Electron scattering from the K-exposed Si(100)(2×1)-H surface

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The interaction of K with the Si(100)(2×1)-H surface has been investigated using high-resolution electron-energy-loss spectroscopy. For a low fractional K coverage ($\Theta_K=0.1$), a broadening of the quasielastic peak was observed. On the basis of its temperature dependence and by a comparison with electron-scattering theory, it is proposed that K adatoms form localized donor levels lying below the conduction band, which is regarded as a two-dimensional electronic system because of the downward band bending near the surface, and that the origin of the broadening is the multiple excitation of plasmons associated with electrons that are thermally excited from the donor levels into the conduction band. A narrowing of the quasielastic peak was observed with increasing Θ_K, and is attributed essentially to the displacement of hydrogen upon K adsorption. The Si-H stretching energy decreases by ~20 meV with increasing Θ_K, which is attributed to the Si-H bond weakening due to charge transfer from the K adatoms. The adsorption of H atoms on the K-covered Si(100) surface is briefly discussed.

I. INTRODUCTION

High-resolution electron-energy-loss spectroscopy (EELS) is one of the most powerful techniques for the study of the physical and chemical phenomena on solid surfaces. EELS has been applied very successfully to the study of vibrations of adsorbates on metal and semiconductor surfaces.[1] Since the observation of the conduction-band surface plasmon by Matz and Lüth[2] for GaAs(110), EELS has also been used for the study of the surface electronic properties, e.g., the band bending and electronic states near the Fermi level of semiconductor surfaces. In particular, from the temperature-dependent study of the linewidth of the quasielastic peak, much information about the electronic properties of semiconductor surfaces are derived. Demuth and Persson[3] carried out experiments and theoretical analyses for the clean Si(111)(7×7) surface and derived information on the electronic states near the Fermi level. Studies on the space-charge layer were made by Strocio and Ho[4] [for the Si(111)(7×7) surface] and Dubois, Zegarski, and Persson[5] [for the GaAs(100) surface] to deduce information on the band bending and position of the Fermi level.

A theoretical analysis for the linewidth of the quasielastic peak has been made by Persson.[3,6] The mechanism of the quasielastic peak broadening is classified into two limiting cases by a parameter β, which will be defined in Sec. III A as follows.

(i) For the case of high carrier concentration where $\hbar\beta \gg k_B T$ (k_B, Boltzmann constant; T, sample temperature), the broadening of the quasielastic peak is attributed to the one-particle excitation which is coupled to phonons, etc. (Drude damping), and the linewidth is proportional to T.

(ii) For the case of low carrier concentration where $\hbar\beta \ll k_B T$, multiple excitation of the two-dimensional plasmon broadens the quasielastic peak, and the linewidth is proportional to $\sqrt{T \ln T}$, and Drude damping is unimportant.

Avci, Dabbousi, and Al-Harthi[7] made EELS measurements for alkali-metal atoms on the H-saturated Si(111) surface and observed a broadening of the quasielastic peak which was attributed to the excitation of electron-hole pairs. However, they did not make detailed measurements of the linewidth (e.g., temperature-dependent study) so that the origin of the quasielastic broadening was ambiguous.

In the present work, we report our study on the K adsorption on the Si(100)(2×1)-H surface with use of EELS and thermal-desorption spectroscopy (TDS). We observed a broadening of the quasielastic peak for low fractional K coverage ($\Theta_K=0.1$) and measured its temperature dependence. Analysis was made of the temperature dependence of the linewidth by using the theoretical formalism developed by Persson.[3,6] The broadening is associated with the multiple excitation of the plasma oscillation of electrons thermally excited from the K-localized levels into the conduction band. Changes of the linewidth of the quasielastic peak, the Si-H stretching energy, etc., with increasing Θ_K have been studied. The H adsorption on the K-covered Si(100) surface is briefly discussed.

