Enhanced Step Waviness on SiGe(001)-(2 × 1) Surfaces under Tensile Strain

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Scanning tunneling microscopy measurements of thermally cleaned, low Ge content SiGe(001) films under an ~1% biaxial tensile strain show large amplitude, quasiperiodic, thermally stable S_B-step undulations alternating with extremely straight S_A steps on extended areas wherever the local step separation $L > 20$ nm. The wavelength λ scales roughly with $L^{1/2}$ for $20 < L < 120$ nm, and reaches a limiting value between 100 and 200 nm on larger terraces. The measured behavior suggests that the wavy steps are stabilized by surface stress relaxation effects which are enhanced by tensile strain.

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The behavior of vicinal (001)-(2 × 1) surfaces on Si and Ge is a subject of great technological and fundamental interest. Much interest results from the highly anisotropic physical properties of these surfaces, due in large part to the "dimerized" nature of the (2 × 1) surface reconstruction [1–4]. Several years ago, Alerhand *et al.* [5] pointed out that the surface stress tensor on these surfaces is quite anisotropic and produces a force imbalance [often referred to as a "force monopole" (FM)] across a single layer (SL) step since the surface reconstruction rotates by 90° across SL steps. Strain relaxation at step edges due to these FM's should lead to a remarkable effect on surfaces with sufficiently low initial step density: *the spontaneous formation of extra up-and-down SL steps* forming a "stripe"-like surface phase. While this stripe phase has not yet been observed, several groups have reported evidence for stable "undulations" of step edges on slightly miscut Si(001) surfaces [6–9] and have pointed out that such undulations should be stabilized by surface stress effects similar to those considered by Alerhand *et al.* [5].

Here we report the first scanning tunneling microscopy (STM) measurements of striking step behavior on (001) surfaces of low Ge content SiGe films under a moderate (~1%) biaxial tensile strain. Step bunching (probably from the strain-relaxed $Si_{0.7}Ge_{0.3}$ substrate) produces extended areas with small local miscut (in the range of 0.05°–0.4°) oriented towards [110] crystal directions. These areas exhibit large amplitude, quasiperiodic "wavy" S_B steps alternating with extremely straight S_A steps, where S_A (S_B) corresponds to SL steps with rows of surface dimers on the upper terrace oriented parallel (perpendicular) to the global step edge [1]. This behavior differs from that reported by Tromp and Reuter [7] for unstrained Si in that the wavelength is an order of magnitude smaller (40–100 nm) in our case, and *only* the S_B-type steps oscillate. While there have been indications that slightly enhanced S_B step undulations may exist on unstrained Si(001) [6,9], we present here the first direct STM observations of extended, thermally stable, multicycle S_B-step oscillations on (001) surfaces, as well as the first investigation of how the amplitude and wavelength of these step undulations vary with local miscut. Our measurements suggest that these wavy steps are related to surface stress relaxation effects [5–9], which are enhanced by the applied tensile strain.

Samples were grown at AT&T by molecular beam epitaxy (MBE). The typical sample structure consists of a 5 nm strained Si layer grown on top of a compositionally graded, relaxed $Si_{1-x}Ge_x$ buffer layer (graded from $x = 0$ to $x = 0.3$) on Si(001) substrates [10,11]. This results in a nominal 1.3% tensile strain in the Si cap layer. STM measurements were performed at The Ohio State University using a custom-built multipurpose STM housed in an UHV system (base pressure $< 1 \times 10^{-10}$ torr) with separate chambers for the STM and for sample/tip preparation and analysis. Etched W tips were cleaned *in situ* with electron-beam heating, and STM images were measured with a typical sample bias of −1.85 V.

Samples were cleaned by first growing a thin (1–2 nm) room-temperature oxide film, then desorbing it in UHV by heating to 1025 °C for several minutes. Figure 1 shows that this procedure [12] produces extended surface areas with very few particle contaminants. Since the Si cap thickness is much less than the ≈12 nm "Matthews-Blakeslee" equilibrium critical thickness for 1.3% strain [13], no strain-relieving dislocations should be introduced during heating. Depth profile x-ray photoemission spectroscopy measurements made after cleaning indicate that there may be a small amount of Ge present near the surface (with concentration <10%), which would reduce the surface tensile strain to a value in the range of 0.8–1.3%.

