

## STEP–STEP INTERACTION ENERGY ON Cu(111) VICINAL SURFACES

MARGRET GIESEN\* and GEORG SCHULZE ICKING-KONERT  
*Institut für Grenzflächenforschung und Vakuumphysik, Forschungszentrum Jülich,  
D 52425 Jülich, Germany*

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We have measured the terrace width distribution on copper (111) vicinal surfaces with (100) steps. For all surfaces, the distribution is well fitted by a Gaussian. The width of the Gaussian scales with the mean terrace width  $L$ , which is indicative of a repulsive  $1/L^2$  interaction potential between steps. We determine an interaction strength of the potential of  $3.2 \pm 0.2$  meV per atom length. From the temperature-dependent analysis of the step–step distance distribution, we find a kink formation energy for (100) steps of  $0.12 \pm 0.03$  eV, which is consistent with previous measurements of the kink energy on copper (100) vicinal surfaces.

### 1. Introduction

The stability of vicinal surfaces has attracted substantial interest in recent years. Stable vicinal surfaces reveal a regular step array and form a near-perfect two-dimensional substrate. The regular step array of vicinal surfaces is stabilized by repulsive interactions between neighboring steps.<sup>1–3</sup>

The interaction potentials can be of a different nature: repulsive entropic interactions arise from the noncrossing condition of adjacent steps. Explicit energetic interactions, repulsive as well as attractive, may be due to dipol–dipol or elastic interactions. Strong repulsive interactions between steps cause regular step arrays with about equally spaced steps, whereas strong attractive interactions may lead to the formation of multiple steps or even large step bunches. However, even for a stable vicinal orientation with strong repulsive step–step interactions, the step array is not perfectly regular. Rather, the step distance distribution has a finite width. The width of this distribution depends on the step density, the temperature and the interaction strength of the potential.

Quite a number of semiconductor and metal surfaces have been investigated in the past.<sup>4–10</sup> Several studies have been performed, for example on copper (11n) surfaces vicinal to the (100) orientation.<sup>8–10</sup> It turned out that most of the surfaces reveal a relatively sharp step–step distance distribution which is well approximated by a Gaussian. This is indicative of an energetic repulsive step interaction potential. Similar results were found on silicon vicinal surfaces, though the interaction strength differs from the Cu(11n) surfaces by about an order of magnitude.<sup>4,5</sup>

Although most of the measurements confirmed the assumption of a repulsive stabilization of the vicinal orientation, some investigations provided evidence for the existence of long-ranged attractive interactions between steps.<sup>8</sup> The attractive interactions may not necessarily lead to an instability of the vicinal surface, but rather to a broader step–step distance distribution.<sup>2</sup> Strong attractive interactions, however, cause a decomposition into different surface orientations or lead to the formation of step bunches.<sup>11</sup> It has been reported that step–step

\*Corresponding author. E-mail: m.giesen@fz-juelich.de

interactions can even be oscillatory with the distance between steps.<sup>7</sup>

In this paper, we present an investigation of the step-step distance distribution of copper surfaces vicinal to the (111) orientation. Depending on the direction of the miscut with respect to the dense orientation, vicinals to the (111) plane have (100) or (111) steps. For miscut angles in low symmetry directions the surfaces may have (100) as well as (111) step segments. It has been shown recently that the (997) surface, which consists of parallel (111) steps along the dense direction, is instable.<sup>12</sup> The opposite surface orientation, (779) with (100) steps, is stable, however. In addition, it was shown that all Cu(111) vicinal surfaces with (100) steps investigated so far are stable and have a rather regular array of parallel steps.<sup>13</sup> The physical reason for the stability difference of the Cu(111) vicinals with (111) and (100) steps is not known yet. Different step energetics as well as different step-step interactions for the two step orientations may play a role.

In this paper, we investigate the step-step interactions of three different Cu(111) vicinal surfaces with (100) steps. We analyze the terrace width distribution as a function of temperature. From this analysis, we determine the step-step interaction strength and, to a limited accuracy, the kink formation energy. A comparison of our results with the Villain model<sup>1</sup> provides an estimate of the roughening temperature of stepped Cu(111) surfaces.

