GaAs(110) terrace-width distributions and kink formation

Y.-N. Yang, B. M. Trafas, R. L. Siefert, and J. H. Weaver
Department of Materials Science and Chemical Engineering, University of Minnesota, Minneapolis, Minnesota 55455
(Received 22 January 1991)

Scanning-tunneling-microscopy studies of $[\bar{1}12]$ and $[1\bar{1}0]$ step structures on cleaved GaAs(110) show that $[\bar{1}12]$ steps are straight whereas $[1\bar{1}0]$ steps are made up of kinks along $[\bar{1}12]$. These step and kink structures are very different from those on Si surfaces. Through quantitative analysis of terrace-width and kink-length distributions, we show that $[1\bar{1}0]$ steps are weakly interacting while kinks are noninteracting.

Steps on surfaces play a key role in determining surface morphologies and stabilities, as demonstrated by studies of Si surfaces.[1,2] For example, the 7×7 reconstruction of Si(111) starts from step edges where the step is believed to act as the source of adatoms needed for the reconstruction.[3] For vicinal Si(111) surfaces, step energies and step-step interactions ultimately determine whether a surface is orientationally stable or will become faceted.[4] For stepped Si(100) surfaces, the surface can have single- or double-height steps, depending on the interplay between step energies and strain energies.[5] Many attempts have been made to model steps using statistical mechanics.[2,6,7] Unfortunately, there has been little experimental confirmation of these models. In particular, it is still an open question as to whether the simple terrace-step-kink model first proposed in 1927 by Kossel[8] is a reasonable description of a real surface. With the invention of scanning tunneling microscopy (STM), there have been experimental attempts to address the question. Wang and coworkers[9] have measured the terrace-width distribution on vicinal Si(111) misoriented toward $[\bar{1}\bar{1}2]$ and have concluded that step-step interactions are short range and repulsive. Swartzentruber *et al.*[10] have studied kink distributions on vicinal Si(100) and have shown that kinks are almost independent.

While there have been a number of excellent studies of steps on Si surfaces, steps on III-V semiconductor surfaces have long been neglected, despite the important role they play for molecular beam epitaxy growth of tilted superlattices.[11] Indeed, little is known about GaAs step structures,[12] the mechanism that creates steps on the cleaved surface, step-step interactions, step energies, step chemistry, and the role of steps in determining Fermi level pinning. In this paper, we present a study of step structures on cleaved GaAs(110). We show two types of steps running along $[\bar{1}12]$ and $[1\bar{1}0]$ where the $[\bar{1}12]$ steps can be either single or double height. The single height steps are stable, and their edges are straight. The $[1\bar{1}0]$ steps are single height, but they always appear rough with kinks along $[\bar{1}12]$. By measuring the terrace width and kink length distributions of $[1\bar{1}0]$ steps, we show there is a weak interaction between steps and that kinks are independent. By parametrizing the kink length distribution, we address the nature of this surprising surface morphology produced by cleaving. We find that the kink distribution of $[1\bar{1}0]$ steps for GaAs(110) is different from that of Si(100) single steps, suggesting that the form of the effective Hamiltonian governing the creation of these kinks is different.

The experiments were carried out in an ultrahigh vacuum chamber at pressures below 1×10^{-10} Torr using a scanning tunneling microscope built by Park Scientific Instruments.[13] GaAs(110) surfaces were obtained by cleaving $3\times4\times10$ mm^3 p-type posts (Zn doped, 3×10^{19} cm^{-3}). All of the surface appeared mirrorlike to the eye, but both types of steps were repeatedly obtained, although with variations in average terrace widths. Moreover, the step structures do not depend on the cleaving direction. Most of the STM images were taken with -1.9-V sample bias and 0.1-nA tunneling current to highlight As atoms.[14]

