

## Thermal stability and structure of the equilibrium clean Si(103) surface

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The Si(103) surface is studied by means of low-energy electron diffraction and scanning tunneling microscopy. It has been found that the clean Si(103) surface is *stable* against faceting, that at the room temperature the thermally equilibrium clean Si(103) surface is, surprisingly, *rough* but *semiconducting* and its topmost thin layer is *disordered*, and that the rough morphology is not a result of the thermodynamic roughening transition but because it has a lower internal energy than that of the flat surface. That Si(103) neither facets to Si(113) facets nor consists of Si(113) nanofacets indicates that it does not belong to the Si(113) family; in contrast, Ge(103) does belong to the Ge(113) family. This difference supports the conclusion that the atomic structure of the Ge(113) surface is different from that of the Si(113) surface. [S0163-1829(99)03020-9]

### INTRODUCTION

Although the first study on the Si(113) surface was reported a long time ago,<sup>1</sup> it has become clear only recently that the annealing of low-index silicon surfaces frequently results in {113} facets,<sup>2</sup> probably through a step-bunching process.<sup>3</sup> The high stability of the surface is a reflection of its low surface free energy.<sup>4</sup> It has also been disclosed that the surface is a stage of the interesting phenomenon of chiral melting,<sup>5</sup> and that it also has some technological importance.<sup>6,7</sup> Thanks to the very recent efforts of many groups,<sup>8-14</sup> it seems to be clear now that the model proposed by Dabrowski and co-workers correctly reflects the structure of the surface.<sup>13,14</sup> Afterwards, investigation of the surface naturally extends to its vicinal surfaces<sup>15-20</sup> and family members, which consist of mesofacets of it, or even their neighbors.<sup>21-24</sup> As a result, the currently determined family territory of the Si(113) surface extends to (114) (Refs. 17 and 24) and (5 5 12) (Ref. 24) towards (001) and (111), respectively, and towards the interior of the unit stereographic triangle.<sup>19</sup>

On the other hand, germanium surfaces have been receiving much less attention than their silicon counterparts,<sup>25</sup> although an early investigation on high index germanium surfaces was reported quite a long time ago.<sup>26</sup> We believe, however, that comparative systematic studies of silicon and germanium surfaces as well as interfaces can be very fruitful, and this has been demonstrated by a series of recent investigations on interfaces of group-III-metal/group-IV-semiconductor systems.<sup>27</sup> In line with this, we have been systematically studying high index germanium surfaces.<sup>28-35</sup> As a result, models have been proposed for the  $3 \times 1$  and  $3 \times 2$  reconstructions of the Ge(113) surface,<sup>28</sup> its subsurface self-interstitial atoms have been disclosed to be migrating frequently below the surface layer even at the room

temperature,<sup>29</sup> and its family territory has been roughly determined.<sup>30,32,34</sup>

Comparing Si(113) with Ge(113), we see not only that their atomic structures are different<sup>13,28</sup> but also that their family territories, as determined so far, are quite different.<sup>24,34</sup> It seems to be that the Si(113) family territory is in all directions smaller than that of the Ge(113) surface. In view of the fact that the Ge(113) territory, crossing the unit stereographic triangle, extends up to (103) and (102) (Ref. 32) and that the Si(103) surface is also very stable,<sup>36</sup> in this paper we investigate the structure of the Si(103) surface to see if this surface also belongs to the (113) family.

### EXPERIMENT

The experiments were carried out in two UHV systems. The first system is equipped with low-energy electron diffraction (LEED), Auger electron spectroscopy (AES), and electron-energy-loss spectroscopy, and has been used and described in recent papers,<sup>27,36,37</sup> while the second system is equipped with field-ion scanning tunneling microscopy (FISTM), LEED, and AES, and has also been used and reported in recent papers.<sup>38,39</sup> The STM tip was made out of a {111} W single-crystal wire with electrochemical etching and then cleaned with field emission *in situ* prior to being used. The bias voltage was applied to the sample and the tip was grounded. The constant current mode was used throughout the work and the scanning rate was set around 2500 Å/sec. The sample was same as the one used previously,<sup>36</sup> i.e., cut with a precision of  $\pm 0.5^\circ$  from a silicon single-crystal rod (*p*-doped, 6–8 Ω cm). To assure that the Si(103) surface was clean and in equilibrium, several measures were taken. Specifically, to avoid contamination from metals, (i) the sample was mounted on the Mo sample holder with W wires (in the first system) or Ta ribbons, and a Si(111) buffer plate was