II. EXPERIMENT

All experiments were made by the use of an ultrahigh vacuum chamber which housed a high-resolution electron-energy-loss spectrometer, a quadrupole mass spectrometer for TDS and gas analysis, a four-grid retarding field analyzer with a normal-incidence electron gun for low-energy electron diffraction (LEED), and a spherical deflector analyzer for Auger electron spectroscopy (AES). For EELS measurements, a primary energy $E_p=7.1$ eV and an incidence angle $\theta_i=60°$ with respect to the surface normal were used. The ionizer of the mass spectrometer was enclosed in a Pyrex-glass envelope with a 4 mm diam aperture. The aperture was located 1 mm from the sample surface during the TDS measurements

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(heating rate, 8 K/s).

The sample used ($7\times8\times0.1$ mm^3) was of p type, doped, and 3000 Ω cm. The sample surface was cleaned by several cycles of Ne^+-ion bombardment and annealing to 1150 K. The sample heating was made by electron bombardment from the rear. The sample cleanliness was checked by EELS and AES. The sample temperature was measured by using an Alumel-Chromel thermocouple inserted between the Si sample and the mount.

The K atoms were deposited on the Si surface by using a well-outgassed chromate dispenser (SAES Getters) which was located 3 cm from the sample surface. The amount of the adsorbed K atoms was controlled by the deposition time keeping the current constant. The fractional K coverage Θ_K was estimated by the K TDS peak area assuming that the room-temperature saturation coverage corresponds to $\Theta_K=1$ on the basis of the double-layer model.[8,9] During deposition, the sample temperature was kept at 300 K and the background pressure below 1×10^{-10} Torr.

The atomic hydrogen was formed by the exposure of H_2 to a hot ($\sim$2000 K) and well-outgassed W filament. Formation of the monohydride phase was monitored by EELS, TDS, and LEED. In our experimental condition, the monohydride phase was observed by the exposure of 10 L H_2 (1 L$\equiv10^{-6}$ Torr sec). The fractional H coverage Θ_H was estimated by the H_2 TDS peak area using the fact that the monohydride phase corresponds to $\Theta_H=1$.

III. RESULTS AND DISCUSSION

A. Theory of electron scattering

We will analyze our EELS spectra (especially, the broadening of the quasielastic peak) using the theoretical formalism developed by Persson.[3,6] In the following is described a relevant part of his theory.

Let us consider a monochromatic electron beam of an incident energy E_p and an incident angle θ_i (measured from the surface normal). In the dipole theory, the single scattering probability $P_s(\omega)$ that an incident electron loses energy in the range between $\hbar\omega$ and $\hbar(\omega+d\omega)$, is given by

$$P_s(\omega)=\frac{2}{(ea_0\pi)^2}\frac{1}{k^2\cos^2\theta_i}\frac{v}{\omega}\times\int_0^\infty dx\frac{1}{x}f(x,\theta_i)\mathrm{Img}\left[\omega\frac{x}{v},\omega\right], \quad (1)$$

where

$$f(x,\theta_i)=\frac{1}{x}\int_0^{2\pi}d\phi\times\left[1+\left[\frac{1/x}{\cos\theta_i}-\tan\theta_i\cos\phi\right]^2\right]^{-2}, \quad (2)$$

a_0 is the Bohr radius, k the wave vector of the incident electron, $v=\hbar k/m$ the velocity of the incident electron, and Img the surface loss function that describes the energy absorption in the medium. If the loss energy of the excitation is very small, the distance $d\sim(2E_p/\hbar\omega)/k$ from the surface at which the excitation process starts will be large, and the multiple scattering must be considered. The scattering probability at a finite temperature including the multiple-scattering event $P(\omega)$ is given by

$$P(\omega)=\frac{1}{2\pi}\int dt\, e^{-i\omega t}\exp\left[\int d\omega' P_s(\omega')\{[n(\omega')+1](e^{i\omega' t}-1)+n(\omega')(e^{-i\omega' t}-1)\}\right], \quad (3)$$

where $n(\omega)=[\exp(\hbar\omega/k_BT)-1]^{-1}$ is the Bose-Einstein factor. Considering the second moment,

$$\langle(\Delta\omega)^2\rangle=\langle\omega^2\rangle-\langle\omega\rangle^2, \quad (4)$$

where $\langle\omega\rangle=\int d\omega\,\omega P(\omega)$, one can estimate the linewidth of the quasielastic peak in terms of the single scattering probability without the numerical calculation of $P(\omega)$ [Eq. (3)]. A simple expression for the linewidth of the quasielastic peak is given by

$$\langle(\Delta\omega)^2\rangle=\int d\omega\,\omega^2(2n(\omega)+1)P_s(\omega). \quad (5)$$

