface by means of low-energy electron diffraction (LEED). To simplify the complicated LEED patterns, atomic hydrogen was adsorbed on the surface at room temperature. As for the LEED patterns, it was reported that the fractional-order spots weaken or disappear in the case of hydrogenation of the Si(111)7×7 (Ref. 8) the cleaved Si(111)2×1 (Ref. 9), and the Si(100)2×1 (Ref. 10) surfaces. These results are interpreted as the hydrogen causing Si atoms in the unit cells to be in the bulklike structural sites.[11,12]

A kinematical LEED calculation is available for analyzing surface structures. Webb and Lagally[13] studied kinematical LEED quantitatively. Defected surfaces were analyzed by means of LEED.[14-16] McRae[11,17,18] analyzed the LEED patterns of several kinds of semiconductor surfaces kinematically using a double diffraction mechanism.

The primary purpose of the present paper is to clarify atomic configuration of the hydrogenated Si(110) surface. In the present LEED data, fractional-order spots disappear with hydrogenation, but integer-order spots and the areas around them remain, when low-energy electron-energy-loss spectra show the hydrogen's saturation of Si dangling bonds on the surface. For this surface we analyzed characteristics of the relative intensities of LEED spots as a function of the primary energy. We propose a step structure for the hydrogenated Si(110) surface structure. Next, we report atomic configuration of the clean Si(110) surface. LEED spot intensities of the clean surface show the same inherent characteristics in the step structure as those of the hydrogenated surface. A step structure model for the clean surface structure is discussed on the basis of the kinematical LEED analysis.

II. EXPERIMENTAL

The present experiment was made in an ultrahigh vacuum of 1×10^{-10} torr. LEED patterns were observed by a four-grid optics for normally incident electrons. A single-pass cylindrical mirror analyzer was used for low-energy electron-energy-loss spectroscopy (LEELS) and Auger-electron spectroscopy (AES).

A sample showed a mirror polished Si(110) surface of a *p*-type wafer with a resistivity of 10–20 ohm cm. The sample was cleaned in a CP4 etchant before being mounted on a tantalum sample holder and heated repeatedly up to 1200 °C by passing electric current through the sample in a vacuum of less than 2×10^{-10} torr. The contamination of the surface was checked by AES. No impurity was found in the clean Si(110) surface. The atomic hydrogen was produced by dissociating H_2 to 2H with the heated W filament of an ion gun. After hydrogenation, AES spectra showed no impurity peak except for a small residual carbon peak at 273 eV and an oxygen peak at 503 eV whose intensities were less than 4×10^{-3} of the silicon peak at 92 eV.

III. EXPERIMENTAL RESULTS AND DISCUSSION

A. Hydrogenated Si(111) surface

Atomic hydrogen was adsorbed on the clean Si(110) surface by the method described in Sec. II. LEELS spectra show that a peak around energy loss 8 eV becomes high with an increase of exposure time of the hydrogen. In the case of the clean surface there is no peak in the energy range.[19] Ibach and Rowe[9] reported that the hydrogen causes a peak around energy loss 8 eV to be higher for the Si(111)7×7, the cleaved Si(111)2×1, and the Si(100)2×1 surfaces forming Si—H covalent bonds. For the Si(110) surface, as well as for these structures, our result indicates that the atomic hydrogen forms Si—H covalent bonds. As for LEED patterns, diffraction spot intensities weaken as the exposure time of the hydrogen increases, but those of the integer-order spots and the areas around them do not. The LEELS spectra and LEED patterns remain unchanged with hydrogen exposure over 1.2×10^{-2} torr sec. It is thought that the hydrogen saturates dangling bonds under this condition.

We observed the LEED patterns of the H-saturated surface with primary energy 20—120 eV. The typical patterns at $E_p = 35$, 50, 65, and 80 eV are shown in Fig. 1(a)—1(d). The characteristics of the LEED spot intensities are as follows.

(i) At every primary energy, intensities of the diffraction spots are always below our detection limit except those of integer-order spots and the areas around them indexed $(p_1 + q/16, p_2)$: p_1 and p_2 are integers and $q = 0$, $\pm 1, \pm 2, \pm 3$. This corresponds to reports that hydrogen makes the fractional-order spots weaken or disappear for the other Si surfaces[8–10] and the surface structures revert to the bulklike structures.[11,12] For the Si(110) surface the present result indicates that the hydrogen causes the silicon atoms to be in a bulklike structural site.