The paper is organized as follows. After a description of the experimental setup and sample preparation in Sec. 2, we present our results in Sec. 3. Then, in Sec. 4, the results are discussed in terms of a simple model for the interaction potential. We conclude with a brief summary in Sec. 5.

## 2. Experimental

The experiments were performed in a standard ultrahigh vacuum chamber with a base pressure of  $5 \times 10^{-11}$  mbar. Our temperature variable scanning tunneling microscope (STM) is of the Besocke type. During the STM measurements the temperature of the sample is changed by radiative cooling and heating.

We used three samples with miscut angles  $2.49^\circ$ ,  $3.05^\circ$  and  $12.75^\circ$  along the  $[11\bar{2}]$  direction. These surfaces have an orientation of (23 21 21), (19 17 17) and

(11 7 7), respectively. The samples consist of parallel monatomic (100) steps along  $[\bar{1}10]$ . The mean terrace widths between adjacent steps are 47.8, 32.3 and 10.2 Å, respectively. These values correspond to 21.63, 14.62 and 4.62  $a_\perp$ , where  $a_\perp = 2.21$  Å is the kink length of a (100) step on a (111) surface.

The samples were cut by spark erosion from a (111) copper single crystal bar. They were mechanically and electrochemically polished and oriented to the desired orientations by diffractometry to within  $0.1^\circ$ . Before mounting in the chamber, the crystals were annealed for 2 h in a H<sub>2</sub>:Ar (1:25) atmosphere at 900°C. After this procedure the crystals are well oriented and largely free of the usual contaminants, like sulfur and carbon. The final preparation was performed *in situ* by about 30 cycles of Ne<sup>+</sup> sputtering (1.3 keV) and annealing to 700°C, with subsequent slow cooling to room temperature (cooling rate 0.8 K/s). This preparation was finished by one cycle of moderate sputtering with 0.6 keV and annealing to 400°C. After this procedure the concentration of contaminants on the surface is far below the Auger detection limit and the surfaces have a regular array of parallel steps.

After the final *in situ* preparation cycle, the surface was carefully checked with respect to residual pinning sites by means of the STM. Residual pinning sites have a large influence on the local mean distance between steps. In our experiments, the concentration of pinning sites was lower than  $10^{-7}$  per atom. For the analysis, we used STM images obtained from areas free of residual contamination. A measured terrace width distribution was taken into account for the analysis only when the average step density found from the distribution was consistent with the nominal step density given by the miscut angle of the surface.

## 3. Experimental Results

Figure 1 shows an STM image of Cu(11 7 7) around room temperature. Images of the (19 17 17) and (23 21 21) surface are similar; however, they display larger step-step distances. The parallel steps run from top to bottom and the upward direction of the steps is from left to right. Monatomic steps on Cu(111) surfaces appear frizzy in STM images at room temperature and higher temperatures. The frizziness is due to kink diffusion along the steps.<sup>14-16</sup>

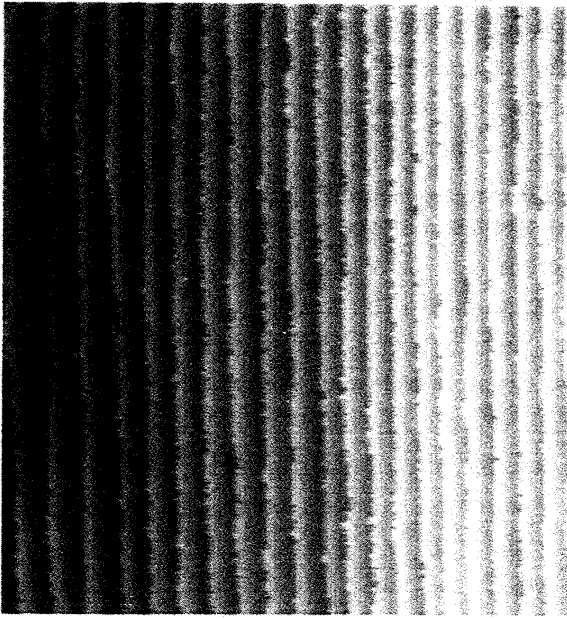


Fig. 1. STM image of the stepped Cu(11 7 7) surface at room temperature. The image shows an area of the sample of about  $24 \times 24 \text{ nm}^2$ .