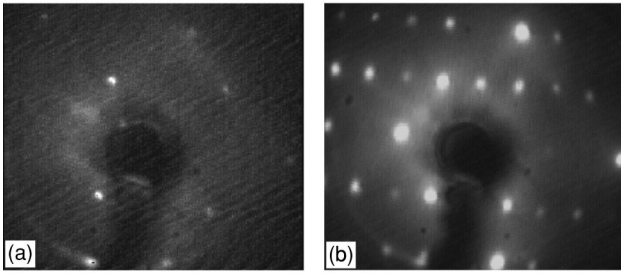


FIG. 1. (a) A typical LEED pattern (84 eV) of the equilibrium clean Si(103) surface. (b) A typical LEED pattern (84 eV) of the Si(103)  $1 \times 1$ -In surface.

put between the sample and the ribbons (in the second system); (ii) no metal tools were allowed to touch the sample; (iii) the UHV systems and the incident geometry of the Ar-ion beam were carefully arranged so as to reduce the possibility of Ni contamination from the sputtering; and additionally, (iv) the sample was thoroughly degassed at 600 °C for more than ten hours at the beginning. To exclude possible kinetic influences to the surface structure, we tried many different ways of surface preparation, including (i) flashing the sample to 1000–1200 °C for about 15 sec and then cooling it down with very different rates; and (ii) sputtering the surface with an Ar-ion beam, annealing it at very different temperatures, and then cooling it down slowly. We also tried to change the morphology of the clean surface by depositing some indium onto the surface and then desorbing the indium to get back the clean surface. In this case the indium evaporation source was made the same as the one used previously.<sup>36</sup>

## OBSERVATION

### The LEED observation

It turns out that the LEED patterns observed from the clean Si(103) surfaces were always poor no matter which manner of surface preparation, mentioned above, and which of the two UHV systems were used. This means that these Si(103) surfaces were very similar and indeed thermally in equilibrium, and kinetic influences on their surface structure were negligible. Thus we simply call them a well-annealed clean Si(103) surface. Since the patterns obtained in the present work are essentially the same as those reported previously<sup>36</sup> we just reproduce the reported images in Fig. 1, rather than showing new ones. The interesting features of the patterns are the following. (i) Never have any diffraction beams of any facets other than (103) been observed at any beam energy. (ii) At any energy only a few weak, though very sharp, diffraction beams of the (103)  $1 \times 1$  pattern can be seen simultaneously. (iii) The background is low.

Since the surface gives rise only to (103) patterns, the first conclusion that one can easily reach is that the Si(103) surface is *stable*. Here, the definition of a stable surface is thermodynamically stable with respect to formation of some sort of hill-and-valley structure<sup>40</sup> or thermodynamically stable against faceting.<sup>41,23</sup> However, from the rest of the characters of the patterns, i.e., only *few sharp weak* beams simultaneously visible on a *low* background, it seems to be not that straightforward to extract further information about the sur-

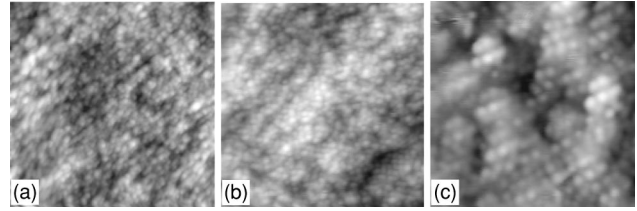


FIG. 2. STM images acquired from the equilibrium clean Si(103) surface. (a)  $1250 \text{ \AA} \times 1250 \text{ \AA}$ , 2.8 V, 0.1 nA. (b)  $310 \text{ \AA} \times 310 \text{ \AA}$ , -2.6 V, 0.25 nA. (c)  $150 \text{ \AA} \times 150 \text{ \AA}$ , -2.6 V, 50 pA.