(ii) Each spot intensity oscillates as the primary energy increases. The intensity depends on the surface-normal

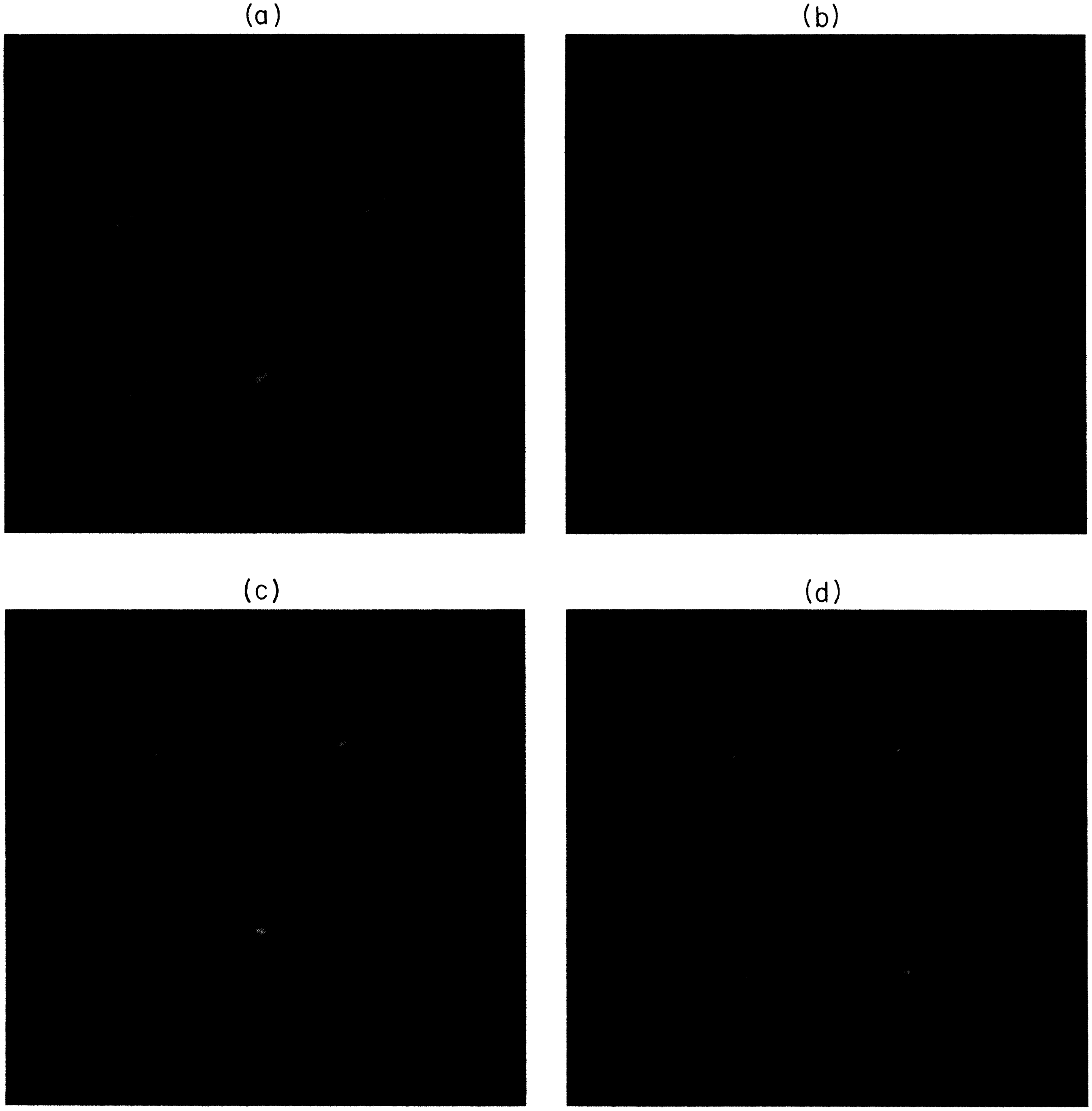

FIG. 1. The LEED patterns observed (photographs) and calculated (drawings) for the Si(110) + H surface at $E_p = 35$ eV (a),(e), 50 eV (b),(f), 65 eV (c),(g), and 80 eV (d),(h). The spots are indexed as shown in (e). The circled area of each calculated spot is proportional to the spot intensity. Weak intensity spots are omitted. In these calculations, it is set that $N_1 = N_2 = 8$ and $d = 1.92$ Å.

momentum transfer. Every spot shows the same period of oscillations corresponding to a bulk Si(110) layer spacing (1.92 Å). The Si(110) surface has a vertical atomic configuration of 1 monolayer.

(iii) When one spot intensity becomes local maxima, intensities of the two nearest-neighbor spots become local minima.

(iv) The fractional-order spot intensities around the (0,0) spot are always symmetric. This contradicts the periodically monotonous step structure for a vicinal surface.

On the basis of kinematical analysis, the fractional-order spots of the Si(110) + H surface are attributable to a periodic one-monolayer step array which is described by an up and down sequence of terraces. The unit cell of the Si(110) + H surface shows that the step boundaries are along a $[\bar{1}\bar{1}2]$ direction. The Si(110) + H surface structure is expected to be the step structure as shown in Fig.