We have analyzed the step-step distance distribution from a large set of STM images similar to the image shown in Fig. 1. The step-step distance distribution was measured for each sample at four different temperatures between 296 and 360 K. At a distinct temperature the distribution was determined from about 20 images scanned in different surface areas. Depending on the surface, the STM images displayed 10–20 steps. The total number of steps analyzed for a terrace width distribution was 100–350, equivalent to a total step length of about 8–13  $\mu\text{m}$ . In Fig. 2 the probability of finding a step-step distance on Cu(11 7 7) for (a) 296 K, (b) 301 K, (c) 306 K and (d) 323 K is plotted in units of the atomic distance  $a_{\perp}$  perpendicular to the step edges. Figures 3(a) and 3(b) show the distributions found on Cu(19 17 17) and Cu(23 21 21) at 353 and 313 K, respectively. The experimental data are shown as open circles.

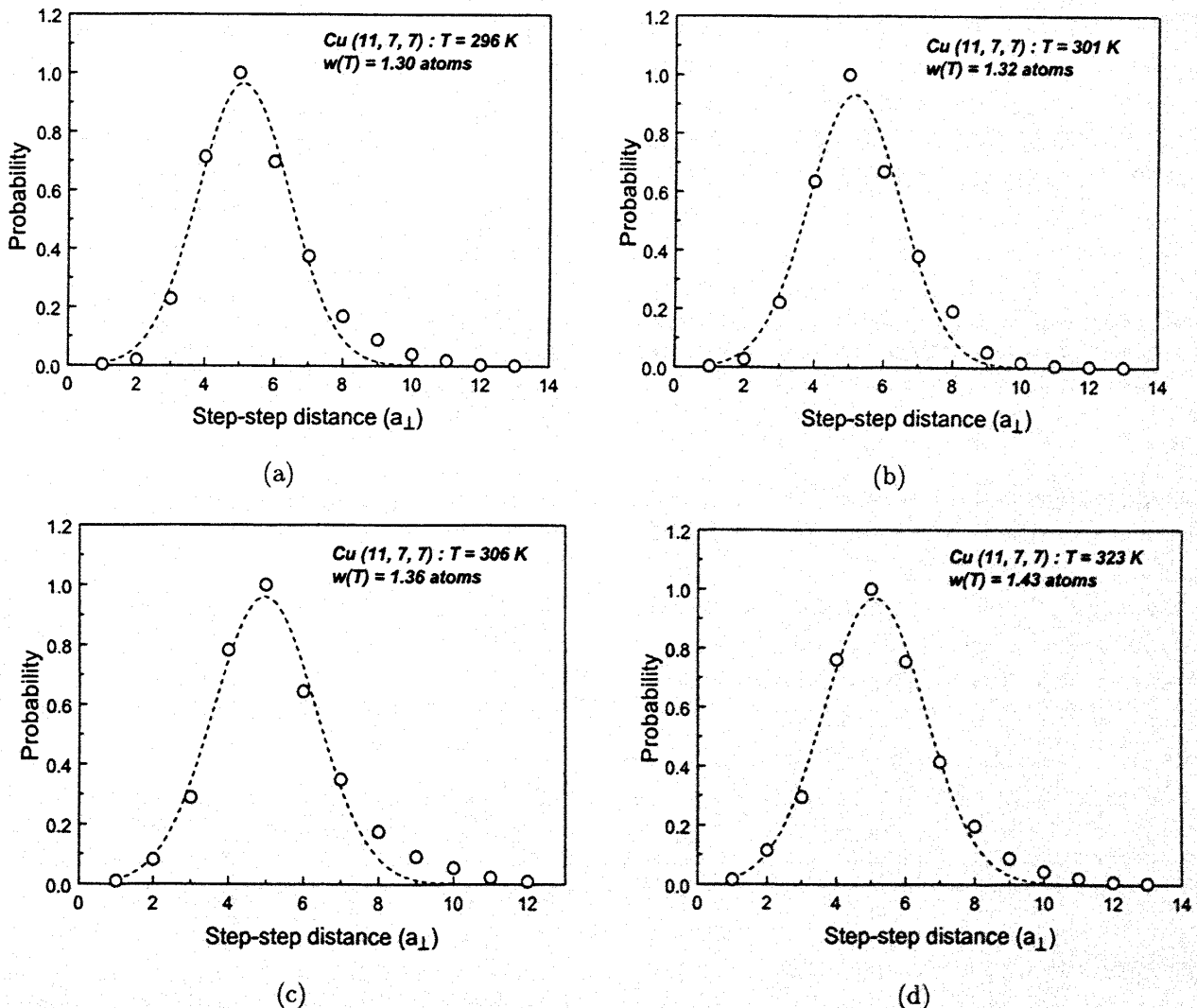