Consider a two-dimensional electronic system on top of a semi-infinite dielectric medium. Assume that Img is well approximated by

$$\mathrm{Img}=-\mathrm{Im}\frac{2}{\epsilon+1-4\pi ne^2q_\parallel/[m^*\omega(\omega+i/\tau)]}, \quad (6)$$

where $\epsilon\approx11.7$ is the bulk dielectric constant of Si, n the electron concentration (electrons per cm^3), m^* the effective mass of an electron, τ the relaxation time for the Drude damping, and $q_\parallel$ is the momentum transfer parallel to the surface. Substituting Eqs. (1) and (6) into Eq. (5), and introducing the dimensionless parameters $\xi=1/\beta\tau$, $\eta=\hbar\beta/k_BT$, and $\beta=4\pi ne^2/[m^*(1+\epsilon)v]$,

$$\langle(\hbar\Delta\omega)^2\rangle=\frac{2C}{\pi}(\hbar\beta)^2\int_0^\infty dy\frac{y}{e^{\eta y}-1}\times\int_0^\infty dx\, f(x,\theta_i)\times\frac{\xi}{\xi^2+(x-y)^2}, \quad (7)$$

where

$$C=\frac{4}{\pi}\frac{1}{\cos^2\theta_i}\frac{1}{ka_0}\frac{1}{\epsilon+1}.$$

[The temperature-independent contribution to $\langle(\hbar\Delta\omega)^2\rangle$

is neglected.] In the limit $\eta \ll 1$, one can use the asymptotic form $f \to (\pi/x)(1+\cos^2\theta_i)\cos\theta_i$ as $x \to \infty$ to obtain from Eq. (7),

$$\langle (\hbar\Delta\omega)^2 \rangle = 2C\pi \cos\theta_i (1+\cos^2\theta_i)\hbar\beta k_B T \times \ln(k_B T/\hbar\beta) \ . \quad (8)$$

B. Quasielastic-peak broadening and analysis of its temperature dependence for $\Theta_K = 0.1$

Figure 1 shows room-temperature EELS spectra in the specular mode of K on the Si(100)(2×1)-H surface (monohydride phase) for various K coverages. In the spectrum for $\Theta_K = 0$ corresponding to the Si(100)(2×1)-H surface, two loss peaks at 80 and 260 meV are observed which are assigned to the Si-H bending and stretching modes, respectively [Fig. 1(a)].[10] Broadening of the quasielastic peak is observed at $\Theta_K = 0.1$ [Fig. 1(b)]. In order to understand the origin of this broadening, measurements of the full width at half-maximum (FWHM) were made as a function of the sample temperature between 150 and 300 K, and the results are shown by the open circles in Fig. 2, where the FWHM corresponding to 0 K is assumed to be the same as that of the Si(100)(2×1)-H surface. It is noted that the FWHM for the Si(100)(2×1)-H surface is 11.5 meV, whereas that for clean Si(100)(2×1) is 12 meV.