Figure 1 shows a mosaic for GaAs(110) that demonstrates the stability of $[\bar{1}12]$-type steps. Two single-height steps run from the lower left and split into a double-height step and a single-height peninsula structure. The direction of the step is determined to be $[\bar{1}12]$ from atomically resolved images.[15] For the double-height step, the macroscopic direction does not exactly follow $[\bar{1}12]$ but is made up of segments of double-height steps along $[\bar{1}12]$ that parallel the peninsula. This suggests that double-height steps along $[\bar{1}12]$ are also stable. Structures consisting of many consecutive single-height steps along $[\bar{1}12]$ have also been observed.[15] The peninsula structure of Fig. 1 is approximately 82 atoms long, one atom high, and two to five atoms wide. Its existence indicates that the energy cost of a $[\bar{1}12]$ step is very low, as discussed below.

Figure 2 shows a mosaic for cleaved GaAs(110) that reveals 4–5 single-height steps with the macroscopic step direction parallel to $[1\bar{1}0]$ stepping upward from lower left to upper right. What makes these steps special is that their edges have large fluctuations around the mean position with kinks made up of $[\bar{1}12]$-type steps. These kinks are often elongated parallel peninsulalike structures extending over a lower terrace and long cuts into the terrace, microscopically resembling the structure of Fig. 1. Although two step edges can be close together, no step crossing has been observed.[5] Only one step collision at

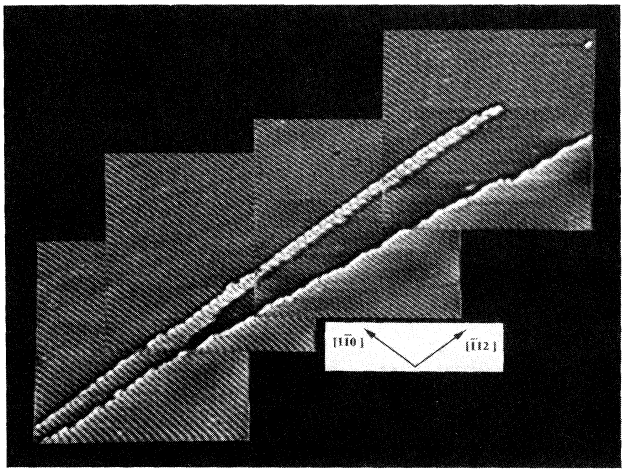

FIG. 1. Mosaic STM image showing two single-height [$\bar{1}$12] steps (lower left) that yield a double-height step and a peninsula one layer high parallel to [$\bar{1}$12]. Each image corresponds to 225 Å×225 Å. The width of the peninsula varies from two to five atoms.

one atom site was found in hundreds of images. To our knowledge, these images present the most irregular step edges ever observed. STM *I-V* measurements show that the Fermi level is pinned in midgap. This may explain the often-observed phenomenon in photoemission experiments where the Fermi level is pinned even for "mirror-like" cleaved surfaces.

For a given stepped surface, the terrace width distribution is largely determined by energetic step-step interactions.[6,15] Strong repulsive interactions result in a sharp distribution that peaks at the mean terrace width while an attractive interaction gives a much broader distribution. In fact, quantitative theoretical investigations of the correlation between terrace width distribution and step-step interaction have been achieved by treating each step mathematically as a fermion for steps that do not cross.[6] Comparison with this theory makes it possible to deduce the nature and the strength of step-step interactions. To do so, we measured the local terrace widths (in units of the distance between As atoms along [$\bar{1}$12], namely 6.92 Å) for surfaces that resulted from cleaving parallel and perpendicular to [1$\bar{1}$0]. Measurements of 828 and 941 terrace widths for these surfaces, with average terrace widths L of 10.7 and 9.7, were used to generate the distributions plotted in Fig. 3(a). The observed creation probability is much broader than for vicinal Si(111) where there was strong short-range repulsion between steps.[9] However, it is sharper than what is expected for noninteracting steps using the kink distribution deduced from the experiment. A weak interaction, $3.7/x^2$ (eV/kT), is obtained from fitting the measured distribution to the theoretical model.[16]