face structure. Therefore, we turn to analyzing first the individual characters to find out the implications of each. Obviously, only surfaces consisting of large domains can give rise to *sharp* LEED diffraction beams. Second, the fact that at any energy always only a *few* integral-order beams are visible indicates that the I-V curve (i.e., the beam intensity versus the beam energy curve) of each beam consists of only a few sharp peaks. This is an indication that the surface is bulklike, because an ideal two-dimensional (2D) surface can give rise only to flat LEED I-V curves, so that all beams of the entire pattern must always be visible. Third, the diffraction beams of a bulklike surface at energies when visible should not be weak, unless the surface is covered by another thin layer. This thin layer itself, of course, must either be completely disordered or consist of very small domains, so that it gives rise to no extra beams. Finally, from the *low* background of the Si(103) surface we know that the thin layer on top of the bulklike substrate must be completely disordered, instead of consisting of very small domains. Because in the case of the latter, superposition of the intensities of the very diffused beams would still result in a high background, while a simple kinematic calculation can easily show that a completely disordered thin layer makes no contribution to the background at all. Consequently, on the basis of the LEED observation, we conclude that a clean and well-annealed Si(103) surface is *stable* but consisting of a *bulklike substrate* covered by a completely *disordered thin top layer*. This conclusion, of course, has to be tested with STM.

### The STM observation

Several typical STM images acquired from the clean and well-annealed Si(103) surface are given in Fig. 2. From these images one can see that the surface obviously is *rough* down to the nanometer scale. This is a new character of the surface that is not seen with LEED. Besides, the topmost layer of the surface is indeed disordered, in accordance with the LEED observation. Moreover, we have also noticed that the surface can be imaged with neither polarity if the bias voltage is smaller than 1.3 V. This indicates that the clean and well-annealed Si(103) surface is *semiconducting*, because a metallic surface on a semiconductor substrate, such as the Ge(001)  $3 \times 6$ -Pb surface,<sup>42</sup> should allow it to be imaged with very low bias voltages of both polarities.

Now, we have to answer the question of how this rough surface can give rise to sharp LEED beams. As mentioned above, since the Si(103) surface consists of a bulklike substrate covered by a disordered thin top layer, only the bulklike substrate makes a contribution to the LEED beams. However, the surface of this bulklike substrate must also be

rough if the disordered top layer has, as expected, a similar thickness everywhere. For a bulklike surface rough means highly randomly stepped, while it has been well established that the reciprocal rods of such a surface must have oscillating cross sections;<sup>43</sup> that is, the diffraction beams from such a surface have nonzero intensities, thus being visible *only* when the scattered electron waves from all its ministepped at different levels are in phase. In this case the entire *rough* surface behaves as if it were a flat truncated surface (i.e., a single domain) and hence gives rise to very *sharp* beams.

Despite these arguments, we still had difficulties in believing that a stable surface could be so rough and its top-most layer could be completely disordered. Contrarily, we would think that the poor LEED patterns and the “bad” STM images were caused by some artifacts. So, before starting to try to understand the strange features of the surface, we tried to further rule out any possibilities that these features were only artifacts of contamination and/or mishandling in surface preparations. Therefore, we have carried out several auxiliary observations.

#### Auxiliary LEED and STM observations

In view of the fact that a small amount of metal, such as Ni, may cause big changes on silicon surfaces,<sup>44</sup> apart from the mentioned careful arrangement inside the UHV system, we always check first the LEED patterns of the Si(111) buffer plates put on *both* ends of the Si(103) sample each time the sample is cleaned. However, what we saw from both buffer plates were always excellent Si(111)  $7\times 7$  patterns, i.e., very sharp and bright beams on a low background, in sharp contrast with the poor patterns of the Si(103) sample. This rules out the possibility of any metal contamination. Moreover, this fact further rules out any kinetic influences on the Si(103) surface structure studied here, because if at temperatures (of about 860 °C the Si(111)  $7\times 7$  reconstruction, which is a large and complicated reconstruction, can develop well, then the Si(103) surface must also be able to reach its equilibrium structure.