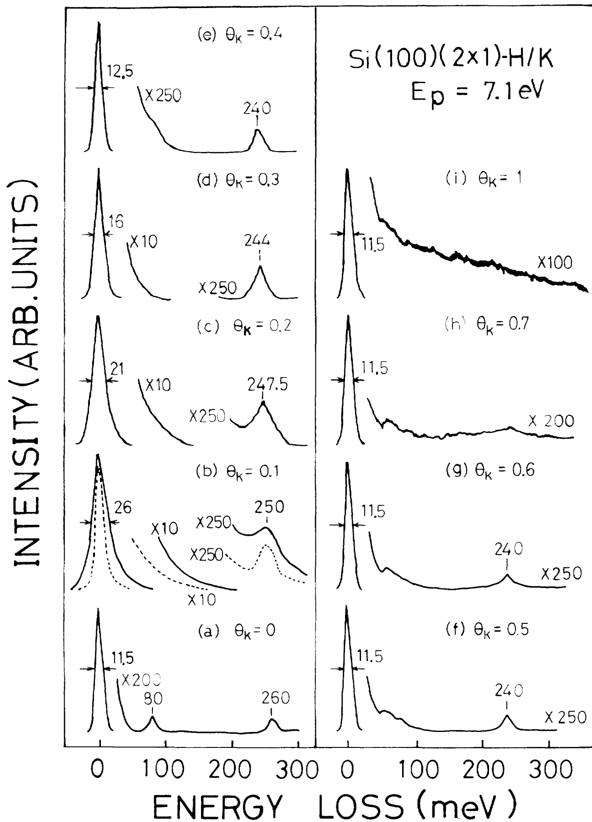

FIG. 1. EELS spectra in the specular mode of K on the Si(100)(2×1)-H surface obtained as a function of the fractional K coverage Θ_K at room temperature. The dashed curve in (b) is recorded at 150 K. $E_p = 7.1$ eV.

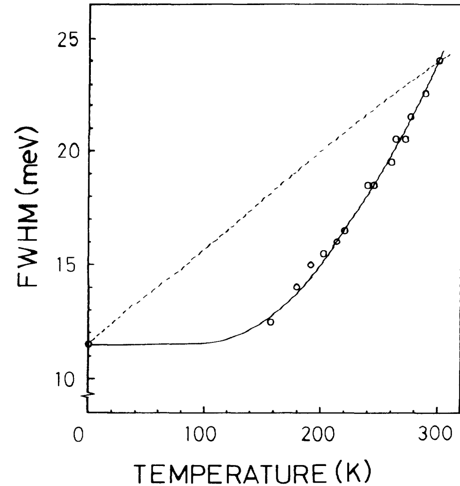

FIG. 2. The measured FWHM of the quasielastic peak is plotted by open circles as a function of the sample temperature of the K-exposed Si(100)(2×1)-H surface ($\Theta_K = 0.1$). The solid curve is calculated by Eq. (8) using the values of $\hbar\beta$ given by the solid line of Fig. 3. The dashed curve is calculated assuming that $\hbar\beta = 0.3$ meV independent of the sample temperature.

Assuming a Gaussian line shape for the quasielastic peak, the FWHM Γ of quasielastic peak obtained experimentally is given by,

$$\Gamma^2 = \Gamma_0^2 + 8\ln 2 \langle (\hbar\Delta\omega)^2 \rangle \ , \quad (9)$$

where Γ_0 is the instrumental resolution of the spectrometer, which is taken to be the value for the Si(100)(2×1)-H surface, $\Gamma_0 = 11.5$ meV. We can calculate $\hbar\beta$ from the experimentally measured FWHM using Eqs. (8) and (9), e.g., $\hbar\beta = 0.3$ meV at 300 K. In Fig. 3 is shown the semilogarithmic plot of $\hbar\beta/\sqrt{k_B T}$ versus $1/k_B T$. Figure 3 indicates that the temperature dependence of $\hbar\beta$ is experimentally described by $\hbar\beta = 0.67\sqrt{k_B T}\exp(-A/k_B T)$ ($A = 60$ meV). The temperature dependence of the FWHM calculated by the use of this relation is shown by the solid curve in Fig. 2, which agrees well with the experimental results shown by open circles in the same figure. It is noted that if $\hbar\beta = 0.3$ meV (the value at 300 K) is used independent of the sample temperature, the dashed curve in Fig. 2 is calculated from Eqs. (8) and (9). As mentioned in Sec. I, the FWHM is proportional to $\sqrt{T}\ln T$, and the experimental results are not reproduced.

