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The structure of vicinal (111) surfaces of perfect and dislocation-rich Ge crystals doped with Ga

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Abstract. We have investigated by means of both scanning tunnelling microscopy (STM) and low-energy electron diffraction (LEED) Ge(111) vicinal surfaces misoriented by 1° and 2° toward the $\langle 11\bar{2}\rangle$ and $\langle \bar{1}\bar{1}2\rangle$ high-symmetry directions. Surfaces of moderately Ga-doped (dopant concentration (DC) $\simeq 1 \times 10^{19}$ cm^{-3}) Ge reconstruct c(2×8). No straight step edges but meandering kinks between terraces are observed with the STM. For highly Ga-doped (DC $\simeq 2 \times 10^{20}$ cm^{-3}) Ge crystals rich in dislocations and Ga inclusions, the vicinal surfaces mentioned exhibit at room temperature the previously reported LEED pattern for a phase of the well oriented clean Ge(111) surface appearing at approximately 300 °C. STM images at room temperature clearly display the incommensurate honeycomb-domain reconstruction, I(2×2), proposed by Phaneuf *et al* in order to explain the LEED pattern. High dislocation density and misorientation appear to be essential in order to observe this reconstruction. This is, to the best of our knowledge, the first real-space observation of such a structure.

1. Introduction

The main strength of the scanning tunnelling microscope (STM) [1] is its ability to study surface structures in real space with atomic resolution. There are many examples of reconstructed surfaces for which more than one possible structural model appears to be consistent with the data obtained with techniques averaging over space, such as low-energy diffraction (LEED) or other Fourier methods. This is the case for the Ge(111) phase at temperatures between approximately 300 °C and 780 °C, whose LEED pattern was interpreted to correspond to an incommensurate structure with either a (2×1) or (2×2) local ordering [2]. Throughout this paper, we will refer to this phase as the moderate-temperature (MT) phase of Ge(111) in order to distinguish it from the non-modulated (1×1) reconstruction, which appears above 780 °C after a further transition [3–5].

In this article we report on STM and LEED observations of vicinal (111) surfaces for high-quality Ga-doped (dopant concentration (DC) $\simeq 1 \times 10^{19}$ cm^{-3}) Ge crystals and those doped at a high level (DC) $\simeq 2 \times 10^{20}$ cm^{-3}) with a high dislocation density. The latter were additionally characterized with wavelength dispersive x-ray (WDX) analysis and transmission electron microscopy (TEM). Surface misorientations were 1° and 2° (±0.25°) toward $\langle 11\bar{2}\rangle$ and $\langle \bar{1}\bar{1}2\rangle$ high-symmetry directions. In the present communication we focus mainly on the I(2×2) (I stands for incommensurate) reconstruction, proposed as the favoured candidate to explain the LEED pattern of the MT phase of Ge(111) [2], which we observe at room temperature for vicinal (111) surfaces of Ga-doped Ge crystals rich in dislocations. In a

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future report, we will discuss results for Ga-dosed Ge(111) surfaces, which show that only Ga deposition and a subsequent annealing can produce at RT the broad splitting of the half-order reflections reported for the MT phase of Ge(111). However, no sharp reflections are observed. Moreover, STM pictures do not show the I(2×2) network but a structure locally (2×2) ordered with quite a few characteristic defects [6].

As far as organization is concerned, we first offer an overview of the previous investigations on the MT phase of Ge(111). After describing the experimental setup in section 3, the LEED and STM results are presented in section 4, comparing the observations of the vicinal (111) surfaces of the two different types of Ga-doped Ge crystal studied. Section 5 is devoted to the discussion of the results, in particular, to the role that dislocations, Ga, and surface misorientation play in the I(2×2) structure.

