Vibration of the Dimer on Si(001) Surface

Excited by STM Current

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Abstract

The vibration of the dimer excited by STM current on Si(001) surface is investigated. We describe this system by the Hamiltonian which has the electron-vibration coupling term as the key ingredient. In order to characterize the transition rates induced by STM current between vibrational states we have introduced the effective temperature of the vibration which differs from the temperature of the substrate. The behavior of the effective temperature depends on the substrate temperature and STM current in highly nonlinear manner and qualitatively changes around 50K of the substrate temperature. At lower temperatures, the effective temperature strongly deviates from the substrate temperature and reaches a few hundred Kelvin for the typical values of STM current. At higher substrate temperatures, the effective temperature reduces to the substrate temperature. On the basis of these behaviors of the effective temperature, we solve the puzzle of the symmetric-asymmetric crossover in dimer images of STM observation in the ordered state of c(4 × 2).

KEYWORDS: Si(001), symmetric image, STM, dimer vibration

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1. Introduction

Intensive studies have been made on the atomic structure of the reconstructed Si(001) surface both experimentally and theoretically. On Si(001) surface, neighboring atoms form buckled dimers which have two stable tilting angles. Along the \langle 110 \rangle direction, the dimer rows is formed by the dimers. The principal features of the surface reconstruction on Ge(001) surface are similar to Si(001) surface. The ground state of the structure of the dimer arrangement of both surfaces is \textit{c}(4 \times 2) and the ordered \textit{c}(4 \times 2) phase turns into a disordered state at room temperature through the order-disorder phase transition.\textsuperscript{1-14} In the ordered state, the dimers are observed as the asymmetric images by scanning tunneling microscopy (STM). In the disordered state, the symmetric appearing images are observed by STM, and these symmetric appearing images have been attributed to the rapid repeat of the orientational change (flip-flop motion).

In the STM observation, semiconductor substrates are doped into n-type ones or p-type ones for the electric conductivity. On Si(001) surface, serious differences in the property of the dimer system between the n-type substrates and p-type ones have not been reported at temperatures higher than 60K.

Recently, p(2 \times 2) phase on Si(001) surface\textsuperscript{15-17} is observed on highly doped n-type substrates below 40K by STM. A phase transition is also observed by low-energy electron diffraction\textsuperscript{18} (LEED) at 40K on highly doped n-type substrates. On the p-type substrates, \textit{c}(4 \times 2) phase on Si(001) surface is observed down to 9K.\textsuperscript{17}

At much low temperatures, the symmetric STM images of p(2 \times 1) structure\textsuperscript{17,19,20} are observed at some conditions of the tip bias voltages $V_t$ and the tip currents $I_t$ in STM observations. Yokoyama\textsuperscript{19} reported that STM images of the dimers at 5K on boron doped (B-doped) p-type Si(001) substrate at the condition of $V_t = \pm 1V$ and $I_t = 50pA$ appear to be symmetric, although most of the dimer images on the substrate are well asymmetric to make the ordered \textit{c}(4 \times 2) structure at 63K, and that the symmetric STM images at 5K are observed also on Antimony doped n-type Si(001) substrate. Kondo\textsuperscript{19} reported subsequently that the STM images at 20K on phosphorus doped n-type Si(001) substrate at the condition of $V_t = 2.0V$ and -1.6V, and $I_t = 300pA$ appear to be symmetric. These observations of the symmetric images in the ordered phase are puzzling and have not been explained yet.

The first-principles calculations (FPC) with high accuracy\textsuperscript{6,7,21} show that the ground state on Si(001) surface is \textit{c}(4 \times 2). The results of FPC show that the energy of the elec-
tronic system decreases, and the energy of the lattice system increases, as the tilting angle of the dimer increases. The equilibrium angle is determined by the competition between the energies of two systems. Thermal equilibrium properties on the surface at temperatures higher than 100K have been successfully explained by Monte Carlo simulations (MCS) with Metropolis algorithm based on the results of FPC\(^6,7\) by mapping the two stable orientations of the dimer onto the Ising system.\(^{6,7,22–25}\) The time-resolving dynamical Monte Carlo simulations (TDMCS) performed for the dimer systems of Si(001)\(^{26,27}\) surface and Ge(001)\(^{28}\) surface show that the most of the long range fluctuations of the dimer arrangement on Si(001) and Ge(001) surfaces are carried by the phase boundary of the c(4 × 2) domain in the dimer row at low temperatures. In order to perform TDMCS on Si(001) surface and on Ge(001) surface, the model potentials for the continuous values of the tilting angle are obtained based on the FPC results\(^{27,28}\). The TDMCS results with the model potentials reproduce well the results of the time-resolving STM observations\(^{12,29}\). Since at temperatures higher than 60K, as mentioned above, serious dopant effect are not reported on Si(001) surface, the reported MCS results based on the results of FPC remain valid.