In order to explain the temperature dependence of $\hbar\beta$, we consider the electronic structure of the K-exposed Si(100)(2×1)-H surface ($\Theta_K = 0.1$). The clean Si(100)(2×1) surface has both filled and empty dangling-bond surface states in the band gap.[11] The hybridization between the (filled) Si dangling-bond band and 1s orbitals of H atoms forms filled Si-H bonding states and empty Si-H antibonding states. The position of the filled surface states is below the valence-band maximum (VBM) according to the band calculation by the empirical tight-binding method and photoelectron spectroscopy mea-

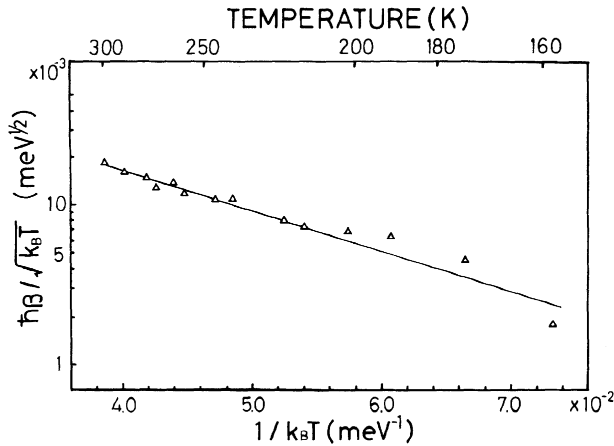

FIG. 3. The value of $\hbar\beta/\sqrt{k_BT}$ is plotted on a semilogarithmic scale as a function of $1/k_BT$. The experimental results (plotted by open triangles) are approximated by the solid line.

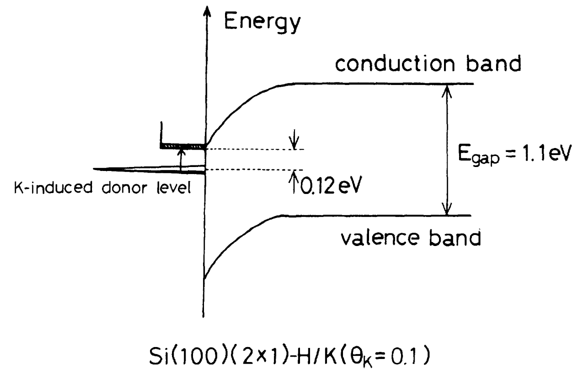

FIG. 4. Schematic representation of the surface electronic state of the K-exposed Si(100)(2×1)-H surface ($\Theta_K=0.1$). The rectangular hatched bar represents two-dimensional density of states of the conduction band, which are occupied by electrons excited from the K-induced donor level.

surements for the Si(100)(2×1)-H surface by Ciraci *et al.*,[12] while the position of the empty surface states is above the conduction-band minimum (CBM) according to the scanning-tunneling-spectroscopy (STS) measurements by Boland[13] which have shown that the empty surface states with Si-H antibonding character are located at 1.2 eV above the Fermi level (E_F). Therefore, the Si(100)(2×1)-H surface has no surface states in the band gap as in the case of the GaAs(110) surface. A large downward band bending is observed upon alkali-metal adsorption for the *p*-type GaAs(110) surface.[14] A similar downward band bending is expected to occur for the case of the Si(100)(2×1)-H/K ($\Theta_K=0.1$) surface. We propose that the K adatoms form localized levels lying below the conduction band similarly to the impurity levels formed in the bulk semiconductor. If the conduction band is regarded as a two-dimensional electronic system because of the downward band bending near the surface, the electron density n is given by

$$n \propto \sqrt{T}\exp(-E_a/2k_BT) ,$$

where E_a is the activation energy for the excitation of electrons from the localized levels to conduction band, and is estimated to be $E_a=120$ meV by comparison with the temperature dependence of $\hbar\beta$.

From the above discussion, the origin of the quasielastic peak broadening is explained as follows. As shown schematically in Fig. 4, K adatoms form localized donor levels lying below the conduction band, and electrons are thermally excited from the donor levels into the conduction band by the increase of the sample temperature. The origin of the broadening is attributed to the multiple excitation of the plasmon formed by electrons in the conduction band. In the EELS spectrum recorded at 150 K [shown by the dashed curve in Fig. 1(b)], the loss corresponding to the transition between the K-induced donor levels and the conduction band was not observed because of the tailing of the quasielastic peak and due probably to the low-excitation cross section. Photoelectron spectroscopy and metastable deexcitation spectroscopy may clear the existence of the K-induced donor levels.