2. The moderate-temperature phase of Ge(111)

Previous work related to the MT phase of Ge(111) will be briefly summarized before we present our results in the next section. This phase is poorly understood in comparison with that stable at RT, the c(2×8), extensively investigated by various techniques such as LEED, medium-energy ion scattering (MEIS), photoelectron diffraction (PED), reflection high-energy diffraction (RHEED), STM, surface x-ray diffraction (SXD), and ultraviolet photoemission spectroscopy (UPS) [2, 3, 7–18]. At approximately 300 °C, the c(2×8) undergoes a reversible transition to the MT phase, as reported in experiments performed with ellipsometry, LEED, MEIS, PED, RHEED, STM, and UPS [2, 3, 5, 10, 17–22]. In 1980, Ichikawa and Ino [3] first observed a twofold splitting of the half-order reflections in the RHEED pattern of Ge(111) at temperatures higher than 300 °C. The splitting was clearly observed between 350 °C and 450 °C, and was believed to correspond to a (2×2) modulation of the (1×1) surface [3]. At RT the same split half-order reflections appeared if small amounts of Sn 0.1 monolayer (ML) or In (0.05 ML) were deposited onto the surface before annealing [3]. Ichikawa *et al* suggested that the reconstructed surface was a mixture of the four different possible types of (2×2) domain on top of a Ge(111) surface [2, 3]. Each of these domains can be generated from a different one via a shift by a primitive bulk translation vector (see figure 15 in [2]).

Yang and Jona [9] reported on a similar observation upon deposition of 1 ML Al onto Ge(111) and subsequent annealing for 10 min at 800 °C. The half-order reflections of the LEED pattern appeared split as observed with RHEED on slightly Sn- and In-covered surfaces. Unlike the authors of [3], Yang *et al* suspected a (2×1) reconstructed surface, with antiphase-domain boundaries (ADBs) perpendicular to the short direction of the unit cell, to be responsible for the spot splitting. From the similarity between their LEED data and the RHEED results of Ichikawa *et al* [3], they claimed to have stabilized the same phase by using Al, instead of Sn or In.

Phaneuf and Webb [2] performed a LEED analysis of intrinsic Ge(111) surfaces for a wide temperature range. In good agreement with the previously mentioned works [3, 9], they found the reversible phase transition from the c(2×8) to the MT structure to occur at about 300 °C. Two possible models for the structure were proposed: three orientationally equivalent domains of a (2×1) structure containing periodic ADBs as suggested by Yang *et al* , and a non-periodic arrangement of (2×2) hexagonal domains similar to that suggested by Ichikawa *et al* [3]. Contrary to that model, however, domain walls, parallel to the $[0\bar{1}1]$, $[10\bar{1}]$, and $[\bar{1}10]$ directions, are c(4×2) reconstructed in the second model proposed by Phaneuf *et al* . Walls are knotted together at locally $(\sqrt{3}\times\sqrt{3})$ reconstructed edges, so that the surface is tiled with hexagons of different sizes. From these two models, called I(2×1) and I(2×2), the second was chosen to be the most likely to explain the diffraction data,

essentially because STM pictures of annealed Ge(111) surfaces had shown the coexistence of c(4×2) and (2×2) phases mixed with perfectly reconstructed c(2×8) areas [11, 12, 14]; thus the transition to I(2×2) should not be costly in energy.

3. Experimental details

Tunnelling pictures were obtained at RT using a commercially available STM [23] in a UHV chamber equipped with facilities for resistive sample annealing, cleaning by Ar bombardment, and surface characterization using an LEED and Auger electron spectroscopy apparatus. The tunnelling tips were prepared from 0.4 mm thick polycrystalline tungsten wire by hydroxide AC etching. Ge crystals with a Ga concentration of 1×10^{19} cm^{-3} to 4×10^{19} cm^{-3} were acquired from MHO [24], whereas we grew those with the highest Ga concentration by means of the Czochralski method. In order to obtain the highest possible Ga concentration, 5.08 wt.% Ga was added to the starting Ge material in accordance with the segregation coefficient of 0.087 [25]. Using a crucible with an inside diameter of 5 cm and a slow pulling rate of 0.5 cm h^{-1}, a hole concentration of 2×10^{20} cm^{-3} was obtained for a crystal diameter of 2.5 cm at a crystal length of about 2 cm. The hole concentration was determined by four-point probe resistivity measurements and atomic emission spectroscopy (inductive coupled plasma) [26] revealed a Ga concentration of 0.63 wt.%, which corresponds to a DC of approximately 2.9×10^{20} cm^{-3}.