The surface localized states of \(\pi\)-band and \(\pi^*\)-band\(^{6,7,17,19,21,30–32}\) are formed mainly through the hybridization of the dangling bonds on the dimers. FPC\(^{6,7,21}\) show that the energies of the top of the \(\pi\)-band and the bottom of \(\pi^*\)-band stay a few ten meV above from the top of the valence band of Si and about 500meV below from the bottom of the conduction band of Si, respectively. The band widths are obtained to be about 1eV in both of \(\pi\)-band and \(\pi^*\)-band. These features are observed by angle-resolved UPS\(^{30}\) (ARUPS) and scanning tunneling spectroscopy \(^{19,31,32}\) (STS). On the n-type substrates, the Fermi level of the system stays near the bottom of the conduction band, which is much higher than the bottom of \(\pi^*\)-band. The large band bending appears near the surface region of the n-type substrate at much low temperatures. On the p-type substrates, the Fermi level stays near the top of the valence band. Therefore, the top of the \(\pi\)-band is near the Fermi level. The large band bending does not appear near the surface region on the p-type substrates. Because the dopant effect on the substrate is not taken into account in the FPC, the results of FPC reproduce well the surface properties of p-type substrate, but some modifications are necessary for n-type substrate at much low temperatures.

In the present study, we take the scope to the vibration excited by STM current on the p-type substrate. We will introduce the Hamiltonian which has the electron-vibration cou-
pling term. The excitation rates by the STM currents for the vibration will be obtained. The rates will be characterized by introducing the effective temperature of the vibration. The mechanism for the symmetric-asymmetric crossover in dimer images of STM observation on Si(001) surface will be presented.

2. Model

We introduce the Hamiltonian \( H \) representing the coupling between the electronic system and the localized vibrational system,

\[
H = H_e + H_{e-v},
\]

\[
H_e = \sum_k \varepsilon_k c_k^\dagger c_k + \sum_p \varepsilon_p c_p^\dagger c_p + \Gamma \left\{ \left( \sum_k \gamma_k c_k^\dagger \right) \left( \sum_p \gamma_p^* c_p \right) + \text{H.c.} \right\}
\]

\[
= \sum_{\alpha} \varepsilon_\alpha c_\alpha^\dagger c_\alpha + \sum_{\alpha} \varepsilon_\alpha a_\alpha^\dagger a_\alpha + \left( \sum_{\alpha} \Gamma_\alpha a_\alpha^\dagger c_\alpha + \text{H.c.} \right) + \sum_p \varepsilon_p c_p^\dagger c_p + \left( \sum_p \Gamma_p a_p^\dagger c_p + \text{H.c.} \right),
\]

\[
H_{e-v} = \hbar \omega \left( b^\dagger b + \frac{1}{2} \right) + \delta \varepsilon (b^\dagger + b) a_\alpha^\dagger a,
\]

\[
\varepsilon_\alpha = \sum_k |\gamma_k|^2 \varepsilon_k,
\]

\[
a_\alpha^\dagger = \sum_k \gamma_k^* c_k^\dagger,
\]

\[
\Gamma_p = \Gamma \gamma_p,
\]

where \( c_k \), \( c_p \) and \( b \) are the annihilation operators for the electronic states in the \( \pi \)-band, for the states in the conduction band of the STM tip, and for the vibrational state in the rocking mode of the dimer on Si(001) surface beneath the STM tip. We assume that the vibrational states are the harmonic oscillator, and the energy of the state with the vibrational number \( n \) is \( \hbar \omega (n + 1/2) \). The energy of the vibrational state \( \hbar \omega \) is measure by the electron energy loss spectroscopy\textsuperscript{33} as 20meV. \( a_\alpha^\dagger = \sum_k \gamma_k^* c_k^\dagger \) and \( \sum_p \gamma_p^* c_p^\dagger \) are the creation operator for the spatially localized states \( |a\rangle \) in the surface dimer and in the prominence of the tip, respectively. The tunneling current is through the the spatial localized states. The coefficients of the spatial localized states are normalized as \( \sum_k |\gamma_k|^2 = 1 \) and \( \sum_p |\gamma_p|^2 = 1 \).