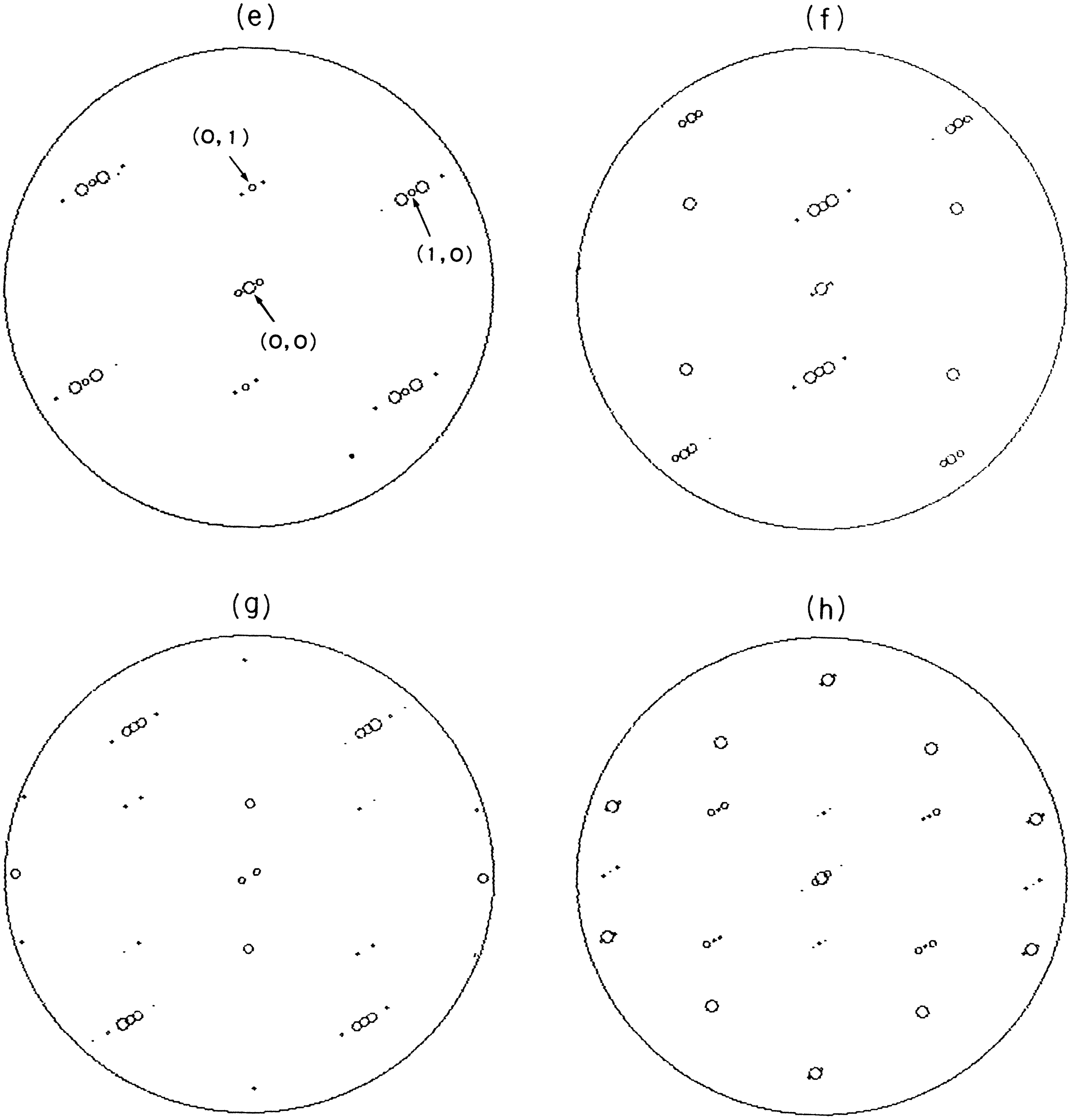

FIG. 1. (*Continued*).

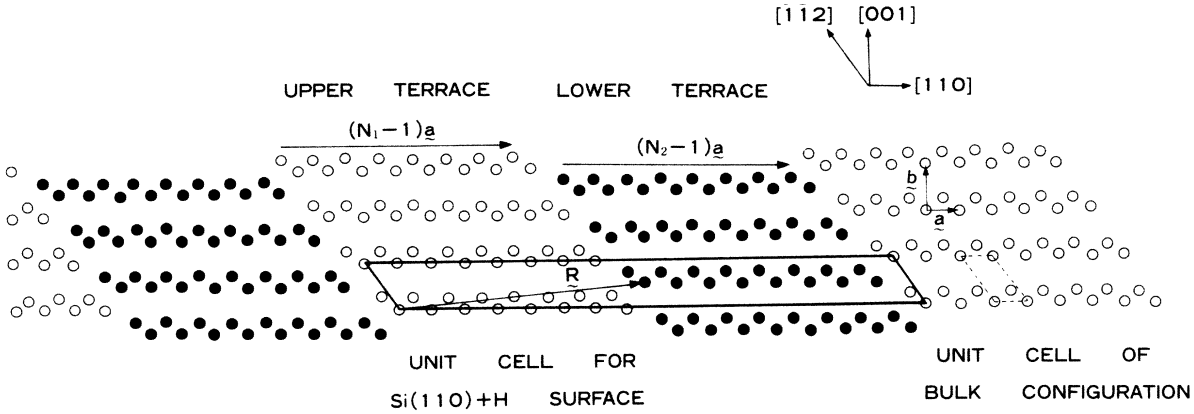

FIG. 2. Model of atomic configuration of the Si(110) + H surface from the top view. Open and solid circles denote the top-layer atoms in the upper and the lower terraces, respectively. The atoms in the underlayers are omitted. The "16×2" unit cell for the Si(110) + H surface is shown by the solid line. The 1×1 unit cell of bulk configuration is shown by the dashed line. In this figure, $N_1 = N_2 = 8$.