Fig. 2. Probability of finding a step-step distance on Cu(11 7 7) at (a) 296 K, (b) 301 K, (c) 306 K and (d) 323 K. The widths of the distributions are indicated as  $w(T)$  in the view graphs.

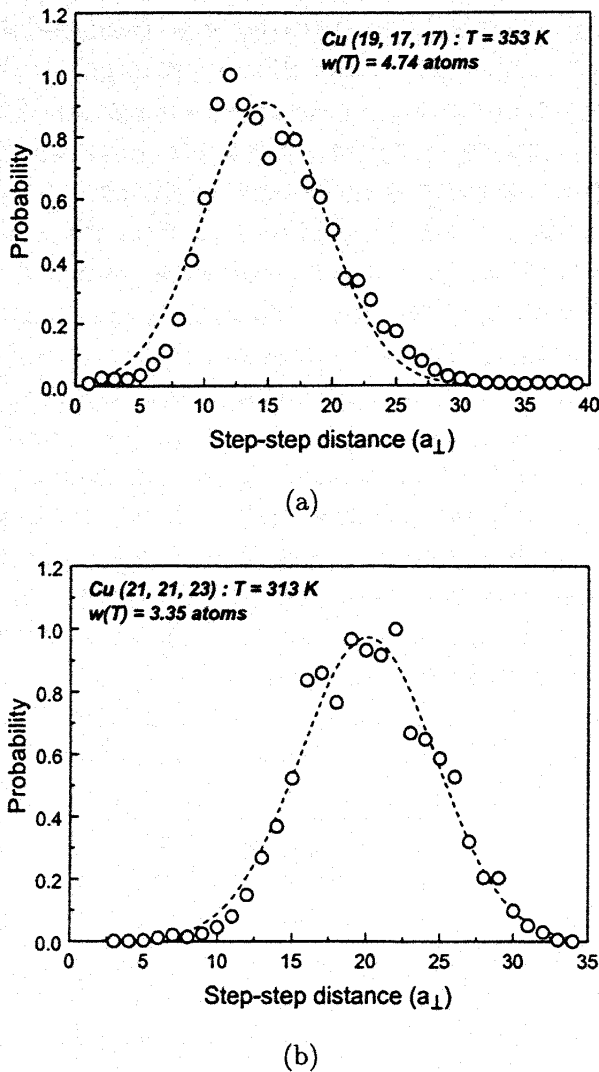


Fig. 3. Probability of finding a step-step distance on (a) Cu(19 17 17) at 353 K and (b) Cu(23 21 21) at 313 K. These terrace width distributions are taken from a set of four measurements at different temperatures for each surface.

The dashed curves in Figs. 2 and 3 are fits to the data with a Gaussian. The Gaussian fit obtained for Cu(11 7 7) shown in Fig. 2 is good despite a small asymmetry of the experimental distribution. This asymmetry becomes obvious especially at larger step-step distances. The data points obtained for the two other surfaces (Fig. 3) slightly scatter though they are also in agreement with a Gaussian distribution. The width of the Gaussian fits  $w(T)$  is given in Figs. 2 and 3 in units of kink lengths  $a_{\perp} = 2.21 \text{ \AA}$ .  $w(T)$  increases with increasing temperature (Fig. 2).