The diagonalized term of \( \sum_k \varepsilon_k c_k^\dagger c_k \) is rewritten by \( a \) and \( c_\alpha \) as the first three terms in the third line of eq. (1), where \( c_\alpha \) is the annihilation operators for the electronic states orthogonalized with \( |a\rangle \). The amplitude of the vibration modifies the one electron energy of \( |a\rangle \), and \( H \) has the electron-vibration coupling term, because the energy of the electronic system, as mentioned above, decreases as the tilting angle of the dimer increases. The term
of $\delta \varepsilon$ represents the electron-vibration coupling. $\delta \varepsilon$ is the coupling constant between the amplitude of the vibration and the energy of the one electron state of $|a\rangle$. The vibration is excited or deexcited through the electron-vibration coupling by the STM current. The similar Hamiltonian of eq. (1) has been used in the precedent studies of vibrations of molecules adsorbed on metal surfaces$^{34-41}$. In the present study, however, the Hamiltonian is applied to totally different system, the surface localized semiconductor state on Si(001) surface.

In the present study, we treat the case that the tip bias voltages $V_t$ is positive and so large that the Fermi level in the conduction band of the STM tip is below the bottom of the $\pi$-band of the p-type Si(001) substrate; $V_t$ is assumed to be slightly larger than 1V, because the band width of the $\pi$-band is about 1eV. The elastic inter-band transition of electrons from the $\pi$-band to the conduction band of the tip is induced by the presence of the tip. The elastic inter-band transition rate $\sigma_{\text{elas}}$ of electrons from the surface to the tip without coupling to the vibration$^{34-41}$ is given by the T-matrix element and the Fermi distribution functions:

$$
\sigma_{\text{elas}} = \frac{2\pi}{\hbar} \sum_{a,p} \left| \Gamma^*_p G_a(\varepsilon) \Gamma_a \right|^2 \\
\quad \times \left( \frac{1}{\exp(\beta(\varepsilon_a - \varepsilon_F)) + 1} \right) \left( 1 - \frac{1}{\exp(\beta(\varepsilon_p + eV_t - \varepsilon_F)) + 1} \right) \delta(\varepsilon_a - \varepsilon_p)
$$

$$
= \frac{4}{\pi \hbar} \Delta_t(\varepsilon) \Delta_s(\varepsilon) |G_a(\varepsilon)|^2 D_{\pi},
$$

$$
G_a(\varepsilon) = \langle a | (\varepsilon + i0^+ - H_e)^{-1} | a \rangle
$$

$$
\Delta(\varepsilon) = \Delta_s(\varepsilon) + \Delta_t(\varepsilon),
$$

$$
\Delta_s(\varepsilon) = \pi \sum_\alpha |\Gamma_\alpha|^2 \delta(\varepsilon - \varepsilon_\alpha),
$$

$$
\Delta_t(\varepsilon) = \pi \sum_p |\Gamma_p|^2 \delta(\varepsilon - \varepsilon_p),
$$

$$
\Lambda(\varepsilon) = \frac{1}{\pi} \int_{-\infty}^{\infty} d\varepsilon' \frac{\Delta(\varepsilon')}{\varepsilon - \varepsilon'},
$$

where $\varepsilon_F$ is the Fermi level of the electronic system, $G_a(\varepsilon)$ is the Green function for the
electron system, $\Delta(\varepsilon)$ is the width of the projected density of states for $|a\rangle$, $\Delta_s(\varepsilon)$ and $\Delta_t(\varepsilon)$ are the components of $\Delta(\varepsilon)$ in the surface and in the tip, respectively, $P$ denotes the Cauchy principal value, and $E_\pi$ and $D_\pi$ are the energy level of the top of the $\pi$-band and the width of the $\pi$-band, respectively. In the present study, $-(E_\pi - \varepsilon_F)$ is assumed to be of the order of a few ten meV and $D_\pi$ is assumed to be large enough $\beta D_\pi \gg 1$. The temperature of the system is assumed to be so low that the broadness of the Fermi distribution around $\varepsilon_F$ in the surface state and around $\varepsilon_F - eV_t$ in the tip state are not contributed to the evaluation of the integration in eq.(2). We assume that $\Delta_t(\varepsilon_a)/\Delta_s(\varepsilon_a)$ is small in the STM observation in the typical conditions enough to be approximated as $\Delta(\varepsilon_a) \approx \Delta_s(\varepsilon_a)$. Because in the STS experiment at 5.5K, the tunneling spectra of the $\pi$-band are observed to be almost symmetric band, we assume that $\varepsilon_a$ stay at the center of the $\pi$-band in energy, and $\Lambda(\varepsilon_a) = 0$. Therefore, $\sigma_{\text{elas}}$ is approximately obtained as