It is considered that contributions from phonons and free bulk carriers to the quasielastic peak broadening are not important.[3,6]

C. Narrowing of the quasielastic peak for $\Theta_K > 0.1$

In Fig. 5 the FWHM of the quasielastic peak is shown as a function of Θ_K. The FWHM has a maximum at $\Theta_K=0.1$ and is decreased gradually with increasing Θ_K. Using the theory of Persson,[3,6] these results might be (incorrectly) interpreted as follows: For low Θ_K, where $\hbar\beta \ll k_BT$, the broadening is caused by the multiple excitation of the plasma oscillation for the two-dimensional electronic system, while with the increase of Θ_K, the transition from the region where $\hbar\beta \ll k_BT$ to the region where $\hbar\beta \gg k_BT$ occurs, and thus, for high Θ_K, the broadening arises from the Drude damping, but the FWHM narrows as $1/\tau \rightarrow 0$.

In Fig. 6 is shown the variation of the fractional H coverage Θ_H as a function of Θ_K for the K deposition on the

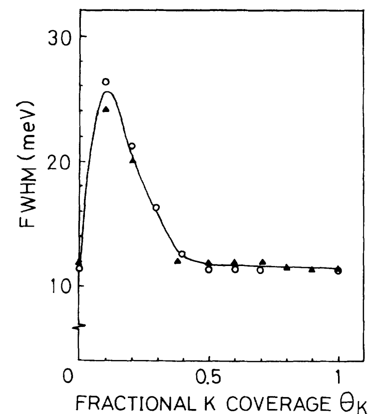

FIG. 5. The FWHM of the quasielastic peak is shown as a function of the fractional K coverage Θ_K. The open circles correspond to the series of EELS spectra shown in Fig. 1, and the solid triangles to other series of EELS spectra.

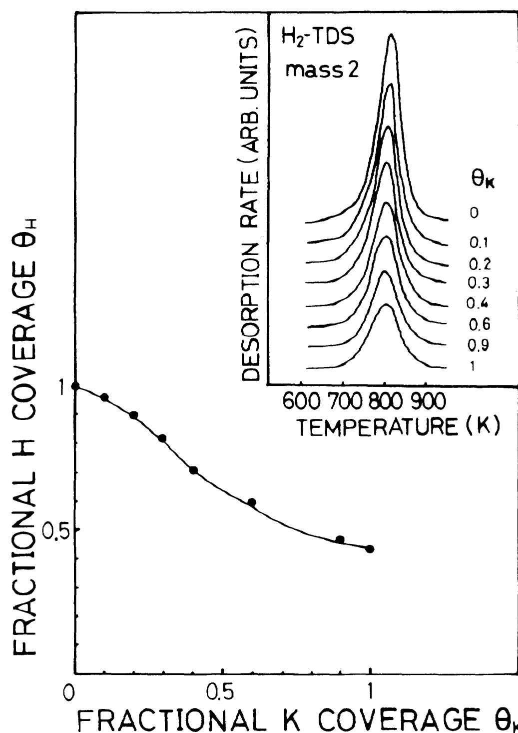

FIG. 6. The fractional H coverage Θ_H estimated by the TDS peak area is shown as a function of Θ_K. The inset shows the corresponding H_2 TDS spectra (heating rate, 8 K/s).

Si(100)(2×1)-H surface at room temperature. The Θ_H was estimated using the corresponding H_2 TDS spectra shown in the inset of Fig. 6. With increasing Θ_K, the Θ_H is decreased, which is interpreted to indicate that the displacement of H_2 is induced by the K adsorption as will be discussed later. The Θ_K dependence of the FWHM is correlated with that of Θ_H, i.e., the FWHM is decreased with the decrease of Θ_H. Thus, the narrowing of the FWHM is associated essentially with the displacement of hydrogen. For low Θ_K, where the broadening is observed, the displacement of hydrogen is negligible, and therefore, the electronic structure schematically shown in Fig. 4 is applicable. For high Θ_K, the displacement of hydrogen is considerable, so that the π and π^* surface bands for the Si-K bonds are partly formed due to the K-K lateral interaction, and therefore, the electronic structure is considerably changed.