2. In this figure, N_1 and N_2 denote the number of Si atoms along a [110] direction on the upper and the lower terraces, respectively.

Local maxima of the fractional-order spot intensities, the indices of which are $(p_1 + q/16, p_2)$: p_1 and p_2 are integers and $q = \pm 2$, are very weak. The number of Si atoms on the upper and the lower terraces along the [110] direction is about eight.

In order to describe the detailed characteristics of the measured spot intensities, we discuss the diffraction mechanism. The measured fractional-order spot intensities are symmetric around each integer-order spot, besides the (0,0) spot. This is inconsistent with calculated results within the single-scattering LEED. The calculated fractional-order spot intensities are asymmetric around each integer-order spot, except the (0,0) spot; they are symmetric only around the (0,0) spot. Consideration of the double diffraction mechanism excludes this discrepancy.

Intensities of all measured spots are modulated with another periodicity which depends on the surface-normal momentum transfer. This periodicity corresponds to a bulk Si(110) layer spacing and can be derived by a reflection diffraction and the uniform attenuation of the primary beam under the top layer.

We assume the double diffraction mechanism reported by McRae,[11] that the fractional-order spots mainly stem from reflection diffraction in the underlayers, with forward diffraction at the top layer. We also assume the same scattering factor for all Si atoms and the uniform attenuation of the elastic beam under the top layer, neglecting the dependence on the scattering angle. The attenuation coefficient α is the ratio of the electron amplitude scattered by the atoms in the $(n+1)$th and nth layers, and is chosen so as to correspond to the measured period of the modulation for spot intensities.

Finally, a total diffraction wave field around an integer-order spot corresponding to the scattering vector $\mathbf{S}_0$ is given by the leading term at the given scattering vector $\mathbf{S}$ corresponding to a 16×2 reciprocal-net vector.

$$\sum_{j=0}^{1} e^{i(\mathbf{S}-\mathbf{S}_0)\cdot\mathbf{r}_j} \left[\sum_{n_1=0}^{N_1-1} e^{in_1(\mathbf{S}-\mathbf{S}_0)\cdot\mathbf{a}} + \sum_{n_2=0}^{N_2-1} e^{in_2(\mathbf{S}-\mathbf{S}_0)\cdot\mathbf{a}+i\mathbf{S}\cdot\mathbf{R}} \right]$$

$$\times \sum_{j=0}^{1} e^{i\mathbf{S}_0'\cdot\mathbf{r}_j} \sum_{l=0}^{1} \alpha^{l+1} e^{i\mathbf{S}_0'\cdot\boldsymbol{\rho}_l} \sum_{m=0}^{\infty} \alpha^{2m} e^{-i(2m\mathbf{S}_0'\cdot\mathbf{C})} ,$$

$$\mathbf{r}_0 = 0, \quad \mathbf{r}_1 = -\tfrac{1}{2}\mathbf{a} + \tfrac{1}{4}\mathbf{b}, \quad \mathbf{R} = (N_1 - \tfrac{1}{2})\mathbf{a} + \tfrac{1}{2}\mathbf{b} - \mathbf{c} ,$$

$$\boldsymbol{\rho}_0 = -\tfrac{1}{2}\mathbf{a} + \tfrac{1}{2}\mathbf{b} - \mathbf{c}, \quad \boldsymbol{\rho}_1 = -2\mathbf{c} ,$$

where $\mathbf{r}_j$ indicates the atom positions in the local 1×1 unit cell, **a**, **b**, and **R** are shown in Fig. 2, and **c** is a unit vector in the surface-normal direction whose length is a Si(110) layer spacing. The $\mathbf{S}_0'$ is a scattering vector in the underlayers for which an inner potential of 12 eV is considered, and corresponds to the vector $\mathbf{S}_0$ for which the inner potential is not considered. The summation over j is carried out to consider the structure factor of the local 1×1 unit cell in each underlayer and over l the shift of Si

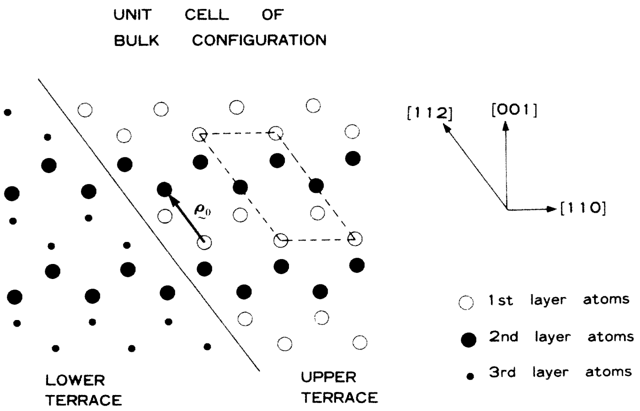

FIG. 3. Enlarged diagram of Fig. 2. Open circles denote the first layer atoms. Large and small solid circles denote the second and third layer atoms, respectively. The 1×1 unit cell of bulk configuration is shown by the dashed line.