$$
\sigma_{\text{elas}} \approx \frac{4}{\pi \hbar} \Delta_t(\varepsilon_a) \Delta_s^{-1}(\varepsilon_a) D_\pi.
$$

The inter-band transition of electrons from the $\pi$-band to the conduction band of the tip induced by the presence of the tip can excite the vibrational state in the dimer through the electron-vibration coupling. The inelastic inter-band transition rate $\sigma_{0\rightarrow1}^{\text{int}}$ of electrons from the surface to the tip coupling with the excitation from the ground state of the vibrational number $n = 0$ to the excited state of $n = 1$ is obtained in the lowest order in $|\delta \varepsilon|$ as

\begin{align*}
\sigma_{0\rightarrow1}^{\text{int}} &= 2 \frac{2\pi}{\hbar} \sum_{\alpha',p'} |\langle p',1|H_{e-v}|\alpha',0\rangle|^2 \delta(E(p') - \hbar \omega - E(\alpha')) \\
&= \frac{4\pi |\delta \varepsilon|^2}{\hbar} \int_{-D_\pi + E_\pi}^{E_\pi} d\varepsilon \rho_s(\varepsilon) \rho_t(\varepsilon) \\
&\quad \times \left( \frac{1}{\exp(\beta(\varepsilon_a - \varepsilon_F)) + 1} \right) \left( 1 - \frac{1}{\exp(\beta(\varepsilon_p - \hbar \omega + eV_t - \varepsilon_F)) + 1} \right) \\
&\approx \frac{4\pi |\delta \varepsilon|^2}{\hbar} \rho_s(\varepsilon_a) \rho_t(\varepsilon_a) D_\pi, \\
\rho_s(\varepsilon) &= \sum_{\alpha'} |\langle \alpha'|a\rangle|^2 \delta(\varepsilon - \varepsilon_{a'}) \\
&= \frac{1}{\pi} \left( \frac{\Delta_s(\varepsilon)}{(\varepsilon - \varepsilon_a - \Lambda(\varepsilon))^2 + \Delta^2(\varepsilon)} \right), \\
\rho_t(\varepsilon) &= \sum_{p'} |\langle p'|a\rangle|^2 \delta(\varepsilon - \varepsilon_{p'})
\end{align*}

6
\[
\sigma_{0\rightarrow1}^{\text{int}} \approx \frac{4|\delta\varepsilon|^2}{\pi\hbar} \Delta_t(\varepsilon_a) \Delta_s^{-3}(\varepsilon_a) D_{\pi}.
\] (5)

The elastic transition rate \(\sigma_{\text{elas}}\) and the inelastic transition rate \(\sigma_{0\rightarrow1}^{\text{int}}\) depend critically on \(I_t\) and do not on \(T\), because in eqs. (3) and (5), \(\Delta_t\) depends critically on the spatial tunneling gap of STM. The fraction of the inelastic transition rate to the elastic transition rate \(W = \sigma_{0\rightarrow1}^{\text{int}}/\sigma_{\text{elas}}\), however, does not depend on \(\Delta_t\), and is obtained from eqs. (3) and (5) as

\[
W = \left(\frac{|\delta\varepsilon|}{\Delta_s(\varepsilon_a)}\right)^2.
\] (6)