Figure 1(a) shows a 5 × 5 μm^2 STM image of such a strained $Si/Si_{0.7}Ge_{0.3}$ sample after surface cleaning. This image is displayed in "derivative mode" [14] and should be viewed as if illuminated obliquely from the

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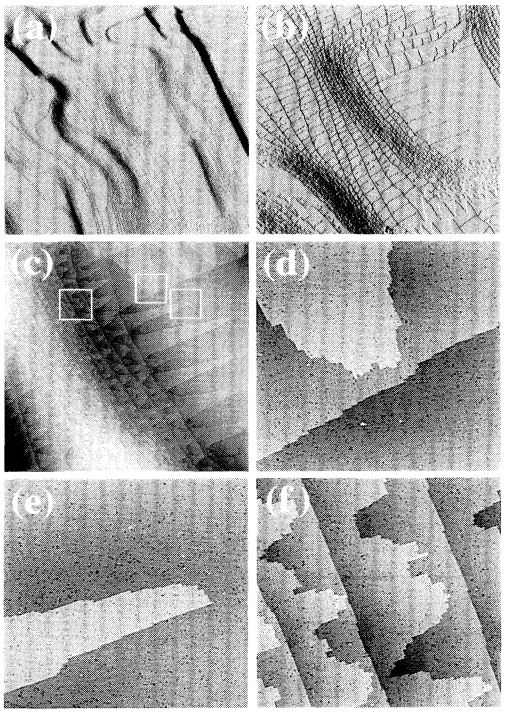

FIG. 1. (a) $5 \times 5\ \mu m^2$ derivative mode image of a strained Si sample following surface cleaning. (b) $1.8 \times 1.8\ \mu m^2$ image of the central part of (a). (c) $820 \times 820\ nm^2$ gray-scale image of the central part of (b). (d)–(f) $100 \times 100\ nm^2$ close-ups of boxed areas in (c).

left. On a large scale, we see localized "step bunched" regions generally running along [110] directions, which are probably related to the [110]-oriented "cross hatching" present on relaxed SiGe surfaces [11]. Away from the step bunched regions are several large (001) terraces, and extended areas with small local miscut (typically 0.05°–0.4°) usually oriented towards a [110] direction. This unique morphology permits a direct investigation of the dependence of the step behavior on local misorientation.

Figure 1(b) is a $1.8 \times 1.8\ \mu m^2$ scan of the central part of Fig. 1(a), showing that the slightly miscut regions are covered with quasiperiodic wavy steps alternating with very straight steps. The local miscut in this scan ranges from 0.02°–0.6°, corresponding to local step separations L in the range 350–13 nm (here $2L$ is the separation between adjacent *straight* steps). Figure 1(c) shows a $820 \times 820\ nm^2$ scan (displayed now as a gray scale keyed to height) of the central part of Fig. 1(b), and Figs. 1(d)–1(f) show atomic resolution close-up scans of the boxed areas in Fig. 1(c). On a large scale, we note that (1) both the amplitude A and characteristic wavelength λ of the wavy steps increase with L, (2) for $L > 20$ nm the wavy steps in general cover most (>80%) of the distance between adjacent straight steps, and (3) for $L < 20$ nm the periodicity becomes suppressed and/or masked by step meander. We also find that λ increases more slowly with L than does A, causing larger step undulations to assume elongated "finger"-like shapes. Analysis of many scans from several samples suggests an approximate empirical relation $\lambda \approx (10 \pm 3\ \text{nm}) \times (L/1\ \text{nm})^{0.5\pm0.1}$ for $20 < L < 120$ nm, with about a ±20% scatter in the data. On much larger terraces ($L > 300$ nm) highly elongated stripelike [5] step fingers are often observed. In this case the lateral separation of the fingers generally falls in the range of 100–200 nm with no systematic variation with terrace width.

The atomic structure of the steps is revealed by the close-up scans in Figs. 1(d)–1(f) and Figs. 2(b)–2(d). We see that the straight steps are nominally of the S_A type, while the wavy steps are nominally of the S_B type. From previous studies of unstrained, thermally cleaned Si(001) it is well known that S_B steps are much rougher than S_A steps [14] due to large step *meander,* with step kinks largely uncorrelated in direction, separation, and length [14–16]. In contrast, it is evident that the kinks on the larger wavy steps on our strained Si samples are highly correlated, particularly in direction.

