

Equilibrium structure of monatomic steps on vicinal Si(001)

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 (Received 28 May 1991)

The equilibrium structure of monatomic steps on vicinal Si(001) is described in terms of anisotropic nearest-neighbor and isotropic second-nearest-neighbor interactions between dimers. By comparing scanning-tunneling-microscopy data and this equilibrium structure, we obtained interaction energies of 0.38 eV between dimers in a row, 0.24 eV between sets of two dimers in adjacent rows, and -0.07 eV for the diagonal interaction between dimers in adjacent rows.

A substantial amount of research has been devoted to monatomic steps on the vicinal Si(001) surface. This interest is due to the great influence of these steps on several surface phenomena, such as preferential reactivity and the growth of epitaxial overlayers.¹ The Si(001) surface reconstructs to form rows of dimerized atoms,² yielding a (2×1) unit cell. A slight misorientation with respect to the [001] direction in the [110] direction (the directions [110] and $[\bar{1}10]$ correspond to the directions of the dimer rows) results in a vicinal Si(001) surface with monatomic steps. Proper cleaning of this surface³ leads to a regular step distribution that reflects the macroscopic misorientation of the sample. Due to the symmetry of the diamond lattice, two types of steps can be distinguished on the Si(001) surface: steps running parallel or perpendicular to the dimer rows of the upper terrace. Steps parallel to the dimer rows of the upper terrace are straight (*A*-type steps⁴), whereas the others are ragged (*B*-type steps⁴),³ i.e., they exhibit a high density of thermally excited kinks.⁵ A slight misorientation Θ with respect to the [001] direction in the $[\bar{1}10]$ direction results in a certain number of forced kinks. Especially in the smooth *A*-type step edge, a large fraction of the kinks can be forced due to the step misorientation Θ . Energy considerations show that at zero temperature, a step edge will tend to be as straight as possible and hence contain only forced kinks. As the temperature rises, the number of thermally excited kinks increases. Recently, Swartztruber *et al.*⁶ analyzed scanning tunneling microscopy (STM) images of vicinal Si(001) with an equilibrium distribution of steps and kinks to determine the distribution of kink separations and kink lengths. From this analysis, step and kink energies were obtained. According to these authors, the kink energy fits the form $E(n) = nE + C$, where E is an energy per unit step length and C a constant effective corner energy, and n is the kink length perpendicular to the step edge, measured in units of the surface-lattice constant a ($= 3.84 \text{ \AA}$). In the analysis of the *B*-type step edge in Ref. 6, no difference between forced and unforced kinks was made, and in the analysis of the *A*-type step edge the problem of forced kinks was eliminated by dealing only with the thermally excited unforced kinks that are in the direction opposite to the kinks caused by the azimuthal misorientation.

In this paper, the equilibrium structure of the step

edges of the vicinal Si(001) surface is described in terms of anisotropic nearest-neighbor interaction and isotropic second-nearest-neighbor interaction between dimers. It will be shown that it is possible to analyze step edges that include forced kinks induced by the misorientation of the step edge. Moreover, it will also be demonstrated, using the Burton, Cabrera, and Frank (BCF) theory,⁵ that neglecting the presence of forced kinks yields incorrect results. The corner energy proposed in Ref. 6 will be reinterpreted as the second-nearest-neighbor interaction between dimers.

As a model appropriate for the dimer reconstructed Si(001) 2×1 surface, we consider a square crystal with anisotropic nearest-neighbor interactions E_x and E_y , respectively, and isotropic second-nearest-neighbor interactions $E_{z,\text{diag}}$ (see Fig. 1), where E_x is the interaction energy between sets of two dimers on the same terrace in adjacent rows, E_y is the interaction energy between dimers on the same terrace in a row, and $E_{z,\text{diag}}$ is the diagonal interaction energy between dimers on the same terrace in adjacent rows. In principle, two different *B*-type step edges can occur because there are two different configurations, depending on where the dimer row of the upper terrace ends with respect to the dimer rows of the

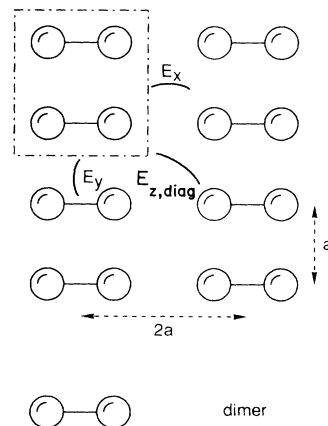


FIG. 1. Interaction energies between adjacent blocks of two dimers on the Si(001) surface. The distance between adjacent rows of dimers and between adjacent dimers in a row is $2a$ and a , respectively ($a = 3.84 \text{ \AA}$).

lower terrace. Both type-*B* monatomic steps have been observed,⁷ and thus, occasionally, kink lengths of an odd number in *a* do occur, but, in general, kinks are found on a (2×2) lattice.^{6,8} The occasional kinks of odd length in *a* are not contained in the model.