Eq. (6) shows that the fraction of \(\sigma_{0\rightarrow1}^{\text{int}}/\sigma_{\text{elas}}\) is given dominantly from the intrinsic property of Si(001) surface, and independent of the STM current. In the present study, as mentioned already, \(V_t\) is assumed to be so large that the Fermi level in the conduction band of the tip is below the bottom of the \(\pi\)-band, and \(\hbar\omega \ll eV_t\). From these assumption, the inelastic inter-band transition rate \(\sigma_{1\rightarrow0}^{\text{int}}\) of electrons from the surface to the tip coupling with the deexcitation from the vibrational number \(n = 1\) to \(n = 0\) is well approximated to take the same value as \(\sigma_{0\rightarrow1}^{\text{int}}\). Thus the inelastic inter-band transition rate \(\sigma_{n\rightarrown\pm1}^{\text{int}}\) of electron from the surface to the tip coupling with the vibrational transition from \(n\) to \(n \pm 1\) is given as

\[
\sigma_{n\rightarrown\pm1}^{\text{int}} = \max(n, n \pm 1) \sigma_{0\rightarrow1}^{\text{int}}.
\]

At finite temperatures \(T\), the deexcitation of the vibrational number \(n = 1\) to \(n = 0\) through the inner-band excitation of the electron-hole pair creation in the \(\pi\)-band can occur. In the inner-band excitation, both the initial state and the final state of the electron are within the states of \(|\alpha'\rangle\), which have dominant component in the \(\pi\)-band on the surface. The
deexcitation of the vibration with the inner-band excitation does not occur at 0K. The rate of the deexcitation \( \sigma_{1\rightarrow 0}^{\text{inn}} \) of vibration through the inner excitation is independent of \( I_t \) and depends on \( T \):

\[
\sigma_{1\rightarrow 0}^{\text{inn}} = \frac{2\pi}{\hbar} \sum_{\alpha_i', \alpha_i} |\langle \alpha_2', 0 | H_{e-v} | \alpha_1', 1 \rangle|^2 \delta(E(\alpha_2') - \hbar \omega - E(\alpha_1'))
\]

\[
= \frac{4|\delta \varepsilon|^2}{\pi \hbar} \int_{-E_\pi + \hbar \omega}^{E_\pi - \hbar \omega} d\varepsilon \rho_s(\varepsilon) \rho_a(\varepsilon + \hbar \omega) \times \left( \frac{1}{\exp(\beta(\varepsilon - \varepsilon_F)) + 1} \right) \left( \frac{1 - \exp(\beta(\varepsilon + \hbar \omega - \varepsilon_F)) + 1}{\exp(\beta(\varepsilon + \hbar \omega - \varepsilon_F)) + 1} \right)
\]

\[
\approx \frac{4\pi |\delta \varepsilon|^2}{\pi} \rho^2_s(\varepsilon_a) \left( \frac{F(T)}{1 - \exp(-\beta \hbar \omega)} \right)
\]

\[
\approx \frac{4}{\pi} \frac{F(T)}{1 - \exp(-\beta \hbar \omega)} \quad (7)
\]

The transition processes of \( \sigma_{\text{elas}}, \sigma_{1\rightarrow 0}^{\text{int}}, \sigma_{0\rightarrow 1}^{\text{int}}, \sigma_{1\rightarrow 0}^{\text{inn}}, \) and \( \sigma_{0\rightarrow 1}^{\text{inn}} \) are schematically shown in Fig. 1. The essential framework of the formalism for \( \sigma_{\text{elas}}, \sigma_{0\rightarrow 1}^{\text{int}}, \) and \( \sigma_{1\rightarrow 0}^{\text{int}} \) is similar to that of theoretical studies\(^{34-41}\) on the STM induced vibration of molecules adsorbed on metal surfaces. In the problems of molecules adsorbed on metal surfaces, tran-
sitions corresponding to the inner-band transitions in the present study have also been treated. The transitions corresponding to the inner-band transitions, however, do not exhibit any temperature dependence in the case of metal surfaces. Eq. (7) shows that \( \sigma_{1\rightarrow 0}^{\text{inn}} \) depend strongly on \( T \); \( \pi \beta \hbar \sigma_{1\rightarrow 0}^{\text{inn}} \approx 4W \exp(\beta(E_\pi - \varepsilon_F)) \) for \( -\beta(E_\pi - \varepsilon_F) \gg 1 \) and \( \pi \beta \hbar \sigma_{1\rightarrow 0}^{\text{inn}} \approx 2W \) for \( -\beta(E_\pi - \hbar \omega - \varepsilon_F) \ll 1 \). The rate of the excitation \( \sigma_{0\rightarrow 1}^{\text{inn}} \) of vibration through the inner-band deexcitation is easily obtained by the essentially same way as \( \sigma_{1\rightarrow 0}^{\text{inn}} \):

\[
\sigma_{0\rightarrow 1}^{\text{inn}} \approx \frac{4}{\pi}W F(T)/(\exp(\beta \hbar \omega) - 1).
\]