#### 4. Discussion

Steps in equilibrium fluctuate in their step position due to the formation of kinks and adatoms. The fluctuations of monatomic steps on stepped surfaces are

restricted by the presence of neighboring steps due to the noncrossing condition. A crossing of steps on a defect-free vicinal surface would include overhangs which are energetically unfavorable. The noncrossing condition leads to an effective entropic repulsion of adjacent steps even when no explicit energetic interactions are present. In that case, steps act like free fermions. In the free fermion model, the terrace width distribution is asymmetric.<sup>2</sup> This asymmetry is always observed in experiments (Figs. 2 and 3) although the distribution is much narrower than the free fermion distribution due to an explicit repulsive interaction between steps. Energetic repulsive interactions may arise from elastic interaction potentials which are caused by the lattice distortion near step edges. Repulsive interactions can also be due to dipole-dipole forces between steps. The dipole-dipole forces arise from the electron distribution near step edges. In the case of energetic repulsive interactions, elastic as well as electric dipole-dipole interactions, the interaction potential is described by a potential<sup>3</sup>

$$V(x, L) = A \sum_{n=1}^{\infty} \frac{1}{(nL + x)^2} + \frac{1}{(nL - x)^2}, \quad (1)$$

where  $x$  is the distance perpendicular to the step edges. The mean distance between steps is denoted as  $L$ , and  $A$  is the interaction strength. In Eq. (1), the summation is over all neighboring steps which are assumed to be straight and nonfluctuating.  $V(x, L)$  is well described by the harmonic approximation of the exact potential in Eq. (1):

$$V(x, L) = \frac{A}{L^2} \left( \sum_{n=1}^{\infty} \frac{2}{n^2} \right) + \frac{\pi^4 A}{15 L^4} x^2 + \dots \quad (2)$$

For a harmonic potential, the step-step distance distribution is a Gaussian

$$P(x) = \frac{1}{w\sqrt{2\pi}} e^{-\frac{x^2}{2w^2}}. \quad (3)$$

For a step fluctuating between straight steps the width  $w$  of the Gaussian distribution is given by<sup>3</sup>

$$w^4 = \frac{b^2(T)k_B T}{8c(L)}. \quad (4)$$

The constant  $c(L)$  is in the harmonic approximation

$$c(L) = \frac{\pi^4 A}{15 L^4}. \quad (5)$$

In Eq. (4), the diffusivity  $b^2(T)$  can be expressed by the kink concentration  $P_k$ :

$$b^2(T) \approx P_k \approx 2e^{-\frac{\varepsilon}{k_B T}} \quad \text{for } \varepsilon \gg k_B T, \quad (6)$$

where  $\varepsilon$  is the kink formation energy. Equation (6) holds for small values of  $k_B T$  compared to the kink energy. Hence, Eq. (4) becomes

$$w^4 \approx \frac{e^{-\frac{\varepsilon}{k_B T}} k_B T}{4c(L)}. \quad (7)$$

Using Eqs. (5) and (7) we obtain

$$\left(\frac{w}{L}\right)^4 \approx \frac{15}{4\pi^4} \cdot \frac{e^{-\frac{\varepsilon}{k_B T}} k_B T}{A} \approx 0.0385 \frac{e^{-\frac{\varepsilon}{k_B T}} k_B T}{A}. \quad (8)$$

The scaling of the width  $w$  with the mean distance  $L$  is characteristic for a  $1/L^2$  repulsive interaction potential. Recently, Ihle *et al.* have calculated the expected terrace width distribution for repulsive interactions considering that steps are not straight but fluctuate in equilibrium.<sup>17</sup> The distribution remains a Gaussian; however, for a given interaction strength the distribution becomes broader:

$$\left(\frac{w}{L}\right)^4 \approx 0.122 \frac{e^{-\frac{\varepsilon}{k_B T}} k_B T}{A}. \quad (9)$$

There is an ongoing discussion as to whether Eq. (9) is the appropriate formula for analyzing step-step distance distributions of fluctuating steps. It was shown<sup>18,19</sup> by the calibration with exact results that the extra factor of about 3 calculated by Ihle *et al.*<sup>17</sup> should not be used, at least for small values of  $\frac{A}{k_B T}$ . Controversy still exists for large values of  $\frac{A}{k_B T}$ . Here, we make use of Eq. (8) to analyze the step-step distance distribution.