The Si-K bond energy is about 56 kcal/mol from the TDS measurement (assuming that the desorption energy is equal to the bond energy),[9] and the Si-H bond energy is about 90 kcal/mol (estimated for various silane molecules).[15] These results indicate that the H desorption does not occur by the adsorption of the K atoms. As the dissociation energy of H_2 molecules is 105 kcal/mol, it is considered that hydrogen is desorbed molecularly by the K adsorption on the Si(100)(2×1)-H surface.

D. Energy shift of the Si-H stretching mode with Θ_K

Energy shift of the Si-H stretching mode is observed in the EELS spectra in Fig. 1, and these results are plotted as a function of Θ_K in Fig. 7, where the range of Θ_K is limited to $\lesssim 0.7$, since the loss peak associated with the Si-H stretching mode is hidden in the loss continuum at high $\Theta_K > 0.7$ (Fig. 1) as will be mentioned in Sec. III E. The Si-H stretching energy is decreased with the increase of Θ_K monotonically. It is considered that the redshift (by ~20 meV) of the Si-H stretching mode is due to the Si-H bond weakening by the charge transfer from K adatoms to the Si-H antibonding orbitals through the Si substrate. It is noted that a similar redshift has been observed for the C-O stretching mode of CO on K-covered Pt(111) [38 (15) meV shift for CO on the bridge (on-top) sites] with the increase of the K coverage, which is caused by the C-O bond weakening induced by the charge transfer from K adatoms to the $2\pi^*$ antibonding orbitals of CO.[16] It is noted that the redshift induced by the self-image effect is estimated to be ~5 meV for the system of CO on Pt(111) surface,[17] which seems inadequate to explain the observed redshift.

The loss peak at 65 meV in Fig. 1(f) is assigned to the Si-H bending mode also shifted to the low energy.

E. EELS spectra for the H-exposed Si(100)-K surface

Figure 8(a) shows an EELS spectrum in the specular mode of the Si(100)(2×1)-K surface ($\Theta_K=1$) at room temperature. A loss continuum is observed that may be attributed to the electronic transitions between the surface-state bands, which are broadened by the electron-phonon coupling (because the loss continuum disappears by the O_2 exposure and is decreased in intensity at 150 K). Figure 8(b) shows an EELS spectrum of the same surface subsequently exposed to 10 L H_2 (which corresponds to $\Theta_H=0.3$ according to the TDS measure-

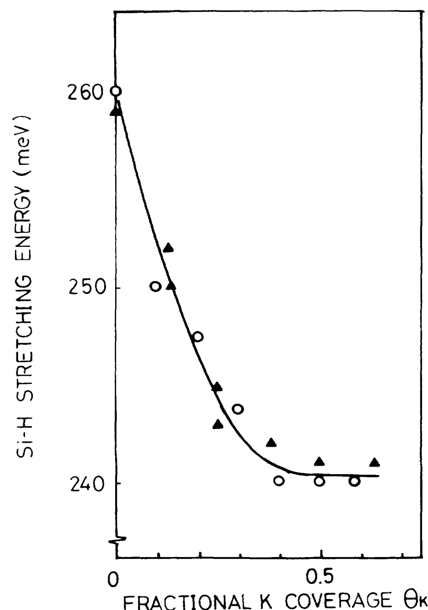

FIG. 7. The Si-H stretching energy is plotted as a function of Θ_K. Open circles correspond to the EELS spectra shown in Fig. 1, and solid triangles to other series.