The total transition rate of the excitation \( R_{0\rightarrow 1} \) of the vibrational number \( n = 0 \) to 1 and the deexcitation \( R_{1\rightarrow 0} \) of the vibrational number \( n = 1 \) to 0 are given by the sum of rates as

\[
R_{0\rightarrow 1} = \frac{1}{\exp(\beta \hbar \omega) - 1} \sigma_{0\rightarrow 1}^{\text{inn}} + \sigma_{0\rightarrow 1}^{\text{int}}
\]

\[
= \frac{1}{\exp(\beta \hbar \omega) - 1} (\tau_0^{-1} + \frac{4}{\pi}WF(T)) + W \sigma_{\text{elas}},
\]

\[
R_{1\rightarrow 0} = \frac{\tau_0^{-1}}{1 - \exp(-\beta \hbar \omega)} \sigma_{1\rightarrow 1}^{\text{inn}} + \sigma_{1\rightarrow 0}^{\text{int}}
\]

\[
= \frac{1}{1 - \exp(-\beta \hbar \omega)} (\tau_0^{-1} + \frac{4}{\pi}WF(T)) + W \sigma_{\text{elas}},
\]

where \( \tau_0 \) is the life time of the vibration through the background phonon system at 0K.

The probability \( P_n \) to find the vibrational state at \( n \) satisfies the rate equation represented by \( R_{0\rightarrow 1} \) and \( R_{1\rightarrow 0} \):

\[
\frac{dP_n}{dt} = (n+1)R_{1\rightarrow 0}P_{n+1} + nR_{0\rightarrow 1}P_{n-1} - (nR_{1\rightarrow 0} + (n+1)R_{0\rightarrow 1})P_n, \quad 1 \leq n,
\]

\[
\frac{dP_0}{dt} = R_{1\rightarrow 0}P_1 - R_{0\rightarrow 1}P_0.
\]

In the stationary distribution of \( P_n \), \( P_n \) is derived as \( P_n = r^n(1 - r) \) from eq. (9), where \( r = R_{0\rightarrow 1}/R_{1\rightarrow 0} \).

The tip current \( I_t \) are given by the sum of the elastic inter-band transitions and the inelastic inter-band transitions:

\[
\frac{I_t}{e} = \sum_{n=0}^{\infty} P_n \sigma_{\text{elas}} + \sum_{n=0}^{\infty} P_n \sigma_{n\rightarrow n+1}^{\text{int}} + \sum_{n=1}^{\infty} P_n \sigma_{n\rightarrow n-1}^{\text{int}}
\]

\[
= [1 + W \frac{1 + r}{1 - r}] \sigma_{\text{elas}}.
\]
When \( T, W, \) and \( I_t \) are given, \( R_{0 \rightarrow 1} \) and \( R_{1 \rightarrow 0} \) are obtained self-consistently with eqs. (8) and (10). The distribution of the dimer vibration in the STM observation is characterized by the effective temperature \( T_{\text{ef}} \) of the dimer vibration defined as

\[
r = \exp(-\hbar \omega / (k_B T_{\text{ef}})).
\]

(11)

Throughout this paper, \( T \) denotes the temperature of the substrate. \( T_{\text{ef}} \) differs from \( T \) in general and depends on \( T \) and \( I_t \) nonlinearly. The key quantity for \( T_{\text{ef}} \) is the fraction \( W = \sigma_{0 \rightarrow 1}^{\text{int}} / \sigma_{\text{elas}} \), which is derived from \( |\delta \varepsilon| \) and \( \Delta_s \) as shown in eq. (6). The coupling constant \( \delta \varepsilon \) between the amplitude of the vibration and the energy of \( |a\rangle \), is approximately estimated as

\[
|\delta \varepsilon| = \Delta \theta \frac{\partial \varepsilon_a}{\partial \theta_{\theta=\theta_0}},
\]