In the BCF theory,⁵ two different types of kinks, which are called positive and negative, corresponding to a “jump” and a “drop,” respectively, are distinguished. Following this theory,⁵ we use the symbol n_{+r} to denote the probability that there is a jump of length $2ar$ at a given position in the step edge in a direction perpendicular to the step edge. The symbol n_{-r} is used to denote the probability that at a given position in the step edge there is a drop of length $2ar$ in a direction perpendicular to the step edge; q is the probability that at a given position in the step edge there is no kink of any kind. We assume that any of the various possibilities ($q, n_{\pm r}$) can occur independently, hence the probability of occurrence of one specific configuration of the step edge is equal to the product of the probabilities of occurrence of the individual situations that make up this specific configuration of the step edge. In the BCF theory,⁵ the equilibrium structure of a step edge is derived for a Kossel crystal (cubic crystal with isotropic first- and second-nearest-neighbor interactions). We have derived the equilibrium structure of a square crystal with anisotropic nearest-neighbor interactions and isotropic second-nearest-neighbor interactions in an analogous manner by apply-

ing the principle of detailed balancing. At any point of the step edge the normalization condition holds:

$$q + \sum_{r=1}^{\infty} (n_{+r} + n_{-r}) = 1. \quad (1)$$

According to the BCF theory,⁵ the following thermodynamic relations can be derived for a step along the *x* axis:

$$E_x/kT = -\ln \left[\frac{n_{+1}n_{-1}}{q^2} \right], \quad (2)$$

$$E_{z,\text{diag}}/kT = -\ln \left[\frac{n_{\pm r}q}{n_{\pm(r-1)}n_{\pm 1}} \right], \quad r \geq 2. \quad (3)$$

Formulas (2) and (3) can be understood as coming from a comparison of two different situations that result in the same overall displacement of the step edge (the principle of detailed balancing⁵). Equation (2) follows from comparing a n_{-1} and n_{+1} pair versus a straight step, while Eq. (3) results from a comparison of a n_{r-1} and n_{+1} kink versus a n_r kink alone. Similar formulas can be derived for a step along the *y* axis, only E_x must be replaced by E_y in (2). Formula (2) shows that the quotient $n_{+1}n_{-1}/q^2$ is independent of the inclination Θ of the step edge. A large inclination corresponds to a large amount of forced kinks in one direction and hence to a low amount of thermally excited kinks in the other direc-