It is important to note that our step structures were ob-

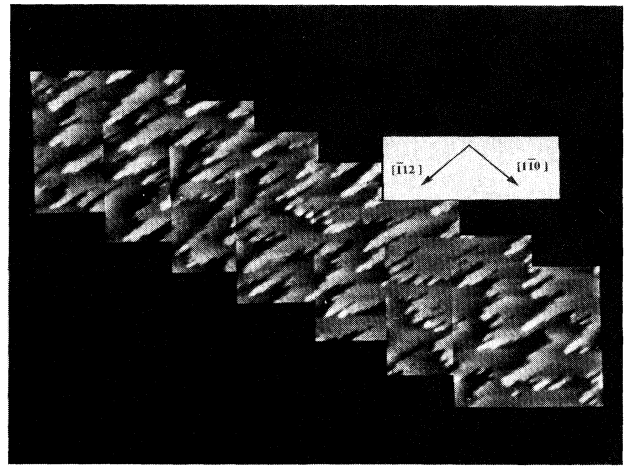

FIG. 2. Mosaic image showing [1$\bar{1}$0] steps on cleaved GaAs(110) with a large number of kinks along [$\bar{1}$12]. Each image is 160 Å×160 Å and L = 10.7.

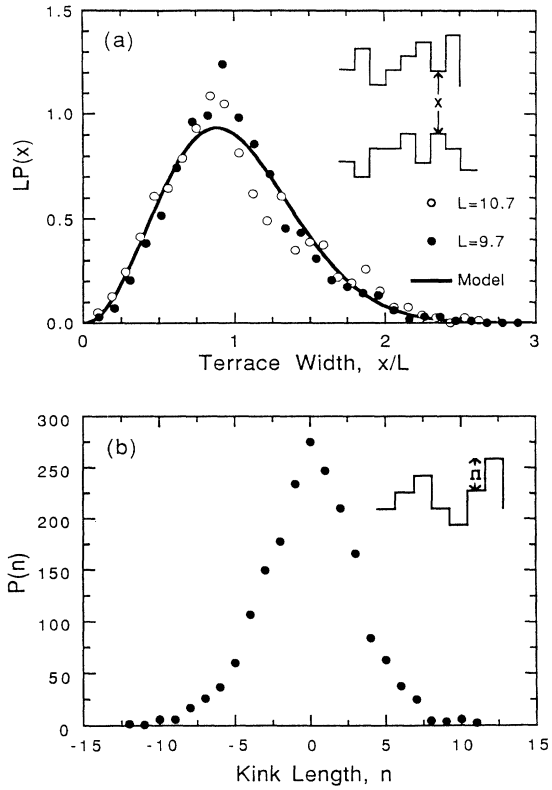

FIG. 3. (a) Terrace width distribution for [$\bar{1}$10] steps on surfaces having average terrace widths L = 10.7 and 9.7 obtained by cleaving perpendicular and parallel to [$\bar{1}$10], respectively. The terrance width x is measured in units of 6.92 Å, corresponding to two As atoms distances along [$\bar{1}$12]. Widths are normalized to the average terrace width L. $P(x/L)$ is the probability of finding a terrace of width x/L. The solid curve is the distribution predicted by a model for weakly interacting steps (Ref. 6). (b) Measured kink length distribution for kinks along [$\bar{1}$12] on [1$\bar{1}$0]-type steps. Kinks are measured in the same units as terrace widths. The symmetric distribution demonstrates that the kinks are independent.

tained by cleaving, in contrast to step structures on vicinal Si surfaces that resulted from misorientation and annealing. In particular, the step structures on vicinal Si can approximate equilibrium step configurations because Si is mobile at high annealing temperature.[9,10] It is not obvious that the GaAs surface can respond fast enough at the moment of cleaving to minimize its surface free energy, thereby putting itself in an equilibrium configuration. However, even if the observed GaAs(110) steps represent nonequilibrium structures, the above analysis should still be valid. In fact, the same terrace width distribution could be obtained by calculating the probability for m random walkers.[15,17]