Carefully oriented surfaces were Syton polished with a few drops of NaClO, degreased in organic solvents, and rinsed in H_2O. Before loading into the UHV chamber, samples were dipped in H_2O_2 in order to oxidize the surface and then rinsed again in H_2O. Samples were degassed for several hours by increasing surface temperature, measured with an optical infrared pyrometer, up to 650 °C, while keeping the pressure below 10^{-9} mbar. At this temperature samples were Ar-ion bombarded for 30 min at a pressure of 5×10^{-5} mbar and left at 650 °C for 15 min until the pressure was down in the low 10^{-10} mbar range again. Only a final postannealing, at 575 °C for 15 min, was incorporated into the already described sample-preparation procedure, successfully used for well oriented Ge(111) surfaces [14, 15]. Three cleaning cycles sufficed to obtain Auger spectra with no impurity signals and sharp c(2×8) and I(2×2) LEED patterns with a very low background. In the case of the I(2×2) reconstruction, the postannealing was essential in order to observe a low background and sharp spots.

4. LEED and STM results

In figure 1(*a*) we show the LEED pattern of surfaces misoriented by 1° toward the $[11\bar{2}]$ direction for high-quality Ga-doped (DC $\simeq 2 \times 10^{19}$ cm^{-3}) Ge. The pattern looks the same as for the 2° misoriented surfaces, as well as for those misoriented by 1° or 2° toward the $[\bar{1}\bar{1}2]$ direction. The nominal width of the terraces for single- and double-height steps on a Ge(111) vicinal surface with 1° miscut is 187.2 Å and 93.6 Å, respectively. In figure 2(*a*), we show an STM constant-current topograph (CCT) of a vicinal surface 1° misoriented toward the $[11\bar{2}]$ direction. The three steps do not align perpendicularly to the $[11\bar{2}]$ direction; they meander by about ±30° and lie locally almost parallel to either the $[\bar{1}2\bar{1}]$ or the $[2\bar{1}\bar{1}]$ directions. Note that the second-highest terrace has a very small width, which may be a precursor structure of double-height steps. The splitting of the integer-order reflections in the LEED pattern, which corresponds to the mixture of double- and single-height steps reported by Jung *et al* in their study of surfaces misoriented by 10° toward the $(11\bar{2})$ direction [27], was not observed. In fact, the majority of steps observed with the STM are of single height.

Three differently oriented domains of the c(2×8) can be clearly observed in a region of smaller size shown in figure 2(*b*). No domain orientation seems to be favoured and (2×2) and c(4×2) ADBs [14, 16] appear more often than for the case of well oriented Ga-doped or intrinsic Ge(111) surfaces [14]. In this CCT, the single-height steps and terraces follow the mentioned common trends: steps do not align along the $[1\bar{1}0]$ direction and the width of the terraces varies considerably along the steps. Concerning the shape of the step edges, we observe an opposite behaviour in the case of Ge(111) surfaces covered with monolayer amounts of Ga [28]. The different discommensurate structures which appear on the surface force step edges to be straight [28] and not meandering like in the Ge(111) vicinal surfaces as discussed.