From Eq. (8) one can roughly determine the kink formation energy  $\varepsilon$ . Figure 4 shows a logarithmic plot of  $(\frac{w}{L})^4 / k_B T$  over  $1/T$ . Here, we have used for  $L$  the measured mean step-step distance determined from the terrace width distribution [about  $L = 5.1, 14.6$  and  $21.5 a_{\perp}$  for Cu(11 7 7), (19 17 17) and (21 21 23), respectively]. The open triangles and circles refer to the data measured on Cu(19 17 17) and (23 21 21), respectively, and the filled squares are the data obtained on the (11 7 7) surface. A least squares linear fit to all data points is given by the dashed line. The data sets lie approximately on the same linear curve. Hence, the step-step interaction potential scales with the mean distance  $L$  between

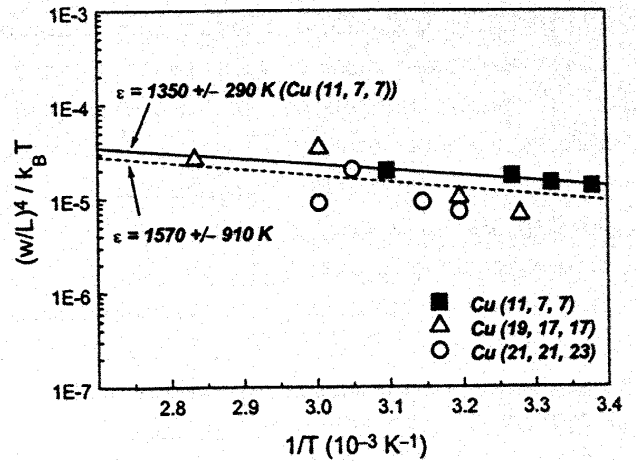


Fig. 4. Temperature dependence of the width of the distribution of all surfaces scaled by the mean distance  $L$  between steps. In this logarithmic plot the slope of the linear fit (dashed curve) yields the kink formation energy  $\varepsilon$ . The solid curve is the best linear fit to the data obtained exclusively from the (11 7 7) surface (solid squares).

steps, i.e. the interaction potential on the Cu(111) vicinal surfaces is a repulsive  $1/L^2$  potential. From the slope of the dashed line we determine the kink energy to be  $\varepsilon = 0.135 \pm 0.078$  eV.

For the solid line we have exclusively used the data from (11 7 7) to determine the kink energy. Here, a value of  $\varepsilon = 0.116 \pm 0.025$  eV is found. In Figs. 2 and 3 we have seen that the best fit to the step-step distance distribution is obtained for the data of the (11 7 7) surface. Hence, the most reliable value for the kink formation energy is  $\varepsilon = 0.116 \pm 0.025$  eV. Recently, we have determined the kink formation energy on Cu(111) by analyzing the equilibrium shape of islands<sup>20</sup> using an Ising model.<sup>21</sup> From this analysis we determine the kink formation energy to  $\varepsilon = 0.11$  eV.

A kink energy of  $0.116 \pm 0.025$  eV is of the same order as the kink energy on Cu(100) vicinal surfaces. For Cu(100),  $\varepsilon$  was determined to be  $0.128 \pm 0.003$  eV.<sup>15</sup> This result is in agreement with theoretical calculations which predict that the kink energy should be about equal for both of the surface orientations (100) and (111).<sup>22,23</sup> The assumption that  $\varepsilon$  is about equal for both surface orientations is supported by our measurements. For the following analysis of the interaction strength  $A$  we assume the kink energy on Cu(111) to be  $\varepsilon = 0.11$  eV.

On vicinals with lower step densities, experimental errors in the determination of the strength  $A$

are larger. The influence of residual contamination is larger on vicinal surfaces with lower step densities. Therefore, the analysis of the terrace width distribution is more reliable for vicinals with a high step density, i.e. with small terraces. On the other hand, Eq. (8) holds when the step-step distance  $L$  is large compared to the interatomic distance. In experiments one has to find a compromise between the two restrictions. It is reasonable to assume that the scattering of the measured terrace widths on the (19 17 17) and (23 21 21) surfaces is due to the enhanced influence of pinning sites. Therefore, we analyze in the following exclusively the data obtained from the (11 7 7) surface. We assume that the terrace width  $L = 5.1$  atoms in the case of the (11 7 7) surface is large enough to justify the continuum approximation.