To rule out the possibility that the rough morphology was the result of a poor polishing of the original sample surface, we deposited some indium onto the clean Si(103) surface and then annealed it, thus making the surface Si(103)  $1\times 1$ -In, which consists of large terraces, as verified by LEED.<sup>36</sup> The STM images (see Fig. 3) acquired from this surface have confirmed this: terraces can be several hundreds of angstroms in width, as Fig. 3(c) shows. Then we heated the sample to about 560 °C so as to desorb the indium. It turns out that right after desorption of the indium the surface changed back to its original rough morphology [see Fig. 3(b)]. This shows clearly that the original polishing of the clean and well-annealed Si(103) surface. Besides, the atomic resolution images [see Fig. 3(d)] also show that neither the STM nor the tip had any problem, and thereby the obtained STM images are reliable, in other words, reflecting the real morphology and structure of the surface. On the basis of all these LEED and STM observations, we must conclude that the clean Si(103) surface is *stable* against faceting, the thermally equilibrium clean Si(103) surface is *rough* but *semi-conducting*, and its topmost thin layer is *disordered*.

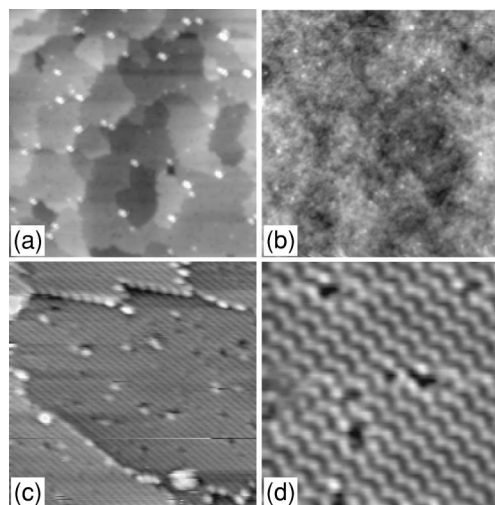


FIG. 3. STM images acquired from the Si(103)  $1\times 1$ -In surface [(a), (c), and (d)] and the surface right after desorption of indium (the desorption temperature was 560 °C) [(b)]. (a)  $1250\text{ \AA}\times 1250\text{ \AA}$ , 2.5 V, 10 pA. (b)  $1250\text{ \AA}\times 1250\text{ \AA}$ , 2.5 V, 5 pA. (c)  $310\text{ \AA}\times 310\text{ \AA}$ ,  $-1.8\text{ V}$ , 1.5 nA. (d)  $77\text{ \AA}\times 77\text{ \AA}$ ,  $-1.5\text{ V}$ , 1.5 nA.

## DISCUSSION

### Not a result of the roughening transition

To our knowledge, never have any stable silicon surfaces at thermal equilibrium been reported to be rough, so it is natural to ask why the Si(103) surface is rough. Since it has been known that metal surfaces, such as some high index surfaces of Ni, Cu, Pb, Bi, Au, In, etc.,<sup>45,46</sup> may become thermodynamically rough at temperatures above the roughening transition temperature  $T_R$ ,<sup>46,47</sup> we have to see first if this mechanism is also responsible for the rough morphology of the Si(103) surface. Actually, it is not difficult to rule out this possibility. First, the Si(103) surface is rough even at the room temperature. If it were thermodynamically rough, then its  $T_R$  ought to be below room temperature. It is hard to believe this because for silicon surfaces the  $T_R$ , though being index-dependent, must be above the melting temperature.<sup>46</sup> In fact, this is why in dealing with the thermodynamics of silicon surface morphology it is always assumed that the surfaces of interest are well below its  $T_R$ .<sup>41</sup> Second and also more importantly, the roughening transition of a crystal surface is characterized macroscopically by the disappearance of a facet of a given orientation from the equilibrium crystal shape. This corresponds to the disappearance of a cusp in the  $\gamma$  plot, a polar plot of surface free energy vs surface orientation.<sup>47</sup> This means that at temperatures above the  $T_R$  of a crystalline surface the surface can no longer exist. Now, our LEED shows that the sample surface was (103) while STM shows it was rough. Consequently, we conclude that the rough morphology of the Si(103) surface is not a result of the roughening transition. Then, we must also conclude that no flat Si(103) surface structures could have a lower surface free energy than that of the rough Si(103) surface, or that the internal energy of the rough surface structure must be lower than that of flat structures because the surface is rough at room temperature while at such temperatures the entropy term of the surface free energy must be negligible.

