

Atomic scale study of strain relaxation in Sn islands on Sn-induced Si(111)-(2√3×2√3) surface

L. L. Wang,^{1,2} X. C. Ma,^{1,a)} Y. X. Ning,¹ S. H. Ji,¹ Y. S. Fu,¹ J. F. Jia,³ K. F. Kelly,² and Q. K. Xue^{3,1}

¹Institute of Physics, The Chinese Academy of Sciences, Beijing 100080, People's Republic of China

²Department of Electrical and Computer Engineering, Rice University, Houston, Texas 77005, USA

³Department of Physics, Tsinghua University, Beijing 100084, People's Republic of China

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Surface structure of the Sn islands 5 ML high, prepared on Si(111)-(2√3×2√3)-Sn substrate, is investigated by low temperature scanning tunneling microscopy/spectroscopy. Due to the elastic strain relaxation in the islands, the in-plane unit cell structure distorts and the apparent height of the surface atoms varies regularly to form an overall modulated strip structure. The quantum well states are observed to depend on the relative position within this structure, which implies the change of the surface chemical potential induced by the elastic strain relaxation as well. © 2009 American Institute of Physics. [DOI: 10.1063/1.3120764]

The epitaxial growth of Sn on Si(111) substrate is very complicated, characterized by varied crystalline orientations due to different crystal symmetries and lattice constants of α -Sn and β -Sn.¹⁻³ At the very beginning of growth, formation of α -Sn with hexagonal structure is favored until phase transition to the thermodynamic stable phase, β -Sn, takes place at a critical thickness of 4 ML. From 5 to 10 ML, the lattice mismatch resulted strain manifests the growth via thickness-dependent modulated strip structures on the island surfaces.³ These modulated strips were shown to disappear gradually with thickness as a result of strain relaxation. However, their atomic structure and how they affect the electronic structure of the islands have not been understood.

In the present work, using a low temperature scanning tunneling microscope (STM), we have investigated the modulated strip structure on the Sn islands at 5 ML, the thickness immediately after the phase transition from α -Sn to β -Sn. Our observation shows that the strain results in great distortion in both the in-plane and out-of-plane structures. The former is characterized by the distortion of unit cell while the latter with periodic height variations. Even at low observation temperature (from 3.2 to 14.2 K), the atoms at special site can move up and down easily with slight fluctuation in temperature. Specifically, we could be able to detect the corresponding response of quantum well states (QWSs) due to local structure change, by which a direct relation between structure relaxation and electronic property change could be studied.

The detail of preparation of Sn islands was described in Ref. 3. Here, 5 ML Sn was deposited on the 2√3 substrate at a temperature of 150 K. Then the sample was transferred to the STM stage. Figures 1(a) and 1(b) show typical high resolution STM images recorded from the 5 ML islands at 80 and 4.6 K, respectively. The line profile below each STM image reveals the change in atom height along the [001]- β -Sn direction. The in-plane unit cells are measured to be 4.31×4.16 Å² with an angle of 79° [see the inserted diagram in Fig. 1(a)] and do not change at 80 and 4.6 K,

while the out-of-plane arrangement changes distinctly and periodically. At 4.6 K, the modulated strip structure remains except some pairs of atoms in the middle of the modulated strip move up and appear 0.1 Å higher than the most background atoms. Hereafter those upward moved and background atoms are called as up and down atoms, respectively, for comparison.

Schematic illustrations of epitaxial orientation and atom arrangement are shown in Fig. 2(a) and Figs. 2(b) and 2(c), respectively. In Fig. 2(a), the dashed rectangles represent the theoretical epitaxial orientation as the β -Sn(100) surface with the rectangle lattice of 5.83×3.18 Å² spreads on a 5.76×3.325 Å² lattice,⁴ while the bold rectangles represent the actual one derived from the atomically resolved image in Fig. 1(a). Consequently, the surface structure of 5 ML island undergoes a ~26% contraction along the [010]- β -Sn direction and a ~30% expansion along the [001]- β -Sn direction accompanied by an angle distortion to 79°. The resulted length of the diagonal along the [011]- β -Sn direction is 6.54 Å, a little bit smaller than the theoretical value of 6.65 Å.