Using  $\varepsilon = 0.11$  eV, we find an average value of  $c(L = 5.1 \text{ atoms})$  for Cu(11 7 7),

$$c(L) = 0.032 \pm 0.001 \text{ meV}, \quad (10)$$

or, in terms of the interaction strength using Eq. (8),

$$A = 3.2 \pm 0.2 \text{ meV (per atom)}. \quad (11)$$

This value is in reasonable agreement with recent measurements of Sánchez *et al.* at room temperature.<sup>24</sup> From the terrace width distribution shown in Ref. 24 one determines an interaction strength of 1.7 meV. We can also compare the value in Eq. (11) with the strength of the potential  $A$  found for Cu(100) vicinal surfaces, which is  $A = 2.8 \pm 1.5$  meV.<sup>9</sup>

Now, we use the value found for the interaction strength  $A$  for the (111) vicinals [Eq. (11)] to estimate the roughening temperature of the Cu(11 7 7) surface. In the Villain model, the roughening temperature  $T_R$  is given by<sup>1</sup>

$$\frac{6A e^{\frac{\varepsilon}{k_B T_R}}}{L^4 k_B T_R} = \frac{\pi^2}{2}. \quad (12)$$

Here, it is assumed that the mean terrace width is large compared to the next nearest neighbor distance. Therefore, the Villain model strictly holds only for surfaces with large indices. Assuming that on Cu(11 7 7) the mean terrace width of about 5.1 nearest neighbor distances is large enough, we find that

$$T_R \approx 164 \pm 1 \text{ K for Cu(11 7 7)}. \quad (13)$$

Table 1. Roughening temperature  $T_R$  determined from the measured interaction strength on stepped copper surfaces vicinal to (111).

Copper (111) Vicinal Surfaces	$T_R$ (K) (Predicted from $A = 3.2 \pm 0.2 \text{ meV}$ )
(11 7 7)	$164 \pm 1$
(19 17 17)	$110 \pm 1$
(23 21 21)	$98 \pm 1$

Table 1 shows the roughening temperatures for all Cu(111) vicinals investigated in our experiment assuming an interaction strength of  $A = 3.2$  meV for all surfaces.

At the end of this discussion we want to estimate the surface stress of the copper surfaces vicinal to the (111) and (100) orientations. Assuming that the elastic Green function has the same form as for an elastic isotropic medium, but with elastic constants pertinent to the crystallographic orientation of the surface, the interaction potential  $V(x)$  for two parallel, equally oriented steps with distance  $x$  can be written as<sup>25</sup>

$$V(x) = \frac{2(1 - \nu_{(hkl)}^2)}{\pi Y_{(hkl)}} (D_x^2 + D_z^2) \frac{1}{x^2}, \quad (14)$$

where  $D_x^2$ ,  $D_z^2$  are the parallel and perpendicular force dipoles arising from the mechanical strain field at the step edges.  $Y_{(hkl)}$  and  $\nu_{(hkl)}$  are the Young moduli and the Poisson ratios for the  $(hkl)$ -oriented surface. For (100)-oriented steps on a (111) vicinal surface and for (111)-oriented steps on (100) vicinal surfaces, the force dipoles can be expressed in terms of the step height  $h_{(hkl)}$  and the surface stress  $\tau_{(hkl)}$ <sup>25</sup> (Fig. 5):

$$\begin{aligned} D_x^2 + D_z^2 &= \frac{5}{6} h_{(100)}^2 \tau_{(111)}^2 && \text{for (111) steps on} \\ &&& \text{(100) terraces,} \\ D_x^2 + D_z^2 &= \frac{5}{6} h_{(111)}^2 \tau_{(100)}^2 && \text{for (100) steps on} \\ &&& \text{(111) terraces.} \end{aligned} \quad (15)$$

Here, we have neglected the contribution of the terraces to the parallel component of the force dipole.<sup>26</sup> Comparing Eq. (14) with Eq. (1) yields

$$\begin{aligned} A_{(111)} &= \frac{5}{3\pi} \frac{1 - \nu_{(111)}^2}{Y_{(111)}} h_{(100)}^2 \tau_{(111)}^2, \\ A_{(100)} &= \frac{5}{3\pi} \frac{1 - \nu_{(100)}^2}{Y_{(100)}} h_{(111)}^2 \tau_{(100)}^2. \end{aligned} \quad (16)$$