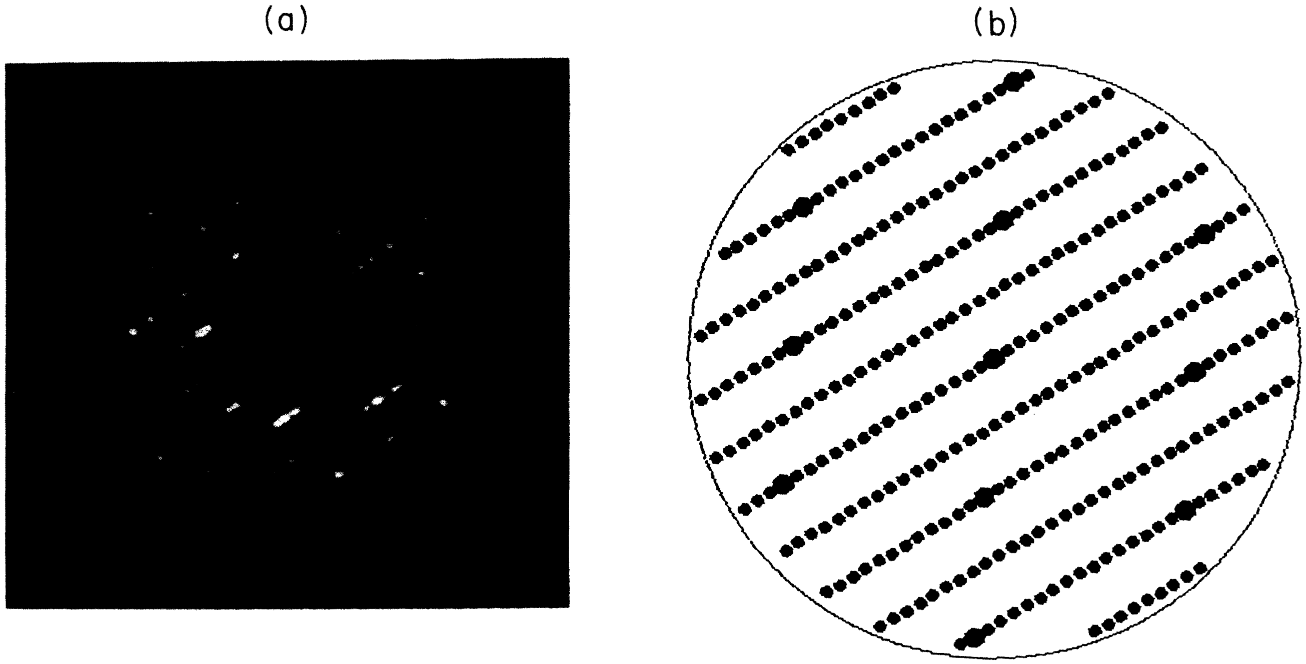

FIG. 4. (a) LEED pattern for the clean Si(110) surface at $E_p = 35$ eV. (b) Scheme of the pattern. Large circles denote integer-order spots and small circles denote fractional-order spots.

atom positions between the nth and the $(n+1)$th layers corresponding to the vector ρ_0, as shown in Fig. 3. We neglect other contributions such as the Debye-Waller factor, because they do not affect the essential characteristics of the spot intensities.

The diffraction spot intensity is proportional to the square of the diffraction wave field. The calculated results show the following parameters: the step height $d = 1.92$ Å within $\pm 5\%$, $7 \le N_1, N_2 \le 9$, and $\alpha = 0.31$, 0.37, 0.42, and 0.46 at $E_p = 35$, 50, 65, and 80 eV, respectively. The typical calculated results are shown in Figs. 1(e)–1(h) under the condition $N_1 + N_2 = 16$. The observed LEED patterns are explained qualitatively by the step structure model and the double diffraction mechanism.

The structure model of the Si(110) + H surface is in good agreement with the experimental results, except for an inconsistency; i.e., the diffraction spots indexed $(0, -2)$ and the areas around them appear [Figs. 1(a) and 1(b)]. These diffraction spots are expected to disappear so as to satisfy the extinction rule when the local surface structure forms a 1×1 structure, because the 1×1 unit cell has two Si atoms. On the contrary, the intensities of diffraction spots indexed $(\pm 1, \mp 1)$ and the areas around them are very weak, satisfying the extinction rule. These results can be explained by considering the slight-lateral displacements of atoms in a few layers from the surface along the [001] direction. These displacements change the structure factor of the 1×1 unit cell and make the $(0, -2)$ spot and the area around it appear, but the other spot intensities are scarcely changed.