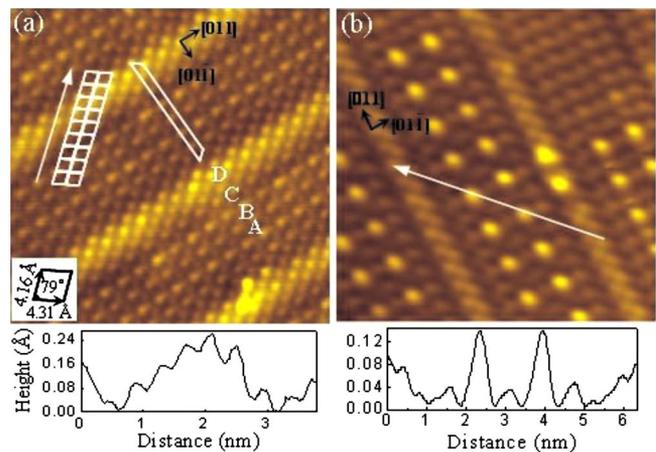


FIG. 1. (Color online) High resolution STM images (10×10 nm²) acquired on 5 ML island at 80 K (a) and at 4.6 K (b). The line profile corresponding to the single-arrowed line is shown just below each image. (a) was acquired with a sample bias of 0.4 V and a constant tunneling current of 0.1 nA, and (b) at -1.0 V and 1 nA.

^{a)}Electronic mail: xma@aphy.iphy.ac.cn.

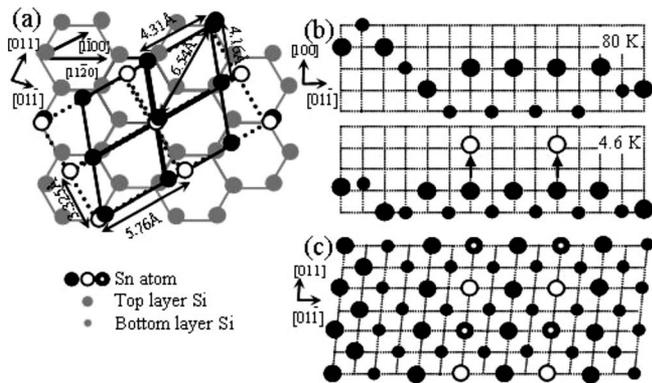


FIG. 2. Schematic illustrations of epitaxial orientation (a), out-of-plane (b), and in-plane (c) atom arrangements. In (b), the solid circles represent Sn atoms at the down positions, the open circles represent Sn atoms at the up positions, and larger circles represent atoms in the outer row. In (c), larger circles represent atoms closer to the surface.

This in-plane distortion can force several rows of atoms along the $[011]$ - β -Sn direction to move up periodically to release the strain. Figure 2(b) shows the out-of-plane atom arrangement in one period, the top one at 80 K and the bottom one at 4.6 K. The periodic unit of the modulated strip, marked by the trapezoid schematics in Fig. 1(a), is composed by 15 atoms in two rows along the $[01\bar{1}]$ - β -Sn direction and defined as starting from the outward stretched atoms. Regardless of the uncertainty in atom height measurement at different scanning parameters, the most dominating change with temperature is that one pair of atoms along the $[01\bar{1}]$ - β -Sn direction and right in the middle of the modulated strip move up to the position labeled by open circles [see Fig. 2(b)]. This upward movement appears every other pair along the $[011]$ - β -Sn direction so that protruding double-atom chain is formed [see Fig. 2(c), the solid circles with white core represent the every other pair of atoms that stay down here].

Figures 3 show a series of typical atomically resolved images acquired in the temperature range of 3.2–14.2 K. It is interesting to note that some pairs of atoms move up and down easily with slight fluctuation in temperature. For example, the double-atom chain A that arranges sparsely at 3.2 K becomes densely at 8.8 K as every pair is up. The sparse arrangement is recovered at 14.2 K, as the every other pair is half-up. The double-atom chain C undergoes similar switch, as it arranges sparsely at 3.2 K and becomes densely at 8.8 and 9.6 K. In contrast, the double-atom chain B becomes discontinuous at 3.2, 9.6, and 14.2 K, as the three pairs of atoms marked by white rectangle are down. All those phenomena can be illustrated in Fig. 2(c), in which the atoms represented by the open circles move up and down with the atoms represented by the solid circles with white core being up (A and C) or down (B).