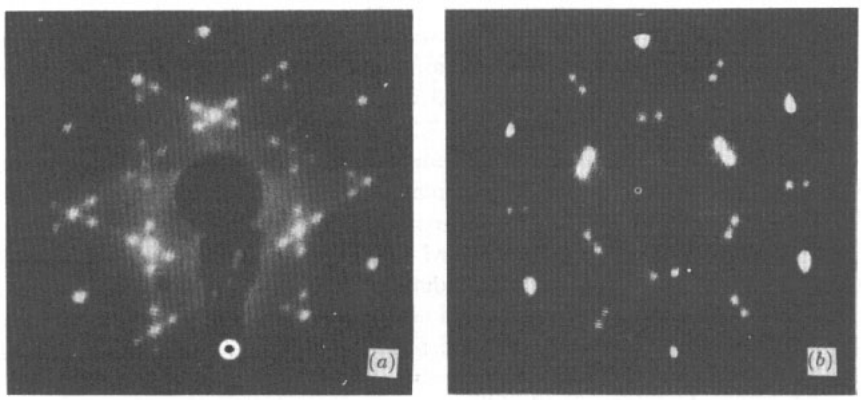

Figure 1. Reproduction of the LEED patterns of vicinal (111) surfaces misoriented 1° toward the $[11\bar{2}]$ direction. Electron beam energy = 33 eV. (*a*) For Ga-doped Ge crystals the surface still reconstructs c(2×8). (*b*) The pattern for Ga-doped Ge crystals rich in dislocations is the same as that reported in [2] and [9].

Well-oriented (111) surfaces of Ge crystals with a DC approximately equal to 2×10^{20} cm^{-3} and a high density of dislocations, for which Ga inclusions (see below) may be partly responsible, exhibit the usual c(2×8) LEED pattern shown in figure 1(*a*); however, those misoriented by 1° (see figure 3(*a*)) or 2° show the LEED pattern reproduced in figure 1(*b*), which exhibits the splitting of the half-order spots, characteristic of the MT phase of Ge(111). As for the highly perfect Ga-doped Ge, varying misorientation directions ($\langle 11\bar{2}\rangle$ or $\langle \bar{1}\bar{1}2\rangle$) or angles (1° or 2°) has no effect. Upon heating, the half-order split spots progressively broaden and become invisible at 475 °C. As shown in figure 3(*a*), step edges appear even more ragged than those of the equivalent surfaces of the perfect Ga-doped Ge crystals. Now, each terrace of the vicinal surface reconstructs in irregular domains with a honeycomb structure as displayed in figure 3(*b*). This atomic honeycomb domain structure can be thought of as a different ordering of the (2×2) and c(4×2) cells, which are the two building blocks of the c(2×8) reconstruction. Domain walls, parallel to the six equivalent $\langle 1\bar{1}0\rangle$ directions, are formed by atomic rows of c(4×2) periodicity. The inside of the domains is reconstructed (2×2) and each wall crossing corresponds to a triangle of three adatoms (a local $(\sqrt{3} \times \sqrt{3})$ arrangement) as shown in figure 4(*a*) and, schematically, in figure 4(*b*). The continuity of the network of domain walls breaks down only at point defects, which explains the low background in the LEED pattern. TEM investigation of these samples revealed a high density of dislocations ($> 10^7$ cm^{-2}) and subgrain boundaries. Ga