B. Clean Si(110) surface

LEED patterns of the clean Si(110) surface at various primary energies usually show a 16×2 structure. As a typical example we show a LEED pattern at $E_p = 35$ eV in Fig. 4. Sometimes the surface shows a "32×2" struc-

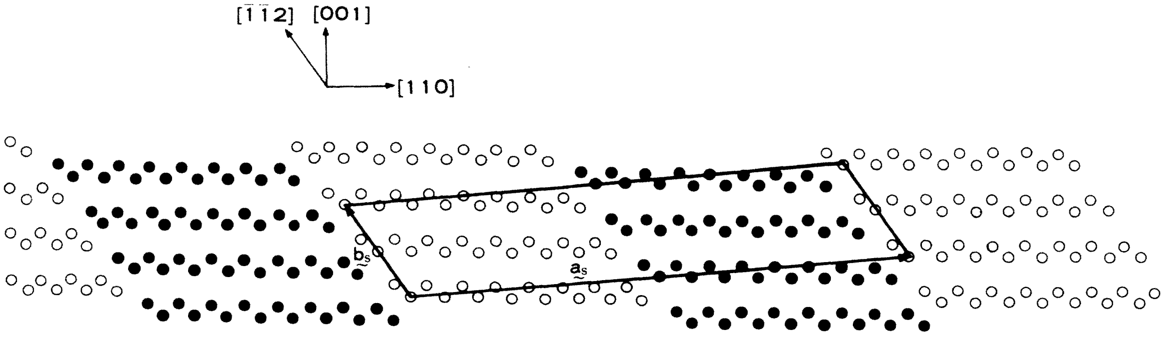

FIG. 5. Unit cell for the clean Si(110)-("16×2") surface. Open and solid circles denote the top layer atoms in the upper and the lower terraces, respectively. The atoms in the underlayers are omitted.

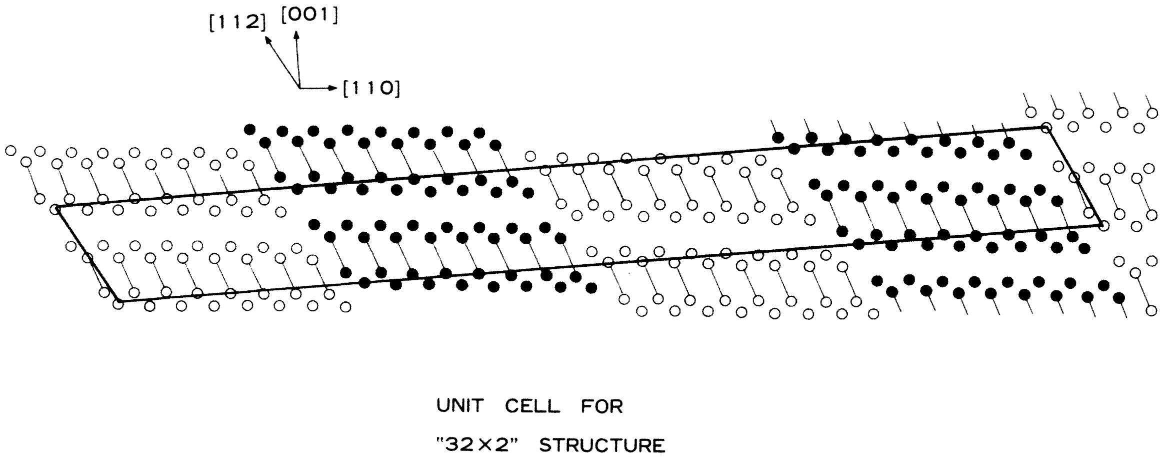

FIG. 6. A possible structure model for the clean Si(110)-("32×2") surface. Two atoms connected with a line make a pair.

ture. First we discuss the 16×2 structure. The structure shows characteristics of the spot intensities similar to those of the hydrogenated surface structure: (i) The clean surface shows the unit vector attributable to the step boundaries for the hydrogenated surface. (ii) Each spot intensity depends on the surface-normal momentum transfer reflecting the Si(110) layer spacing. (iii) When one spot intensity becomes local maxima, intensities of the two nearest-neighbor spots become local minima. Therefore the fractional-order spots of the clean surface are inherent in the step structure that the hydrogenated surface has. We conclude that the clean Si(110) surface mainly consists of the same step structure as the Si(110) + H surface.

On the other hand, the clean surface shows characteristics of the LEED spots different from those of the hydrogenated surface. The unit cell of the clean surface in a real space is shown in Fig. 5. (In this figure silicon atoms are on the bulk structural sites for the sake of simplicity.) The unit vector $\mathbf{b}_s$ along the $[\bar{1}\bar{1}2]$ direction disappears with the hydrogenation, at room temperature. No large transport of Si atoms is thought to occur with the hydrogenation. Therefore the periodicity is not caused by the surface defect, but by surface rearrangement.