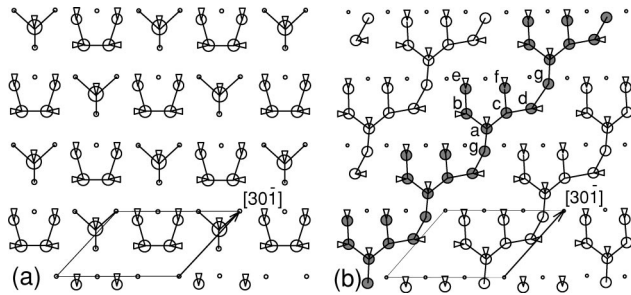


FIG. 4. (a) Model of the atomic structure of the Si(113)  $3 \times 1$  surface,<sup>13</sup> with the triangles representing the dangling bonds. A  $3 \times 1$  unit cell is outlined. (b) Same as (a) but for the Ge(113) surface (Ref. 28). Note that this structure is qualitatively different from that of the Si(113) surface, and that the topmost atoms of the surface form rows parallel to the  $[30 - 1]$  direction, and atoms belonging to the row running from lower-left to upper-right are shaded for clarity.

Obviously, to answer why a rough silicon surface can have such a low internal energy, atomistic calculations are necessary.

#### Why not the Si(103) $1 \times 1$ -III structure

Qualitatively, however, it is useful to find out why the Si(103) surface likes neither the flat structure of the Si(103)  $1 \times 1$ -III surfaces<sup>27,36</sup> nor that of the Ge(103)  $1 \times 4$  surface.<sup>30</sup> It has been reported recently that group-III metals not only can form very well-ordered and stable flat  $1 \times 1$  structure on the Si(103) surface, but also can make the Si(001) and (113) surfaces facet to Si{103}  $1 \times 1$ -III facets.<sup>36</sup> Our experiment confirms this again, as shown by Fig. 3. This indicates that this surface is energetically very favorable. A unit cell of this structure consists of a III adatom and a silicon adatom;<sup>36,27</sup> then what could be wrong if only the III adatom is replaced by a silicon adatom, thus making the surface a clean Si(103)  $1 \times 1$ ? We believe such a Si(103) surface would contain too much tensile stress, which does not exist in the Si(103)  $1 \times 1$ -III surface because group-III atoms not only are larger than silicon atoms but also tend to form planar  $sp^2$ -like back bonds, thus occupying a larger space.<sup>48</sup> Moreover, different from the case of the Si(001) surface, where the coexistence of different stress domains may reduce the otherwise high strain energy,<sup>49</sup> the low symmetry of (103) does not provide this possibility and hence such a Si(103)  $1 \times 1$  surface is energetically unfavorable.

#### Why not the Ge(103) $1 \times 4$ structure either

It has been shown very recently that not only is the Ge(103) surface stable and has a well-ordered  $1 \times 4$  structure<sup>30</sup> but also that its neighboring surfaces, such as (102), may completely facet to include facets of it.<sup>32</sup> A natural question then is, why does Si(103) not like the Ge(103)  $1 \times 4$  surface structure either? To answer this question we recall that Ge(103) belongs to the Ge(113) family because the Ge(103)  $1 \times 4$  reconstruction consists of nanofacets of (113)  $3 \times 1$  and  $(1 - 13) 3 \times 1$ .<sup>30</sup> For the reader's convenience, the models of the relevant structures are reproduced in Figs. 4 and 5. From these models one can see that in the Ge{113}  $3 \times 1$  surfaces the surface atoms form rows in the