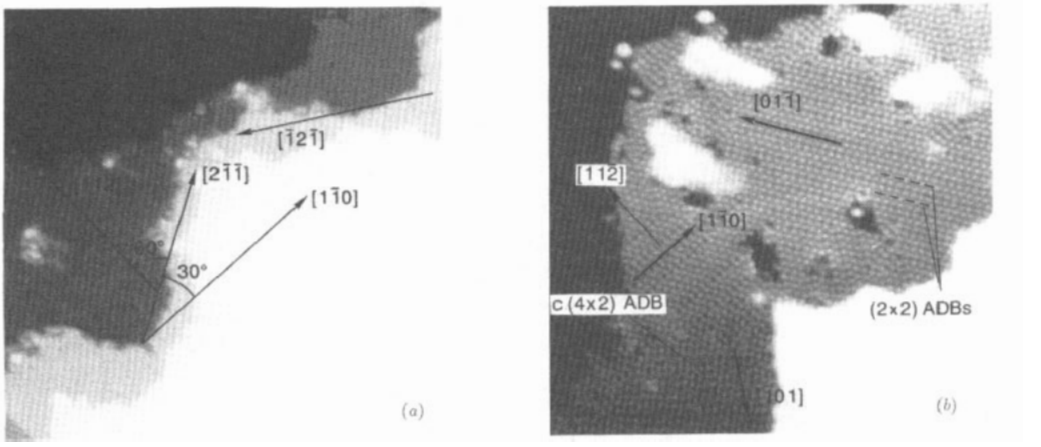

Figure 2. (*a*) STM CCT of an ~720 × 660 Å^2 section of a vicinal (111) surface (misoriented by 1° along the [$11\bar{2}$] direction) of a high-quality Ga-doped Ge crystal. During the scan, performed at +1.1 V sample bias, the tunnelling current was 4.8 nA. Three single-height (3.27 Å) steps can be observed. Their edges are not straight, perpendicular to the [$11\bar{2}$] direction, but meander by about ±30°. (*b*) STM CCT of a section of smaller size on the same vicinal surface as that in (*a*). Arrows, parallel to the [$\bar{1}01$], [$1\bar{1}0$], and [$01\bar{1}$] directions, show the three different domains of the c(2×8) reconstruction. Two (2×2) and one c(4×2) ADBs are indicated. Black–white contrast in (*a*) and (*b*) is adjusted in order to maximize the corrugation on the second-lowest terrace.

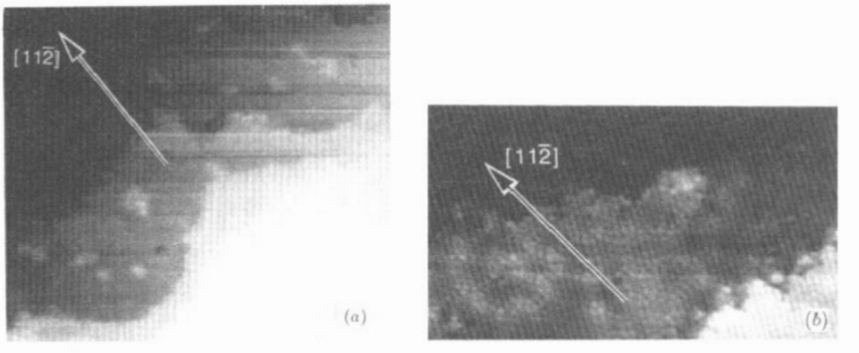

Figure 3. (*a*) STM CCT of an ~780 × 660 Å^2 section of a vicinal (111) surface misoriented by 1° along the [$11\bar{2}$] direction of a Ga-doped Ge crystal rich in dislocations. The scan was performed at +1.0 V sample bias and with a tunnelling current of 9.9 nA. Black–white contrast is adjusted in order to maximize the corrugation on the third-highest terrace. (*b*) STM CCT of an ~400 × 250 Å^2 section of a vicinal (111) surface misoriented by 1° along the [$11\bar{2}$] direction of a Ga-doped Ge crystal rich in dislocations. The scan was performed at +1.05 V sample bias and with a tunnelling current of 4.2 nA. Black–white contrast is adjusted in order to maximize the corrugation on the second terrace.

inclusions were observed on the surface with element-specific WDX analysis.

5. Discussion and conclusions

We have studied vicinal (111) surfaces, misoriented by 1° and 2° toward the [$11\bar{2}$] and [$\bar{1}\bar{1}2$] directions, for both high-quality Ga-doped Ge crystals and those doped to a higher level,