In passing, we also note another remarkable aspect of these samples—the smooth S_A steps have extremely few "unforced" kinks [14,16], i.e., kinks which are opposite in direction to those "forced" by a slight azimuthal misorientation of the local miscut away from [110]. Along the S_A steps in Figs. 1(d), 1(f), 2(b), 2(c), and 2(d), we count 0, 6, 2, 0, and 1 unforced kinks, respectively—a

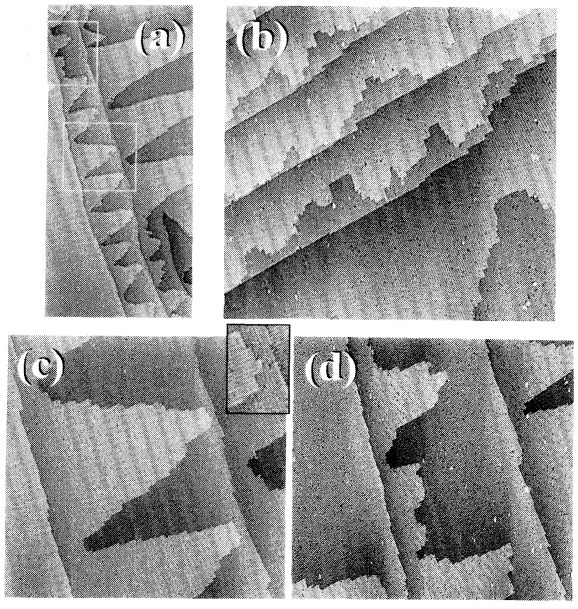

FIG. 2. (a) $320 \times 720\ nm^2$ image of a second strained Si sample. (b) $100 \times 100\ nm^2$ image of a different area on the same sample. (c),(d) $150 \times 150\ nm^2$ images of the boxed areas in (a). Magnified inset in (c) shows that the finger is *not* a kissing site.

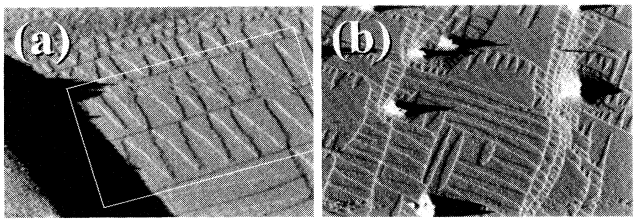

FIG. 3. (a) 780 × 570 nm^2 derivative mode image of a third strained Si sample after a 2 h anneal at 720 °C. Boxed area indicates two S_B steps with peak-to-trough alignment. (b) 3.1 × 2.3 μm^2 area of another strained Si sample, showing the stripelike region. An alternate cleaning model (Ref. [12]) resulted in the larger surface particle density.

total of only nine unforced kinks out of more than 1600 possible kink sites. This is roughly a factor of 5 lower probability of finding unforced kinks than previously reported for unstrained Si(001) [14,16]. This may be due to a tensile-strain-induced *increase* in the energy of S_B-terminated kinks on S_A steps, consistent with recent calculations of Xie *et al.* [10]. This will be discussed in detail elsewhere [12].

We now consider the possible origin of the waviness in the S_B steps. Our atomic-resolution scans show that the vast majority of the fingers are *not* caused by defect-related step "pinning" [17]. We also find that they are *not* in general "kissing sites" [7], i.e., step protrusions which extend completely to the next step edge and which are stabilized by antiphase boundaries (APB's) [18] in the (2 × 1) reconstruction on the lower terrace. Figures 1(d)–1(f) and Figs. 2(c) and 2(d) directly show that there are no APB's present under many of the fingers. This is also evident from Fig. 1(c) and Fig. 2(a), which show that many fingers do not extend to the next step edge. Some APB's can be found, but wavy S_B steps many cycles long clearly do not exist without them.

We have used exactly the same cleaning procedures to study unstrained vicinal Si(001) substrates with surface miscuts of 0.1°–0.3° aligned towards a [110] direction and found essentially random S_B step undulations, in agreement with previous studies [14,15,19]. We also examined samples with a 5 nm thick $Si_{0.9}Ge_{0.1}$ layer grown compressively on Si(001) substrates and cleaned in the same way and again found no evidence of wavy S_B steps. This suggests that the wavy steps are not simply due to a small local miscut or small amounts of Ge present near the surface.