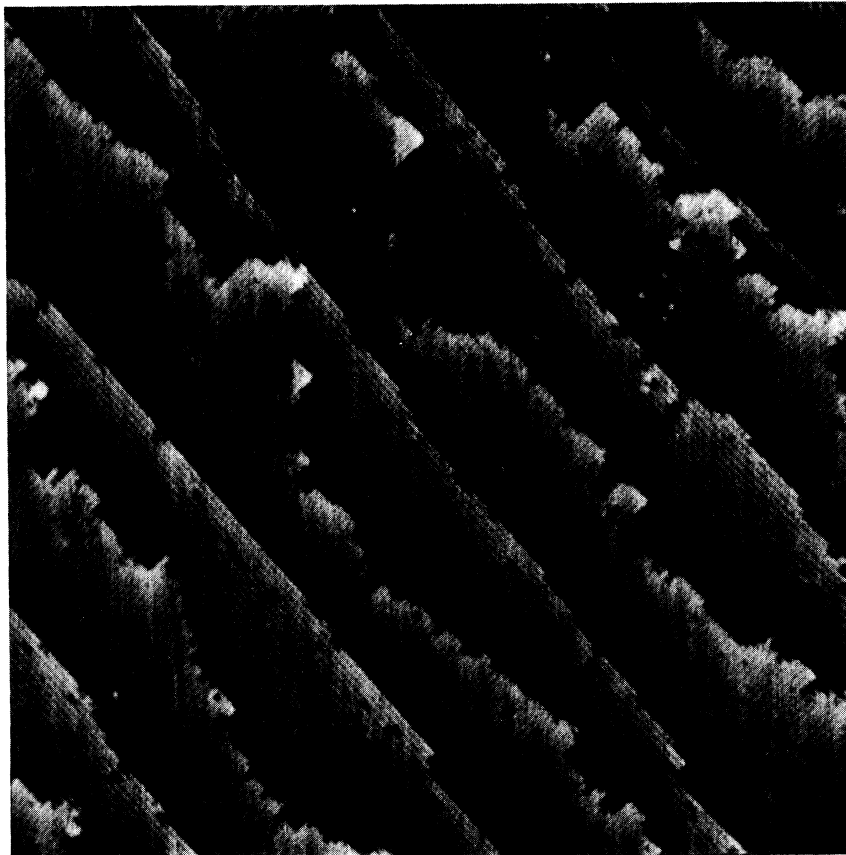


FIG. 2. Large-area STM image ($100 \times 100 \text{ nm}^2$) of Si(001) 0.5° misoriented towards the [110] direction, obtained at -2.0-V sample bias and 0.5-nA tunneling current.

TABLE I. Measured number of kinks ($n_{\pm r}$) vs r obtained from our own data (A - and B -type step edges) and determined from the data of Ref. 6.

r	A step (this work) total length, $1489 \times 2a$		B -step (this work) total length, $1504 \times 2a$		B step (Ref. 6) $n_{+r} + n_{-r}$
	n_{+r}	n_{-r}	n_{+r}	n_{-r}	
0	1297		974		0.52
1	59	100	157	163	0.21
2	7	20	51	57	0.077
3			20	24	0.035
4			9	12	0.0156
5			4	7	0.0077
6					0.0038
7					0.0019
8					0.0009

tion, and vice versa. So only counting the kinks in the direction opposite to the inclination results in a too-low number and hence overestimation of E_y . The distributions of q , n_{+r} , and n_{-r} , as a function of r , as obtained from several images like Fig. 2, together with the data of the B -type step edge of Ref. 6, are presented in Table I. Using these distributions and formulas (2) and (3), the interaction energies $E_{x,y}$ and $E_{z,\text{diag}}$ can be obtained. The data of Ref. 6 have been extracted from the distributions shown in Figs. 1 and 3 of that paper. Using n_{+1} , n_{-1} , and q from Table I and formula (2), we find $E_x/kT = 3.6 \pm 0.2$ for the B -type step edge [compared to $E_x/kT = 3.2$ for the data of Ref. 6, assuming that $n_{+1} = n_{-1} = \frac{1}{2}(n_{+1} + n_{-1})$] and $E_y/kT = 5.7 \pm 0.3$ for the A -type step edge. The error bars are determined using the statistical error \sqrt{n} . According to formula (3), $E_{z,\text{diag}}/kT$ can be determined for different values of r . Using our model, the second-nearest-neighbor interaction $E_{z,\text{diag}}$ must be independent of r . For both the data in Ref. 6 and our own data, this results in a value of -1 ± 0.3 for $E_{z,\text{diag}}/kT$.

It is interesting to note that the value of $|E_{z,\text{diag}}/kT|$ determined from the B -type step edge increases with r at low- r values, both for the data in Ref. 6 as well as for our own data. To overcome this problem, Swartzentruber *et al.*⁶ proposed to fit the data with an additional negative term inversely proportional to r , which can be interpreted as the attractive interaction between the ends of a kink.

In order to translate the parameters, $E_{x,y,z,\text{diag}}/kT$, as obtained from our analysis, to interaction energies, a reasonable quench temperature at which the step configuration is frozen in has to be taken. Our Si(001) samples were held at a temperature of about 775 K for several hours, followed by quenching to room temperature. We know from STM measurements of the Si(001) surface⁹ performed at about 725 K that at this temperature the step edges change significantly on a time scale of minutes. Furthermore, we know that the quench rate is very rapid for the first 100 K. Hence a good estimate

(upper limit) of the temperature at which our step configuration is frozen in is 775 K. Using this temperature of 775 K, we obtain the following interaction energies: $E_x = 0.24 \pm 0.01$ eV, $E_y = 0.38 \pm 0.02$ eV and $E_{z,\text{diag}} = -0.07 \pm 0.02$ eV. Using a lower limit of 575 K (Ref. 6) for the temperature at which the step edges are frozen in lowers the measured values of the interaction energies by 25%.