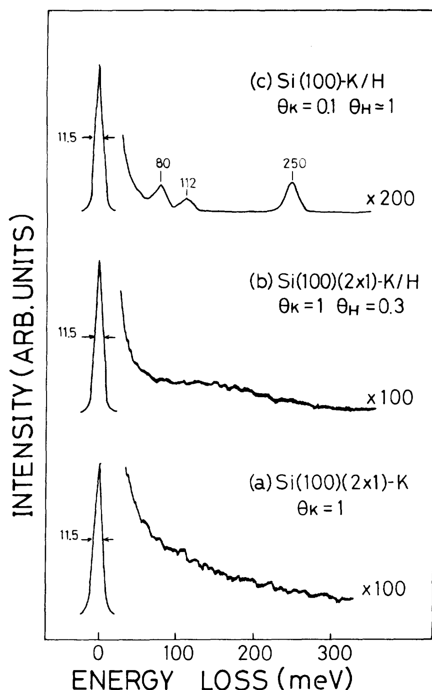

FIG. 8. EELS spectra in the specular mode of (a) the Si(100)(2×1)-K surface ($\Theta_K=1$), (b) the Si(100)(2×1)-K surface ($\Theta_K=1$) exposed to H atoms ($\Theta_H=0.3$), and (c) the Si(100)-K surface ($\Theta_K=0.1$) exposed to H atoms ($\Theta_H \simeq 1$) at room temperature. $E_p=7.1$ eV.

ments). A loss continuum is observed. At 150 K, the loss continuum was reduced in intensity, and a broad peak was observed at around ~170 meV, which is attributed to the electronic transitions induced by the H adsorption. It is noted that the loss continuum shown in Fig. 1(i) has a temperature dependence similar to that in Fig. 8(b). No loss peaks were observed, which are clearly associated with the potassium hydride species that have been observed at 97 and 205 meV (deformation and stretching modes, respectively) for H adsorption on the K-modified Al(100) surface[18] or with the silicon hydride species. Thus, the location of H atoms is not determined yet. It is noted, according to the scanning-tunneling-microscope (STM) measurements, that the Si(100)(2×1) surface has a defect density of approximately 10%.[19] If H atoms are located in the defect sites, $\Theta_H=0.3$ seems too large.

The EELS spectrum of the Si(100)-K ($\Theta_K=0.1$) surface exposed to 10 L H_2 (which corresponds to $\Theta_H \simeq 1$) is shown in Fig. 8(c). Compared with the EELS spectrum shown in Fig. 1(b), no broadening of the quasielastic peak is observed, though the surface composition is similar. This is probably attributed to the difference in the adsorbed state of K atoms, but the details are not understood yet. [From the STM measurements of K on Si(100)(2×1),[20] K atoms form linear chains perpendicular to the Si dimer rows at $\Theta_K \sim 0.1$, which suggests that there is an attractive interaction between K atoms. However, K atoms on Si(100)(2×1)-H might be randomly located.] Three peaks are observed at 80, 112, and 250 meV and are assigned to the bending mode of the SiH (monohydride) species and wagging mode of the SiH_2 (dihydride) species, scissors mode of the SiH_2 species, and stretching modes of the SiH and SiH_2 species, respectively.[10] The existence of the dihydride species for 10 L exposure (which corresponds to the formation of the monohydride phase for the clean surface) is interpreted to indicate that the Si-Si bonds near K adatoms become weak (due, perhaps, to the charge transfer from K atoms to the Si-Si antibonding states) and that the Si-Si bond scission is promoted. The redshift of the Si-H stretching energy (10 meV) is related to the bond weakening by the charge transfer from K atoms similarly to the case discussed in Sec. III D.

IV. SUMMARY

We made EELS and TDS measurements for K adsorption on the Si(100)(2×1)-H surface. Some of the important results are as follows.

(i) For $\Theta_K=0.1$, broadening of the quasielastic peaks is observed, and from its temperature dependence and by comparison with the theory, it is proposed that the K adatoms form localized donor levels lying below the conduction band, which is regarded as the two-dimensional electronic system because of the downward band bending near the surface. It is also proposed that the broadening is caused by the multiple excitation of plasma oscillation of electrons thermally excited from these levels.

(ii) Narrowing of the quasielastic peak was observed with increasing Θ_K, which is attributed essentially to the displacement of hydrogen molecules upon the K adsorption.

(iii) The redshift of the vibrational energy (~20 meV) of the Si-H stretching mode was observed, which is ascribed to the Si-H bond weakening by the charge transfer from the K adatoms to the Si-H bond through the Si substrate.

(iv) The Si(100)(2×1)-H surface exposed to K atoms ($\Theta_K=0.1$) is different from the Si(100)-K surface ($\Theta_K=0.1$) exposed to H atoms ($\Theta_H \simeq 1$).

ACKNOWLEDGEMENTS

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