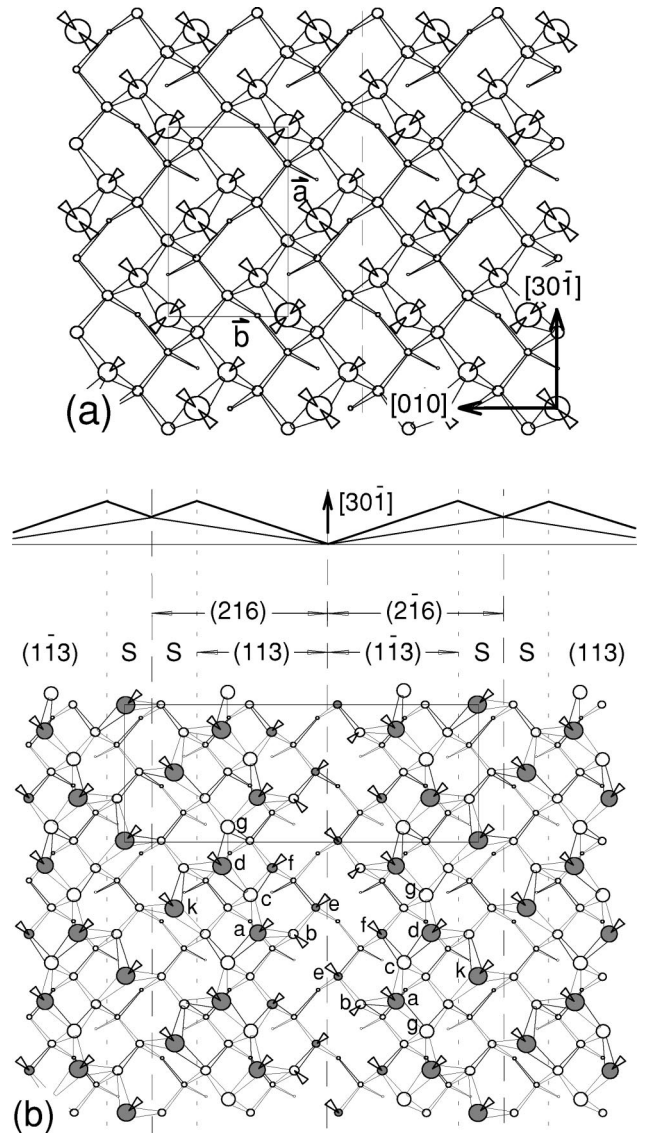


FIG. 5. (a) The truncated Ge(103) surface, with a  $1 \times 1$  unit cell outlined. (b) Model of the atomic structure of the Ge(103)  $1 \times 4$  surface (Ref. 30), with a  $1 \times 4$  unit cell outlined. Note that the structure consists of stripped nanofacets of (216) and  $(2 - 16)$ , which in turn consist of stripped nanofacets of (113) and  $(1 - 13)$ , respectively. Shown on top is the side view of the surface morphology. Note that in this figure and in Fig. 4(b) the atoms that carry a same lower-case character are equivalent, and  $s$  stands for step.

$[30 - 1]$  directions (see Fig. 4) and that the Ge(103)  $1 \times 4$  reconstruction consists of just such rows along with some steps (see Fig. 5). Now, looking at the atomic structure of the Si(113)  $3 \times 1$  surface,<sup>13</sup> which is different from that of the Ge(113)  $3 \times 1$  surface, one can find that its surface atoms do not form any rows, and thus any (103) surface consisting of nanofacets of Si{113}  $3 \times 1$  would be energetically too costly. We believe this is why Si(103) does not belong to the Si(113) family. Besides, the fact that the Si(103) surface does not consist of nanofacets of Si(113)  $3 \times 1$  while the Ge(103) surface does consist of nanofacets of Ge(113)  $3 \times 1$  seems to support the conclusion that the atomic structure of the Ge(113)  $3 \times 1$  surface is different from that of the Si(113)  $3 \times 1$  surface, although a very recent paper disagrees with this.<sup>50</sup>

### Why not faceting

If the Si(103) surface cannot find a flat structure that has a reasonably low surface free energy, then why does it not facet either? Yes, faceting is a possible way of reducing the free energy of an initially flat but energetically unfavorable surface; however, whether a surface facets depends not only on the free energy of the surface but also on that of its neighboring surfaces: in the case where either the surface itself has a reasonably low free energy or the nearest surface that has a deep-enough cusp in the  $\gamma$  plot is not close enough to it or the nearest cusp is not deep enough the surface will not facet.<sup>40</sup> As mentioned in the Introduction, the territory of the Si(113) family<sup>24</sup> is in all directions smaller than that of the Ge(113) family,<sup>34</sup> thus indicating a shallower deep cusp in the  $\gamma$  plot of silicon. This seems to be the major reason why the rough Si(103) surface is stable against faceting.