The integer-order spot intensities are weak and the fractional-order spots can be observed not only around the integer-order spots but also between these spots. The silicon atoms on the clean surface are not in the bulk structural sites.

The clean Si(110) surface sometimes shows a 32×2 structure, of which periodicity along a [15 15 1] direction is twice as large as that of the 16×2 structure. The hydrogenated surface has not been shown periodicity along the [15 15 1] direction.

We discuss a possible structure model for the clean surface. Each terrace consists of atom rows (zig-zag chains) parallel to the [110] direction. The periodicity along the $[\bar{1}\bar{1}2]$ direction, which is twice as large as that of the hydrogenated surface, may be attributable to paired rows of atoms parallel to the [110] direction, the structure of which is similar to that of the dimer model of the Si(100)2×1 structure.[20,21] When the adjacent rows are paired, the surface unit cell has periodicity along the $[\bar{1}\bar{1}2]$ direction. The paired rows are thought to induce large lateral displacements for the Si atoms a few layers from the surface.

A possible model for the 32×2 structure is shown in Fig. 6. With hydrogenation the periodicity along the [15 15 1] direction is thought to disappear because of the relaxation for the paired rows.

We sometimes observed a two-domain 16×2 structure on the clean surface. The step boundaries of the surface are along the $[\bar{1}\bar{1}2]$ and a [112] direction. The structure is thought to be the same as the X structure reported by Jona.[1]

For clean Ge(110) surfaces, Noro and Ichikawa[22] reported the same unit cell as that for the clean Si(110) surface. The structure may be explained by the step structure model proposed in this paper.

IV. CONCLUSION

For the Si(110) + H surface we propose the step structure model which consists of a periodic step array restricted to two layers, as shown in Fig. 2. This structure model is specified as follows: the step boundaries are along the $[\bar{1}\bar{1}2]$ direction, the step height is within $\pm5\%$ of the bulk Si(110) layer spacing, the number of atoms N_1 along the [110] direction on the upper terrace is in the range $7\leq N_1\leq9$, the number N_2 on the lower terrace is in the range $7\leq N_2\leq9$, and silicon atoms on the surface are in the bulklike structural site.

For the clean Si(110) surface the step structure model is also proposed. The surface structure consists of the same outline ascribable to the step structure as to the hydrogenated surface structure. Silicon atoms in the 16×2 unit cell are not in the bulklike structural site. The paired-rows model is suggested for the reconstructed structure.

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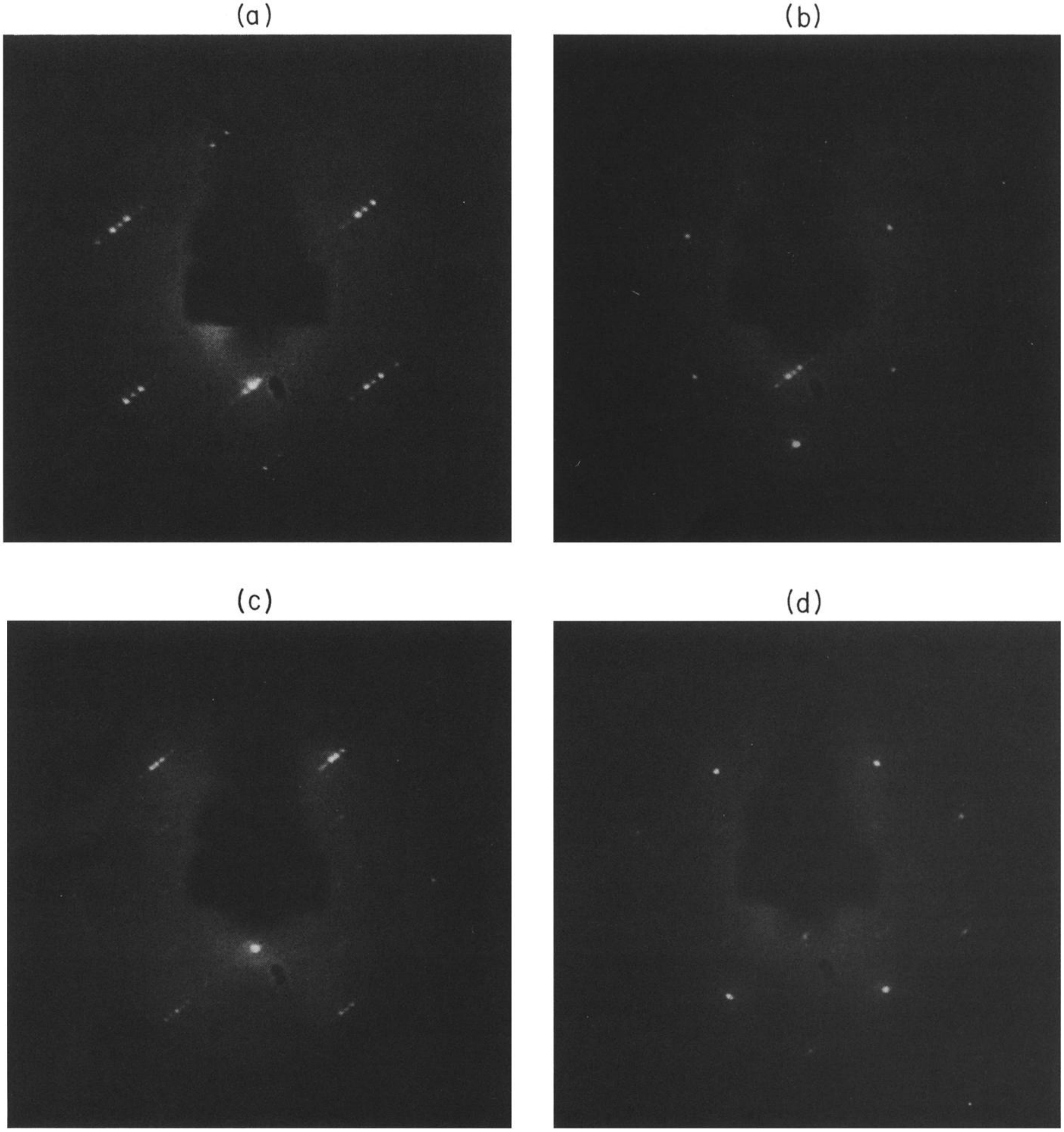