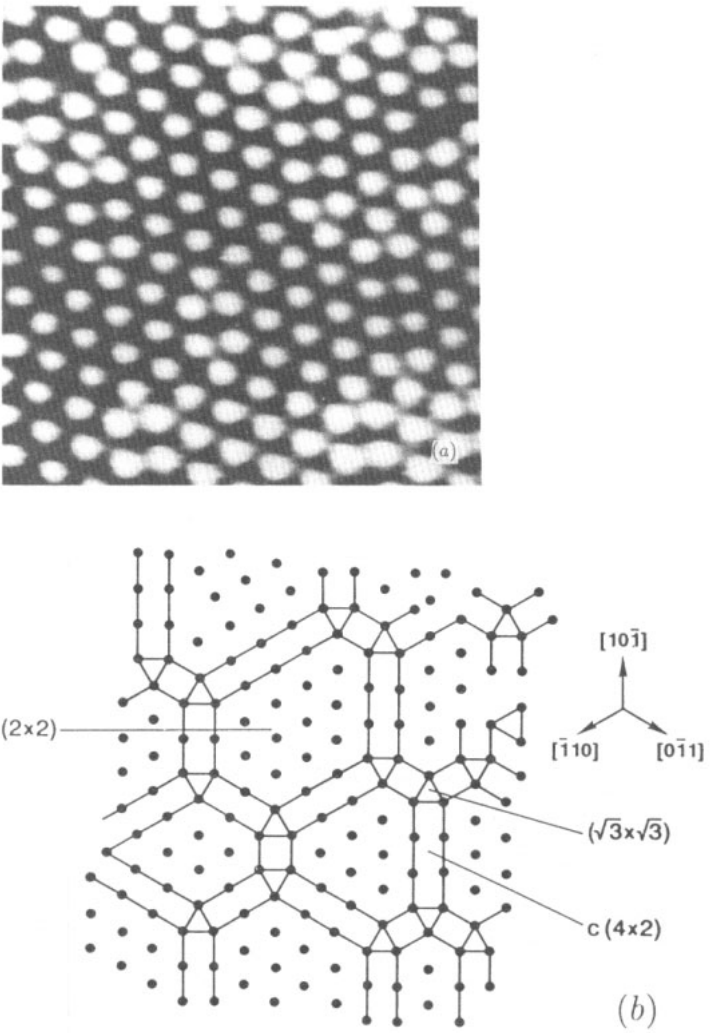

Figure 4. (*a*) STM CCT of an ~90 × 90 Å^2 section of a vicinal (111) surface of a Ga-doped Ge crystal with a high-density of dislocations. The surface misorientation angle toward the [11$\bar{2}$] direction is 1°. The sample bias was +1.1 V and the tunnelling current 5.8 nA. Black–white contrast in this detailed picture of the I(2×2) reconstruction corresponds to a corrugation of 0.9 Å. (*b*) Schematic representation of (*a*), emphasizing the honeycomb topology of the network.

which show a high density of dislocations. For the former, vicinal surfaces reconstruct c(2×8) and no domain orientation is preferred. Step edges meander along the direction perpendicular to the miscut direction and the width of the terraces varies considerably from the nominal value. An irregular honeycomb structure formed by hexagons of different sizes, reconstructed (2×2), appears for the vicinal surfaces of the second type of crystal. Domain walls between hexagons reconstruct c(4×2). This non-periodic reconstruction appears to be structurally equivalent to the (2×2) incommensurate structure, I(2×2), predicted by Phaneuf and Webb [2] to be the most likely candidate for the MT phase of the intrinsic Ge(111) surface. Ga inclusions, observed with WDX on the surface, may be responsible for large strains giving rise to the large density of dislocations observed with TEM. For high-quality Ge crystals with a Ga DC five times lower, the I(2×2) does not appear at RT, even in the case of