Now we can understand why so far only three types of equilibrium clean silicon and germanium surfaces have been observed at room temperature: flat surfaces, stepped surfaces, and faceted or nanofaceted surfaces, but never rough and disordered surfaces,<sup>26,51,24,34,41</sup> although reversible order-disorder transitions do occur on some silicon and germanium surfaces at certain high temperatures.<sup>26,51</sup> We think this is mainly because such surfaces rarely appear for silicon and probably could not appear at all for germanium, since for germanium it has been shown very recently that almost all surfaces must belong to one or more major stable surfaces, meaning that the cusps are deep enough to make all surfaces faceting or nanofaceting to facets of one or more major stable surfaces.<sup>34,35</sup> Silicon, at least Si(113),<sup>19,24</sup> seems to have smaller family territories than that of its germanium counterparts and thus may allow some rough stable surface to appear. That Si(103) is stable also indicates that the territory of the Si(113) family does not extend to (103), or Si(103) does not belong to the Si(113) family.

### Why rough but energetically favorable

Of course, if the free energy of the rough Si(103) surface were higher than those of its neighboring surfaces, then it still could not be stable. Now we see that, if it is stable, then it must have a reasonably low surface free energy, very likely only few percent higher than that of Si(111) and close to that of the other low-index silicon planes because the anisotropy of the  $\gamma$  plot of silicon is only about 4%.<sup>4</sup> Although rough semiconductor surfaces probably have never been studied theoretically, the nature of such surfaces should also be determined by the balance between the energy gain due to

the reduction of dangling bonds and the energy cost due to induced strain.<sup>25</sup> Generally, rough surfaces may have a higher density of dangling bonds, and this seems to be their drawback. However, we see three possible advantages in being rough. (i) It allows a variety of different building entities to exist and thus gives more chances to reduce the dangling bonds. (ii) The rough morphology and the disordered top layer of the Si(103) surface may provide more opportunities for charge transfer between surface atoms and thus for further reduction of the surface energy, so that the Si(103) surface is semiconducting. (iii) As has been demonstrated, the existence of many different building entities,<sup>52</sup> steps,<sup>53</sup> or domains<sup>49</sup> may also provide more opportunities for relief of the surface strain. Actually, it has been shown very recently that two major stable surfaces of germanium, Ge(101) $c(8 \times 10)$  (Ref. 31) and Ge(313)  $5 \times 1$ ,<sup>33</sup> are also very rough, and the only difference is that they are ordered. Of course, despite these qualitative arguments, to prove quantitatively that surfaces with a rough morphology and a disordered top layer may indeed be energetically favorable is still a challenge to further theoretical studies.

### SUMMARY

In summary, on the basis of our LEED and STM observations, it has been found that the clean Si(103) surface is *stable* against faceting, that at room temperature the thermally equilibrium clean Si(103) surface is *rough* but *semiconducting* and its topmost thin layer is *disordered*, and that the rough morphology is not a result of the thermodynamic roughening transition but because it has a lower internal energy than that of the flat surface. To our knowledge, these kinds of silicon and germanium surfaces have never been reported before; thus it is discussed why a rough and disordered surface may have a reasonably low surface free energy.

That the Si(103) surface neither facets to Si(113) facets nor consists of Si(113) nanofacets indicates that it does not belong to the Si(113) family. In contrast, the Ge(103) surface does belong to the Ge(113) family, as it consists of nanofacets of the latter. We believe that this difference is because the atomic structures of the Ge(113) and Si(113) surface are qualitatively different.

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