FIG. 1. The LEED patterns observed (photographs) and calculated (drawings) for the Si(110) + H surface at $E_p=35$ eV (a),(e), 50 eV (b),(f), 65 eV (c),(g), and 80 eV (d),(h). The spots are indexed as shown in (e). The circled area of each calculated spot is proportional to the spot intensity. Weak intensity spots are omitted. In these calculations, it is set that $N_1=N_2=8$ and $d=1.92$ Å.

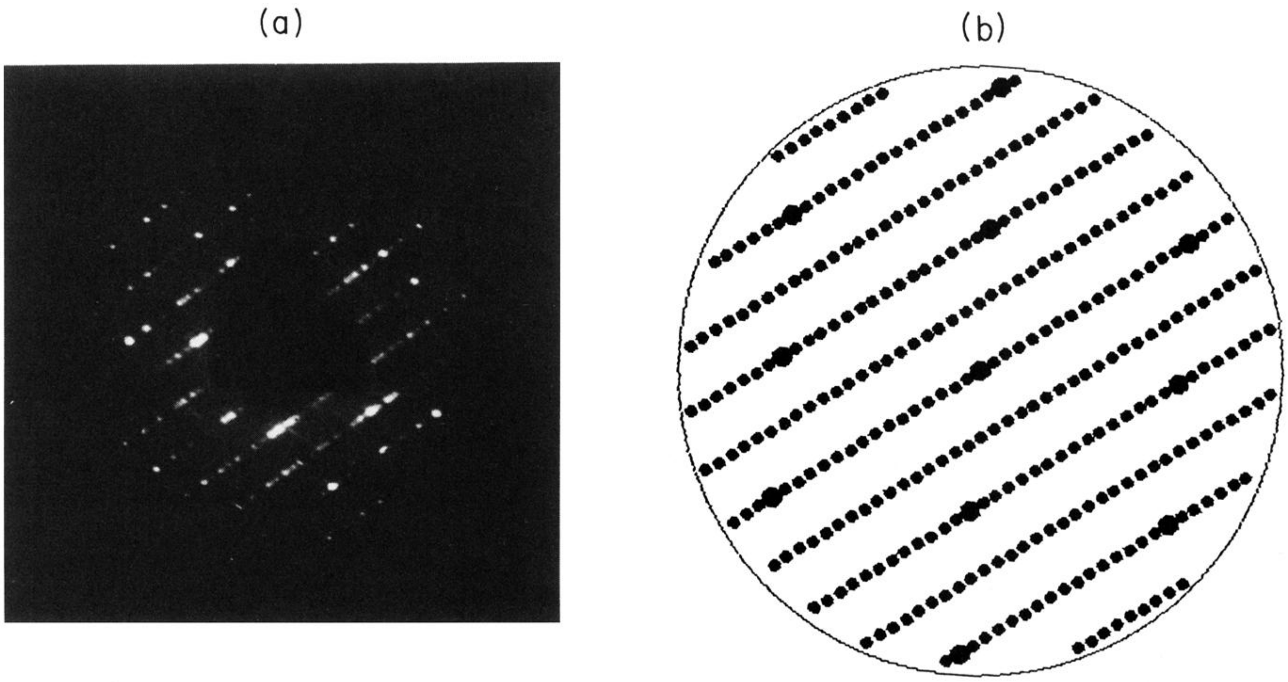

FIG. 4. (a) LEED pattern for the clean Si(110) surface at $E_p = 35$ eV. (b) Scheme of the pattern. Large circles denote integer-order spots and small circles denote fractional-order spots.