$\langle 11\bar{2}\rangle$ and $\langle \bar{1}\bar{1}2\rangle$ Ge(111) vicinal surfaces. Well oriented surfaces of the same highly doped crystals rich in dislocations do not show the I(2×2) reconstruction, therefore the surface misorientation seems to be necessary for this structure. In order to allow comparison with Sn-, In-, and Al-dosed Ge(111) surfaces [3, 9] where these impurities were found to produce a LEED pattern similar to that of the I(2×2) subsequent to annealing, work on Ga-dosed surfaces is in progress. Neither the obtained LEED pattern nor the STM pictures on these surfaces [6] show the quality of the I(2×2) structure observed in the present work for vicinal surfaces of Ga-doped Ge crystals rich in dislocations. The reconstruction observed on Ga-dosed surfaces also consists of domains surrounded by walls, c(4×2) reconstructed, however, these are far from being a continuous hexagonal network like the I(2×2). The surface exhibits some structural similarities with the reconstruction predicted by Sakamoto and Kanamori for the MT phase of clean Ge(111) by means of Monte Carlo (MC) calculations for a lattice gas model [29].

Remarkable overall resemblances exist between the I(2×2) reconstruction and some discommensurate phases observed during commensurate–incommensurate (C–I) phase transitions of certain surfaces, in particular for some chemisorbed and physisorbed systems [30], e.g. Kr on graphite. Increasing the Kr coverage on graphite beyond $\frac{1}{3}$ ML, an irregular honeycomb network of domain walls, which separate the three different possible $(\sqrt{3}\times\sqrt{3})$ domains on the hexagonal substrate, appears [31–33]. Theoretical studies for physisorbed noble gases on hexagonal substrates predict that, depending on the value of the energy, Λ, of a crossing between three ADBs, these walls either align ($\Lambda > 0$), in which case the surface shows a striped phase, like Xe on Pt(111), or forms a network of walls with the topology of a honeycomb ($\Lambda < 0$) [31]. These walls may be either light or heavy depending on whether the material density within the wall is smaller or larger, respectively, than that within the domains. Here, it is important to mention that the I(2×2) reconstruction has a slightly larger adatom density than the c(2×8) [2, 34], just like the discommensurate phase of Kr on graphite with respect to the C-phase [30], i.e., it displays heavy walls.

This discommensuration, in the case of physisorbed systems, results from the competition of two types of interaction: a Van der Waals attraction between the physisorbed atoms and the substrate, and Van der Waals attractions or hard-core repulsions at short distances between adsorbed atoms. In other words, the substrate tries to force the adsorbate to adopt a lattice constant which is does not like. Although not immediately obvious, the mechanism for the formation of the I(2×2) may be similar despite the fact that the magnitude of the interaction energies is different. The bulk truncated (111) surface of Ge is under strong compressive stress since the surface tries to adopt a planar, sp^2-like configuration [35]. If the surface is decorated with adatoms, the stress becomes tensile [35], i.e. the surface would try to adopt a smaller lattice constant. This is a prerequisite for discommensuration and exactly the condition for the formation of heavy walls.

In fact, the c(2×8) reconstruction looks like a striped phase since the rows of c(4×2) cells can be considered as ADBs which separate two non-equivalent (2×2) domains. Although there is as yet no support for this assumption, the c(2×4) structure may be able to partly release the stress created by the (2×2) domains. Ga impurities could influence the energy of the domain-wall crossings. A change in sign for this energy could produce the observed I(2×2) honeycomb domain structure. The stress induced in the substrate by dislocations may even increase this tendency for incommensuration.

Breathing modes are predicted for physisorbed discommensurate structures [32]. However, interaction energies for the physisorbed systems (of the order of 50 meV) [36] are much lower than common energies for chemical bonding (of the order of 1 eV) [35]. Therefore, the expected energies to roughen a domain wall or change its length in Ge(111)–

Ga-I(2×2) are much higher and these *breathing* modes [32] may be observed above RT. Actually Feenstra *et al* showed the high mobility of the adatom rows on the c(2×8) reconstruction slightly above RT [21]. Adatom rows were observed to slide along the $[10\bar{1}]$, $[\bar{1}10]$, and $[0\bar{1}1]$ directions. Assuming the same behaviour for the I(2×2) reconstruction, this would correspond to the wall fluctuations or breathing modes suggested by Phaneuf and Webb [2]. STM investigations of breathing dynamics could be an exciting future prospect.