For kinks on each noninteracting $[1\bar{1}0]$ step, like the terrace width itself, their distribution reflects the interaction between kinks. We measured the probability of finding two adjacent kinks as a function of their separation the same way as was done for the stepped Si(001) by Swartzentruber *et al.*[10] and we obtained similar results.[15] This suggests that the kinks were independent, but the test is not stringent enough to ensure their independence. For example, consecutive kinks may tend to run in the same direction due to kink-kink interactions. Visual inspection of published STM images[10,18] suggests that kinks on single-height steps of Si(100) may be an example of such interacting kinks. Therefore we measured the kink distribution as a function of both the length and the direction where consecutive kinks going in the same direction are counted as positive kinks while those that reverse direction are defined as negative kinks. The plot shown in Fig. 3(b) demonstrates that the kink distribution is symmetric and, hence, the creation of kinks on $[1\bar{1}0]$ steps is independent.

In an equilibrium picture, the kink-length distribution is determined by the minimization of step free energy. The probability of creating a kink of length n along the step edge is proportional to $\exp(-E_n/kT)$,[7] where E_n is the energy cost of a kink of length n. In Fig. 4, we plot $-\ln[N(n)/2N(0)]$ as a function of kink length. The factor of 2 results from the assumption that kinks with the same length cost the same amount energy regardless of the direction. The data are fitted to a form $E_n = n\varepsilon + C$, where ε is the energy of the smallest kink.[19] The best fit gives $\varepsilon/kT = 0.478 \pm 0.023$ and $C/kT = -0.65 \pm 0.10$. C has been interpreted as the corner energy.[10]

Large amounts of energies must be supplied to the crystal to cleave and produce a stepped surface. As a result, it is conceivable that the surface free energy is minimized to produce an equilibrium configuration of kinks. Because of the large energy, the equilibrium configuration should be equivalent to a frozen high-temperature configuration of a surface obtained by annealing. This speculation is supported by the resemblance of the observed step surface morphology and the high-temperature step configuration generated by Monte Carlo simulations.[6,15] In the equilibrium picture, the kink energy ε is also the step energy for $[\bar{1}12]$ steps. To estimate the magnitude of the step energy, we assume room temperature and obtain $\varepsilon = 0.012 \pm 0.006$ eV. This is comparable to the energy for stable steps on vicinal Si(001).[10] Even if the kinks correspond to a nonequilibrium configuration, the length distribution is expected to be the same as long as the probabilities for smallest kinks in a long kink are the same.[20]

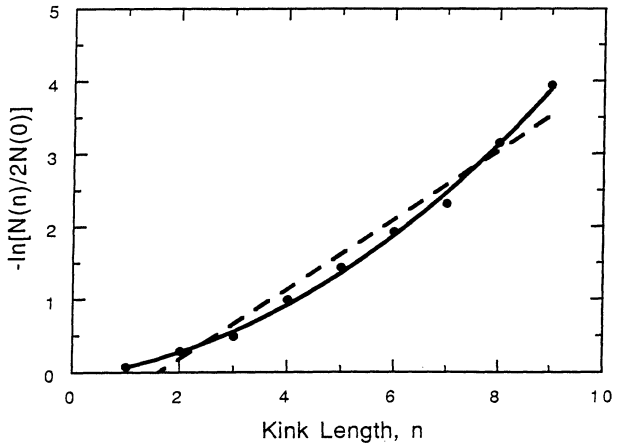

FIG. 4. Experimental lot of $\ln[N(n)/2N(0)]$ as a function of kink length n. Here the sign of the kink is not distinguished. The dashed line is the fit to the form $n\varepsilon + c$ and solid line is the fit to the form $(an)^2$.