We should also consider whether the wavy S_B steps are *nonequilibrium* structures formed by a kinetically limited process during surface cleaning. This is important since various "kinetic instabilities" [20] could produce wavy step fronts during growing or etching and since the longer step "fingers" do look qualitatively similar to growth structures observed during MBE [21] or chemical vapor deposition [22] homoepitaxy. To address this, we have performed annealing experiments. The wavy step structures are quite robust and are still found after annealing for 2 h at 720 °C [as shown in Fig. 3(a)], 10 min at 875 °C, or even after several 2 min "reflashes" at 1025 °C. For comparison, steps on unstrained Si(001) surfaces with miscuts in the range of 1°–0.1° are commonly assumed to equilibrate during time scales of minutes at temperatures in the range 600–710 °C [3,6,14,16,18]. *This suggests that the steps on our samples are in local equilibrium,* at least for local miscuts down to 0.1°. We do note that finite-duration annealing experiments do not prove *long range* equilibration, since equilibration times increase strongly with terrace width [23]. On very large terraces (>500 nm) we do observe long fingers which do not completely cross the terrace, suggesting a kinetically limited structural evolution. We also note that other kinetic processes (such as Ge evaporation [12] or dynamic step bunching [24]) could result in nonequilibrium conditions even during extended high temperature annealing. At present, we cannot directly monitor step motions with our STM, but we do plan high-temperature measurements using low energy electron microscopy to investigate their importance. Nevertheless, the fact that the wavy steps survive annealing under a *range* of temperatures which equilibrate steps on unstrained Si(001) strongly suggests that step *energetics* are very important in determining step.

We propose that the wavy S_B steps on our samples are stabilized by surface stress relaxation effects similar to those previously proposed for unstrained Si(001) [5–9], which in our case are *enhanced* by the applied tensile strain. Several aspects of these wavy S_B steps are consistent with surface stress effects. First, the waviness is confined to S_B steps. Since kinks in S_B steps cost much less energy than kinks in S_A steps [14,16,25], one would expect most strain-relieving undulations to be confined to S_B steps [6,8,9]. Second, the strength of the waviness increases as the local step separation L increases, consistent with the idea of a "critical" terrace width for the onset of step undulations [5,8]. Third, we often find that the "peaks" of a wavy step on one terrace are aligned with the "troughs" on an adjacent terrace, particularly when L (and hence λ) is nearly the same on both terraces. The boxed area in Fig. 3(a) shows an example of this effect. This peak-to-trough alignment results in a pattern of roughly triangular terraces *which border on all three sides extended SL steps* and hence should be a particularly effective in relieving surface stress. Finally, we find that on very large terraces (>300 nm) the wavy steps become elongated fingers with nearly parallel S_A-type edges, and their separation approaches a limiting value in the range of 100–200 nm. In this limit the local step structure appears to approach the stripe phase originally proposed by Alerhand *et al.* [5], i.e., *an array of nearly parallel, periodic, alternating up and down S_A steps.* The lower-central part of Fig. 3(b)

shows a particularly striking example of this stripelike appearance.

The next question is why should this type of step waviness be enhanced by tensile strain? Here we note that on strained Si(001) surfaces the FM at a step actually has *two* components. The first component F_o is due to surface stress anisotropy [5,26], which on Si(001) produces a FM directed towards the upper (lower) terrace at an S_A (S_B) step. The second component F_a is present at a surface step on *any* film under a net applied strain [27] and is simply due to the fact that there is more material under stress on one side of the step than the other. This FM is directed towards the upper (lower) terrace for tensile (compressive) strain and has approximate magnitude [27] $F_a \approx \sigma_a h = B\varepsilon h$, where $h \cong 0.14$ nm is the SL step height, and the elastic modulus B [28] relates in-plane film stress a to applied biaxial strain ε. Hence, *an applied tensile strain should increase the magnitude of the total FM at S_A step edges,* resulting in a larger driving force for step undulations. With this total FM, the optimum terrace width for the Alerhand stripe phase [5] should become