(12)

where \( \theta_0 \) (\( = 19.1^\circ = 0.333 \text{rad} \)) is the equilibrium tilting angle of dimer in the c(4 \times 2) structure, and \( \Delta \theta \) is the mean value of the amplitude of the vibrational number \( n = 1 \). \( \Delta \theta \) is obtained by \( \omega \) and the effective value of the moment of inertia \( I \) as \( \Delta \theta = (3\hbar / (2I \omega))^{1/2} \). As mentioned already, the model potentials for the continuous values of the tilting angles of the dimers on Si(001) surface are obtained based on the FPC results. We can get approximate values of \( I \) and \( \partial \varepsilon_a / \partial \theta \) at \( \theta = \theta_0 \) by the model potentials:

\[
\frac{\partial \varepsilon_a}{\partial \theta_{\theta=\theta_0}} = -k \theta_0,
\]

\[
I = \frac{k}{\omega^2},
\]

(13)

where \( k \) is the value of the second partial derivative of the model potentials for the tilting angle of the dimer beneath the tip at \( \theta = \theta_0 \). We derive the value of \( k \) from the model potentials, as \( k = 1.1 \times 10^4 \text{meV/rad}^2 \). Using eq. (13), we get approximate values as \( I = 1.2 \times 10^{-23} \text{meVs}^2/\text{rad}^2 \), \( \partial \varepsilon_a / \partial \theta = -3.7 \times 10^3 \text{meV/rad} \), and \( \Delta \theta = 5.2 \times 10^{-2} \text{rad} \). From eq. (12), \( |\delta \varepsilon| \) is approximately estimated to be \( 1.9 \times 10^2 \text{meV} \). From the half width of half maximum of STS for \( \pi \)-band of Si(001) at 5.5K, \( \Delta_s \) is roughly estimated to be \( 2.5 \times 10^2 \text{meV} \). From these values, the key quantity \( W \) is obtained to be about \( 0.6 \).

3. Results and Discussions
In the present study, we take the scope on the p-type substrate. The Fermi level of the p-type substrate is well approximated to be at the center of the top of the valence band of the substrate and the acceptor level of dopant at low temperatures. At temperatures low but higher than a few Kelvin, $E_\pi$ is practically fixed at the top of the valence band. In the present study, $E_\pi - \varepsilon_F$ is approximated to be $-22.5\text{meV}$ for B-doped substrate and $-32.5\text{meV}$ for Ga-doped substrate, respectively. The life time of the vibration $\tau_0$ through the background phonon system at 0K is expected to be of the order of $10^{-9}\text{s}$ for semiconductors. We assumed for $\tau_0$ to be 8ns.

The excitation rate $R_{0\rightarrow1}$ and the deexcitation rate $R_{1\rightarrow0}$ for B-doped substrate are shown in Fig. 2. Both rates are monotonically increasing function of $T$ and $I_t$ in highly nonlinear manner. The rates scarcely depend on $T$ for $T < 20\text{K}$, because the inter-band transitions are dominant in them and the inner-band transitions scarcely contribute to them. When $T$ increases around 20K, the excitation and deexcitation of the vibration through the inner-
band transitions of electrons become effective and the rates increase steeply for $T$. The deexcitation rate $R_{1 \to 0}$ increases much steeper for $T$ than $R_{0 \to 1}$ around $20K \sim 40K$. The rates scarcely depend on $I_t$ for $T > 70K$, because the inner-band transitions are dominant in them and the inter-band transitions scarcely contribute to them.

Since the magnitudes of the rates are smaller enough than the frequency of the vibration $4.8$THz derived from $\hbar \omega = 20$meV, the effective temperature of the dimer vibration $T_{ef} = -\hbar \omega / (k_B \log(R_{0 \to 1}/R_{1 \to 0}))$ well characterizes the distribution of the vibration. $T_{ef}$ for B-doped substrate are shown in Fig. 3. At low temperatures of $T < 20K$, $T_{ef}$ scarcely depending on $T$, increases steeply with $I_t$, becomes about $250K$ at $I_t = 50pA$, and reaches about $500K$ at $I_t = 200pA$. The rapid flip-flop is expected in such high $T_{ef}$. These high $T_{ef}$ appearing

![Figure 3: The effective temperature of the dimer vibration ($T_{ef}$) for B-doped substrate. $T_{ef}$ reaches about 500K at $I_t = 200pA$ at low temperature $T < 20K$. $T_{ef}$ decreases steeply around $T \approx 20K \sim 40K$, as $T$ increases.](image)


at low temperatures of $T < 20\text{K}$, essentially explains why the symmetric STM images are observed at low temperatures. When $T$ increases around 20K, $T_{\text{ef}}$ starts to decrease steeply, because of steep increase of $R_{1\rightarrow0}$. $T_{\text{ef}}$ becomes 70K around $T \approx 40\text{K}$ and $I_t \approx 150\text{pA}$. At higher temperatures $T > 60\text{K}$, $T_{\text{ef}}$ increases gradually with $T$, scarcely depends on $I_t$ within the typical values of $I_t$, and takes the nearly same value as $T$. These low $T_{\text{ef}}$ explains why the asymmetric STM images recover in temperature range higher than 50K.