Although the linear fit adequately describes the data, it is interesting that much better agreement is obtained when the data are fitted to a quadratic form $(an)^2$ as shown by the solid line in Fig. 4.[21] The best fit gives $a = 0.21 \pm 0.026$, where $1/\sqrt{2}a$ is the half width of the normal distribution. The implication for the equilibrium picture is that the kink energy E_n is not linearly proportional to the kink length n but is proportional to n^2. In the nonequilibrium picture, the fit indicates that a different random process is responsible for kink formation where the smallest kinks that make up a long kink are no longer identical. A possible cause of the kink formation is random propagation of cleaving. In this case, $[\bar{1}12]$ represents the direction that is preferred for cleave propagation, i.e., the direction that costs the least bond-breaking energy. Although the mechanism capable of explaining the observed kink distribution is not known in either picture, the fact that the same surface morphologies are obtained independent of the cleaving direction suggests that it is the energy, not the stress field, that is responsible for the creation of kinks.

In conclusion, through quantitative analysis of the terrace-width and kink-length distributions, we have laid the groundwork for understanding step structures on cleaved III-V semiconductor surfaces. We have shown that the terrace width distribution is different from those for vicinal Si(111) (Ref. 9) and the steps are weakly interacting. Kink creation events are shown to be independent. The kink distribution for cleaved GaAs(110), unlike kinks on Si(100),[10] is best described by a normal distribution, indicating that a different form of Hamiltonian is responsible for the creation of kinks.

We thank N. C. Bartelt for many discussions and for providing the theoretical curve for Fig. 3(a). This work was supported by the National Science Foundation under Grant No. DMR-86-10837.

[1]N. C. Bartelt, E. D. Williams, R. J. Phaneuf, Y.-N. Yang, and S. Das Sarma, J. Vac. Sci. Technol. A **7**, 1898 (1989); E. D. Williams and N. C. Bartelt, Ultramicrosc. **31**, 36 (1989).

[2]C. Herring, Phys. Rev. B **82**, 87 (1951); C. Jayaprakash, C. Rottman, and W. F. Saam, *ibid.* **30**, 6549 (1984).

[3]W. Telieps, Appl. Phys. A **44**, 55 (1987); R. M. Feenstra and M. A. Lutz, Surf. Sci. **243**, 151 (1991).

[4]R. J. Phaneuf and E. D. Williams, Phys. Rev. Lett. **58**, 2563 (1987).

[5]O. L. Alerhand, A. N. Berker, J. D. Joannopoulos, D. Vanderbilt, R. J. Hamers, and J. E. Demuth, Phys. Rev. Lett. **64**, 2406 (1990).

[6]N. C. Bartelt, T. L. Einstein, and E. D. Williams, Surf. Sci. **240**, L591 (1990).

[7]W. W. Mullins, Phys. Rev. **114**, 389 (1959); E. E. Gruber and W. W. Mullins, J. Phys. Chem. Solids **28**, 875 (1967).

[8]W. Kossel, Nachrbl. Ges. Wiss. Göttingen, 135 (1927).

[9]X.-S. Wang, J. L. Goldberg, N. C. Bartelt, T. L. Einstein, and E. D. Williams, Phys. Rev. Lett. **65**, 2430 (1990).

[10]B. S. Swartzentruber, Y.-W. Mo, R. Kariotis, M. G. Lagally, and M. B. Webb, Phys. Rev. Lett. **65**, 1913 (1990).

[11]J. M. Gaines, P. M. Petroff, H. Kroemer, R. J. Simes, R. S. Geels, and J. H. English, J. Vac. Sci. Technol. B **6**, 1378 (1988); M. Tsuchiya, P. M. Petroff, and L. A. Coldren, Appl. Phys. Lett. **54**, 1690 (1989).

[12]R. Moller, R. Coenen, B. Koslawski, and M. Rauscher, Surf. Sci. **217**, 289 (1989).