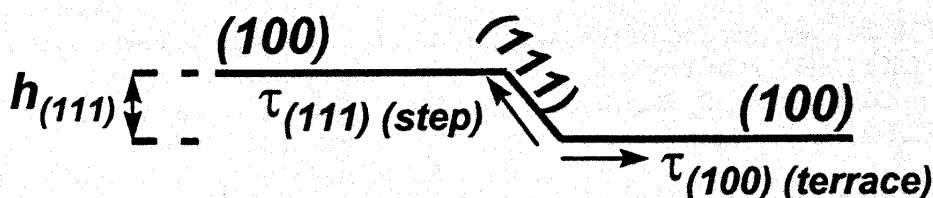


Fig. 5. Geometry used for the calculation of the surface stress  $\tau_{(hkl)}$  in Eq. (15) for the case of a Cu(100) vicinal surface with (111)-oriented steps. For stepped Cu(111), the orientations of the terraces and step edges are (111) and (100), respectively. In both cases, we have neglected in Eq. (15) the contribution  $\tau_{(hkl)(terrace)}$  of the terraces to the parallel component of the surface stress.<sup>26</sup>

$A_{(111)}$  and  $A_{(100)}$  are the interaction strengths found on the (111) and (100) vicinal surfaces, respectively. For both surfaces, the Young modulus and the Poisson ratio can be expressed in terms of the elastic compliances:<sup>25</sup>

$$\begin{aligned} Y_{(111)} &= \frac{4}{2s_{11} + 2s_{12} + s_{44}}, \\ \nu_{(111)} &= -Y_{(111)} \frac{2s_{11} + 10s_{12} - s_{44}}{12}, \\ Y_{(100)} &= \frac{1}{s_{11}}, \\ \nu_{(100)} &= -\frac{s_{12}}{s_{11}}. \end{aligned} \quad (17)$$

For copper, the elastic compliances are  $s_{11} = 15.0 \times 10^{-12} \text{ m}^2/\text{N}$ ,  $s_{12} = -6.3 \times 10^{-12} \text{ m}^2/\text{N}$  and  $s_{44} = 13.3 \times 10^{-12} \text{ m}^2/\text{N}$ .<sup>27</sup> Then, one finds for the Young moduli and the Poisson ratios  $Y_{(111)} = 13.0 \times 10^{10} \text{ N/m}^2$ ,  $Y_{(100)} = 6.7 \times 10^{10} \text{ N/m}^2$ ,  $\nu_{(111)} = 0.50$  and  $\nu_{(100)} = 0.42$ . Using these values in Eq. (16) and  $A_{(111)} = 3.2 \text{ meV}$  and  $A_{(100)} = 2.8 \text{ meV}$ ,<sup>9</sup> the surface stresses on (111) and (100) surfaces are determined to be

$$\tau_{(111)} = 1.15 \text{ N/m}, \quad \tau_{(100)} = 0.64 \text{ N/m}. \quad (18)$$

Using EAM potentials, the surface stresses for Cu(100) and (111) have been calculated by Gumbsch and Daw to be  $\tau = 1.38 \text{ N/m}$  and  $\tau = 0.86 \text{ N/m}$ ,<sup>28</sup> respectively. These values are in good agreement with our estimation of  $\tau$  from the terrace width distribution. However, the results obtained in Ref. 28 for silver are far too low according to first principles calculations [ $\tau = 0.82 \text{ N/m}$  for Ag (100) (EAM)<sup>28</sup> vs.  $\tau = 1.8 \text{ N/m}$  (LDA)<sup>29</sup>]. Hence, the value of  $\tau$  we obtained for Cu(111) in Eq. (18) may be lower than the true value. This conclusion is in agreement with our previous result on Cu(100).<sup>9</sup> There we have found that in contrast to results on silicon all results

on copper are about one order of magnitude smaller than the calculated value.

## 5. Summary

In summary, we have analyzed the step-step distance distribution on copper surfaces vicinal to (111) with (100) steps. The distributions can be described by a repulsive  $1/L^2$  interaction potential. We find that the interaction potential scales for all surfaces with the mean terrace width  $L$ . The interaction strength of the potential is determined to be  $A = 3.2 \text{ meV}$  per atom. The values found for the surface stress for the Cu(111) and the (100) planes using the measured values of  $A$  are smaller than reasonable values for the surface stress of both surfaces. From a temperature-dependent analysis of the distribution width we find a kink energy of  $\varepsilon = 0.116 \text{ eV}$ , which is about equal to the kink energy measured on Cu(100).

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