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References

[1] Binnig G, Rohrer H, Gerber Ch and Weibel E 1982 *Phys. Rev. Lett.* **49** 57
[2] Phaneuf R J and Webb M B 1985 *Surf. Sci.* **164** 167
[3] Ichikawa T and Ino S 1980 *Solid State Commun.* **34** 349
[4] McRae E G and Malic R A 1988 *Phys. Rev.* B **38** 163
[5] Denier van der Gon A W, Gay J M, Frenken J W M and van der Veen J F 1991 *Surf. Sci.* **241** 335
[6] Molinàs-Mata P, Böhringer M and Zegenhagen J to be published
[7] Lander J J, Gobeli G W and Morrison J 1963 *J. Appl. Phys.* **34** 2298
[8] Marée P M, Nakagawa K and van der Veen J F 1988 *Phys. Rev.* B **38** 1585
[9] Yang W S and Jona F 1982 *Solid State Commun.* **42** 49
[10] Patthey L, Bullock E L and Hricovini K 1992 *Surf. Sci.* **269–270** 28
[11] Becker R S, Golovchenko J A and Swartzentruber B S 1985 *Phys. Rev. Lett.* **54** 2678
[12] Becker R S, Swartzentruber B S, Vickers J S and Klitzner T 1989 *Phys. Rev.* B **39** 1633
[13] Hirschorn E S, Liu D S, Leibsle F M, Samsavar A and Chiang T C 1991 *Phys. Rev.* B **44** 1403
[14] Molinàs-Mata P and Zegenhagen J 1993 *Surf. Sci.* **281** *10*
[15] Molinàs-Mata P and Zegenhagen J 1992 *Solid State Commun.* **84** 393
[16] Feidenhans'l R, Pedersen J S, Bohr J, Nielsen M, Grey F and Johnson R L 1988 *Phys. Rev.* B **38** 9715
[17] Aarts J, Hoeven A-J and Larsen P K 1988 *Phys. Rev.* B **38** 3925
[18] Hricovini K, LeLay G, Abraham M and Bonnet J E 1990 *Phys. Rev.* B **41** 1258
[19] Palmerg P W 1968 *Surf. Sci.* **11** 153
[20] Feenstra R M, Slavin A J, Held G A and Lutz M A 1991 *Phys. Rev. Lett.* **66** 3257
[21] Feenstra R M, Slavin A J, Held G A and Lutz M A 1992 *Ultramicroscopy* **42–44** 33
[22] Abraham M, Le Lay G and Hila J 1990 *Phys. Rev.* B **41** 9828
[23] Omicron Vakuumphysik GmbH, Taunustein, Federal Republic of Germany
[24] MHO, Hoboken, Belgium
[25] Trumbore F A, Probansky E M and Tartaglia A A 1959 *J. Phys. Chem. Solids* **11** 239
[26] Welz B 1983 *Atomabsorptionsspektroskopie* (Weinheim: Chemie) p 270
[27] Jung T M, Phaneuf R J and Williams E D 1991 *Surf. Sci.* **254** 235
[28] Molinàs-Mata P, Böhringer M, Artacho E and Zegenhagen J to be published
[29] Sakamoto Y and Kanamori J 1991 *Surf. Sci.* **242** 119
[30] Persson B N J 1992 *Surf. Sci. Rep.* **15** 1 and references therein
[31] Villain J 1980 *Ordering in Two Dimensions* ed S K Sinha (New York: North-Holland) p 123
[32] Villain J 1980 *Surf. Sci.* **97** 219
[33] Villain J 1980 *J. Physique* **41** L267
[34] Both the c(2×8) and the (2×2) reconstructions have the same adatom density, $\frac{1}{4}$ monolayer
[35] Meade R D and Vanderbilt D 1989 *Phys. Rev.* B **40** 3905
[36] Villain J and Gordon M B 1983 *Surf. Sci.* **125** 1