[13]Park Scientific Instruments, Mountain View, CA.

[14]R. M. Feenstra, J. A. Stroscio, J. Tersoff, and A. P. Fein, Phys. Rev. Lett. **58**, 1192 (1987).

[15]Y.-N. Yang, B. M. Trafas, R. L. Siefert, N. C. Bartelt, and J. H. Weaver (unpublished).

[16]Such distribution is indistinguishable from that of noninteracting steps with shorter kinks. The weak interaction introduced compensates for the small kink energy. See Ref. 6.

[17]M. E. Fisher, J. Stat. Phys. **34**, 667 (1984).

[18]R. J. Hamers, U. K. Kohler, and J. E. Demuth, J. Vac. Sci. Technol. A **8**, 195 (1990); Y.-W. Mo, R. Kariotis, B. S. Swartzentruber, M. B. Webb, and M. G. Lagally, *ibid.* **8**, 201 (1990).

[19]The size of the smallest kink is 6.92 Å. The energy unit is eV per this length.

[20]Emile Borel, *Elements of the Theory of Probability* (Prentice-Hall, Englewood Cliffs, NJ, 1965), p. 23.

[21]χ^2 for the normal fit is 0.54 and 21.6 for the exponential fit.

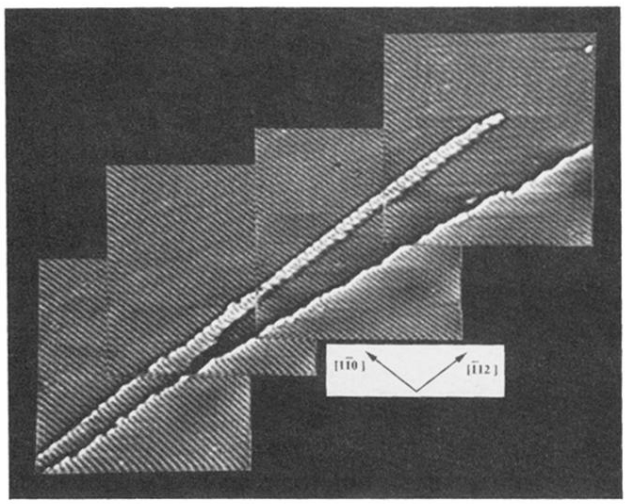

FIG. 1. Mosaic STM image showing two single-height [$\bar{1}$12] steps (lower left) that yield a double-height step and a peninsula one layer high parallel to [$\bar{1}$12]. Each image corresponds to 225 Å$\times$225 Å. The width of the peninsula varies from two to five atoms.

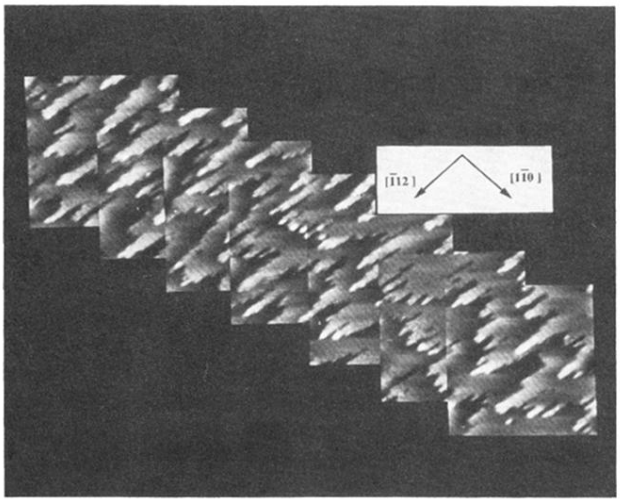

FIG. 2. Mosaic image showing [1$\bar{1}$0] steps on cleaved GaAs(110) with a large number of kinks along [$\bar{1}$12]. Each image is 160 Å$\times$160 Å and $L = 10.7$.