$T_{\text{ef}}$ for Ga-doped substrate are shown in Fig. 4. The essential feature of $T_{\text{ef}}$ shown in Fig. 4 is same as in Fig. 3. The steep decrease of $T_{\text{ef}}$ in Fig. 4, however, is starting around $T \approx 30\text{K}$ which is higher than for B-doped substrate shown in Fig. 3. The temperature where the inner-band transitions exceed the inter-band transitions in magnitude on Ga-doped substrate, is higher than that on B-doped substrate and the ratio of these two temperatures is almost the same value as the ratio of $\varepsilon_F - E_\pi$, $32.5/22.5=1.44$, since $\sigma_{1\rightarrow0}^{\text{inn}}$, as mentioned already, is approximated as $\sigma_{1\rightarrow0}^{\text{inn}} \approx 4W \exp(\beta(E_\pi - \varepsilon_F))/(\pi\beta\hbar)$ for $-\beta(E_\pi - \varepsilon_F) \gg 1$.

At low temperature $T < 20\text{K}$, the atom at the up-position beneath the tip is rapidly transferred to the down-position through the dimer flip-flop motion by quasi-thermal excitation of the vibration of high $T_{\text{ef}}$. After the flip-flop motion to the down-position, $T_{\text{ef}}$ becomes much lower than at the up-position, because tip current is expected to be much smaller at down-position than at up-position. Because of the low effective temperature $T_{\text{ef}}$, the transition rate of the atom from the down-position to the up-position is much smaller than that of the opposite transition; the fraction of the staying time at the down-position is much larger than that at the up-position. The spatial STM gap between the prominence of the tip and the surface dimer is tuned for $I_t$ to be the STM condition. The tip current $I_t$ is time averaged one, and is tuned almost at the down-position at low temperatures. In the scanning of STM tip at much low temperatures, the atoms beneath the tip are almost always tied to the down-positions, and the atoms at the up-position scarcely contribute to the STM images. As the result of the large fraction at the down-position, the symmetric dimer images of the p(2 × 1) structure is observed even in the ordered state of c(4 × 2). These feature that the tip ties the atom to the down-positions in STM observation on Si(001) surface corresponds to the experimental results reported by Mitsui and Takayanagi\textsuperscript{42}.

In the present study, we demonstrate that the inner-band transitions play the important role to decrease $T_{\text{ef}}$ at the temperatures of a few ten Kelvin where deexcitation of the vibration through the inner-band excitations of the electron-hole creation occur. This de-
Figure 4: Fig. 4 The effective temperature of the dimer vibration ($T_{ef}$) for Ga-doped substrate. $T_{ef}$ reaches about 500K at $I_t = 200pA$ at low temperature $T < 30K$. $T_{ef}$ decreases steeply around $T \approx 30K \sim 60K$, as $T$ increases. The decreases on Ga-doped substrate appears in higher temperatures than on B-doped substrate.

excitation through the inner-band excitation can occur also when enough amount of holes in the $\pi$-band or enough amount of electrons in the $\pi^*$-band is induced. For example, when the electrons and holes are induced by infrared photons or by other methods, $T_{ef}$ will be expected to decrease in much low temperature in STM observation. Here we propose the notion of “the excitation-induced cooling”, namely, the decrease of $T_{ef}$ essentially induced by the electronic excitation in $\pi$-band or $\pi^*$-band.

4. Conclusion

In order to explain the symmetric-asymmetric crossover in dimer image of STM observa-
tion on Si(001) surface, we calculate the effective temperature $T_{ef}$ of dimer vibration. The crossover behavior is semiquantitatively understood by the nonlinear dependence of $T_{ef}$ on the substrate temperature and STM current. The symmetric image in the ordered state of c($4 \times 2$) results from the large fraction of the atom at the down-position induced by STM current. We have proposed the notion of “the excitation-induced cooling” under more general situations than that induced by the substrate temperature.

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