$$L_o \approx \pi a \exp[1 + E_A/\alpha(F_o + B\varepsilon h)^2], \qquad (1)$$

where E_A is the step energy, α depends on bulk elastic constants, and $a \cong 0.38$ nm is the surface lattice constant. If we assume the experimental values $E_A \cong 0.028$ eV/a [14,25], $F_o \approx 1.2$ eV/a^2 [2,26], $\alpha \approx 0.0033a^3$/eV [5,28], and $B \approx 64$ eV/a^3 [28] then Eq. (1) gives the *order of magnitude* estimates $L_o \approx 1$ μm for Si(001) with no strain, and $L_o \approx 200$ nm with a 1% tensile strain. This compares with the typical values $\lambda \approx 50$–200 nm for wavy S_B steps measured on our strained samples. Although these estimates are quite rough and depend strongly on the actual parameter values which are used, they nevertheless indicate that moderate biaxial tensile strain should enhance step waviness on Si(001) surfaces. Finally, we note that recent molecular dynamics calculations [29] are consistent with a tensile-strain-induced *increase* in the total FM at S_A steps of roughly 50% of the amount estimated above. More detailed calculations are in progress.

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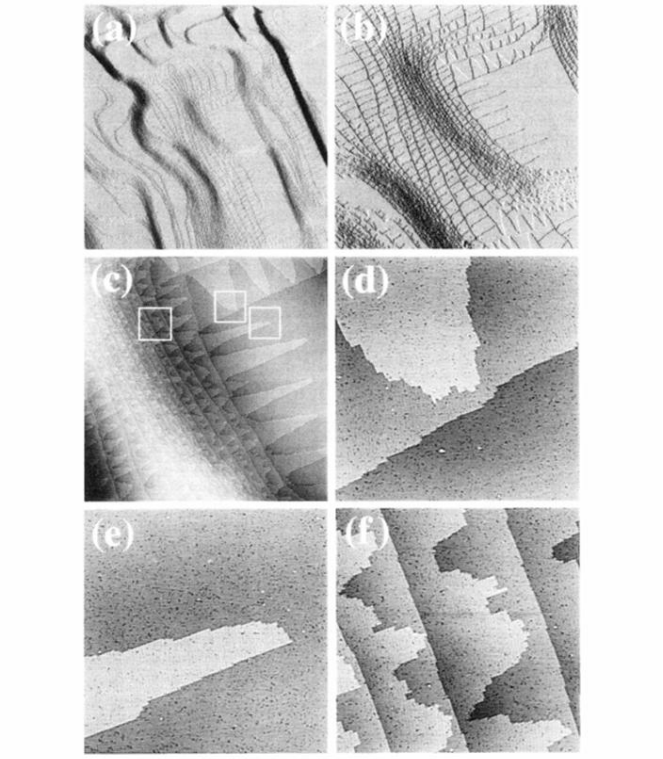

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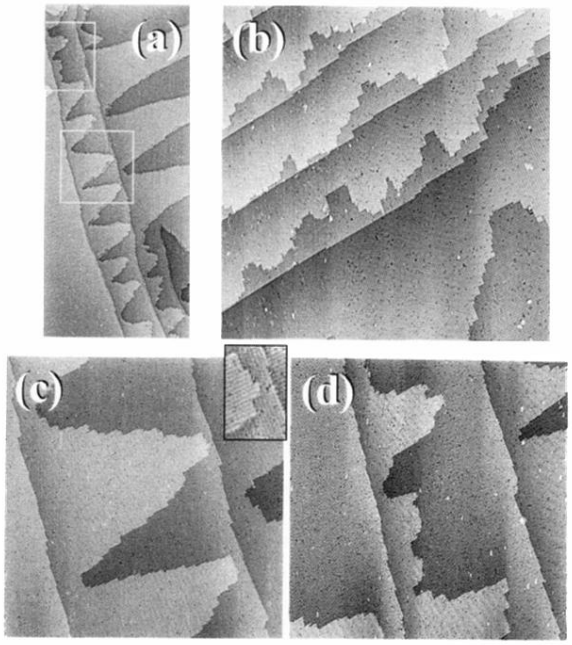

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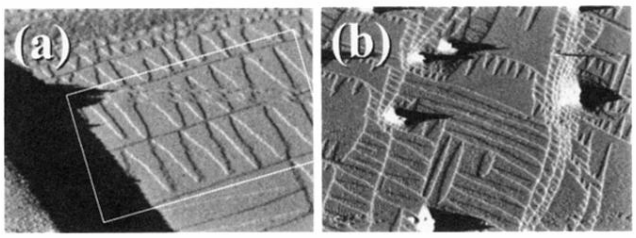

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