In order to compare our results with the data in Ref. 6, $E_{x,y}$ must be divided by a factor of 4; one factor of 2 comes from sharing the interaction between two blocks, and the other comes from using energy per $2a$ instead of energy per a (which is related to the size of the building block). The diagonal interaction $E_{z,\text{diag}}$ has to be divided by a factor of 2 only, due to the translation from interaction energy between two dimers to energy per corner of a block. The energy of a kink with a length of $2ar$, $n_{\pm r}$, for a step edge with no forced kinks ($\Theta = 0$) with respect to no kink is according to our model $E = r(E_{x,y}/2) + (r-1)E_{z,\text{diag}}$. As mentioned before, the data in Ref. 6 were fitted with an expression of the form $E = 2rE_{SB,SA} + C$, so the values $\frac{1}{4}E_x + \frac{1}{2}E_{z,\text{diag}} = 0.026$ eV and $\frac{1}{4}E_y + \frac{1}{2}E_{z,\text{diag}} = 0.06$ eV should be compared with 0.028 and 0.09 eV, respectively, as given in Ref. 6. As expected, in particular the interaction energy related to E_y , as determined from the A -type step edge differs from the data in Ref. 6 due to the presence of a sizeable fraction of forced kinks induced by the misorientation.

To summarize, we have determined the effective interaction energies between dimers by examining the distribution of kink lengths and applying the BCF theory, which explicitly includes forced kinks induced by step misorientations. The corner energy proposed in Ref. 6 has been reinterpreted as the second-nearest-neighbor interaction between dimers.

The support of Dr. J. Dieleman is gratefully acknowledged, and we thank Dr. G. H. L. Brocks for several valuable suggestions.

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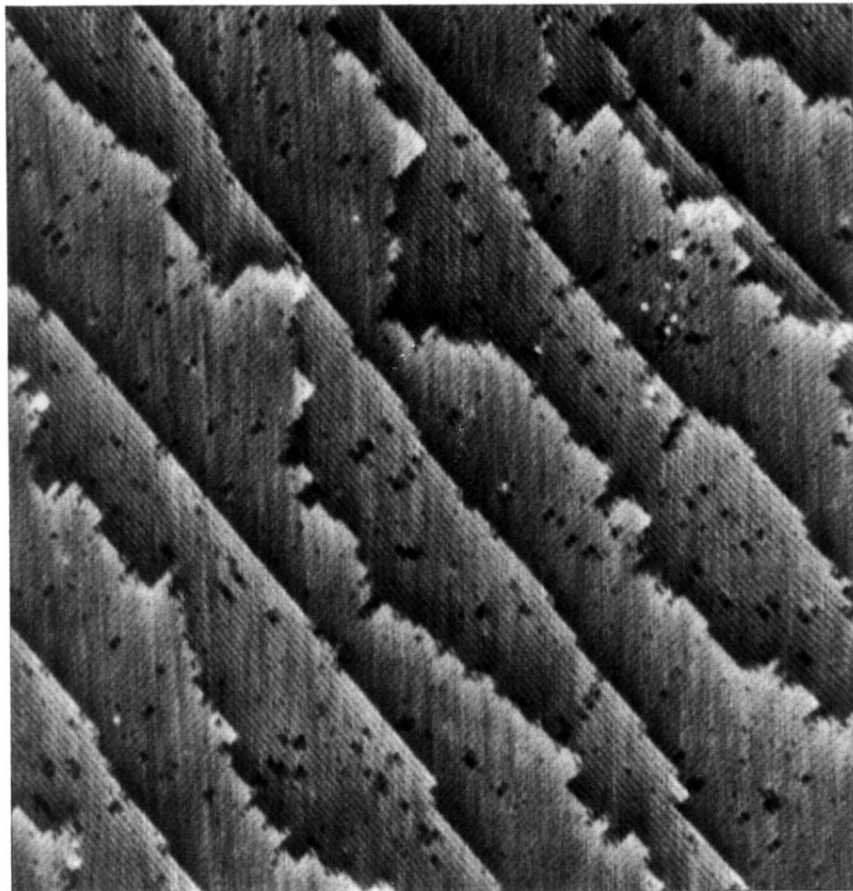


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