Surface structure is controlled by a delicate balance between the electronic energy and the elastic energy involved in the distortion. Especially in reduced dimensions at low temperature, the decrease in electronic energy can outweigh the increase in elastic energy, which is the origin of charge-density wave (CDW) transition and Peierls transition. This is the case of $1/3$ ML Sn on Ge(111) where CDW transition with a structure distortion from $(\sqrt{3} \times \sqrt{3}) R30^\circ$ to (3×3) symmetry was observed.^{5,6} While in the case of $1/3$ ML Sn

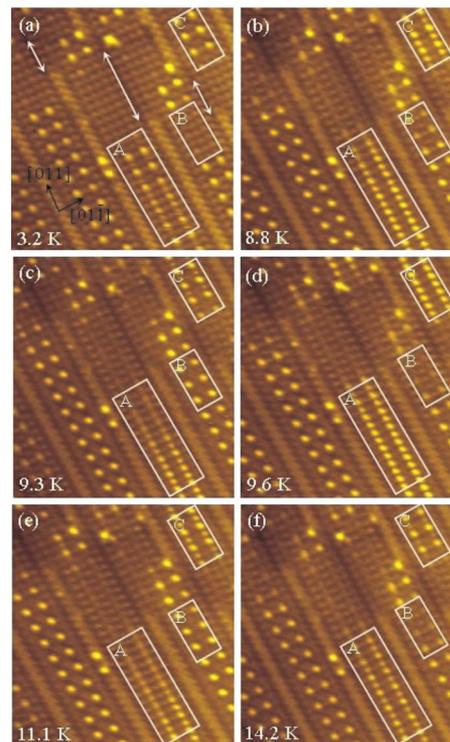


FIG. 3. (Color online) A series high resolution various temperature STM images acquired in the temperature range of 3.2–14.2 K. The image size is $15 \times 17 \text{ nm}^2$. The white rectangles mark the double-atom chains in which some atoms move vertically with slight change in temperature. The white double-headed lines in (a) marked the stagger joints of the modulated strips. All images were acquired at -1.0 V and 1 nA .

on Si(111), although photoelectron spectroscopy study shows some evidence of a similar phase transition, low-energy electron diffraction study at 70 K (Ref. 7) and our STM study at 4 K show $\sqrt{3} \times \sqrt{3}$ symmetry. In this work, the series STM images of 5 ML Sn islands are not bias dependent or complementary and the basic in-plane unit cell remains unchanged at 80 and 3.2–14.2 K, so the atomic up-down movement seems not to be CDW transition or Peierls transition.

We argue that the temperature-related atom up-down movement is a result of elastic relaxation. First, the up-down movement happens on the surface of 5 ML island, which is the thinnest and most strained β -Sn surface and right around the stagger joints, marked by white double-headed lines in Fig. 3(a). It is possible that the strain is enhanced with decreased temperature and induces the vertical movement of single atoms in the middle and near the stagger joint of the modulated strips where strain is large. Second, both the temperature range in which the switching happens and the amount of up-down movement atoms vary in double-atom chains. The up-down movements take place rather randomly in atomic scale, which most likely pertains to strain rather than electronic structure which usually exhibits some collective behaviors.

The strain relaxation induces not only the distortion of surface structure but also the local change in the surface chemical potential accordingly, which can be confirmed by measuring the energy of the QWSs. Figure 4 shows the scanning tunneling spectra A–D taken on the points labeled by the same letters in Fig. 1(a), respectively. Evidently, the lowest unoccupied QWS (LUQWS), the first peak just above the Fermi level, is position dependent. From A to B, to C, and to

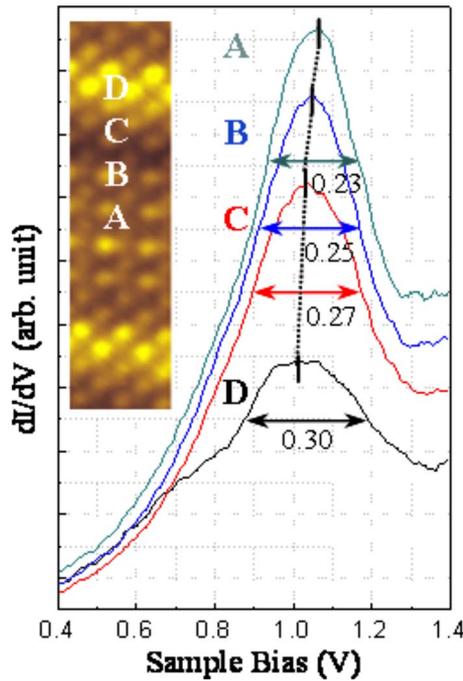


FIG. 4. (Color online) A series dI/dV - V spectra A–D taken on those points labeled by the same letters in Fig. 1(a). All the spectra were obtained at 0.4 V and 0.1 nA.

D, the peak of LUQWS shifts from 1.06 to 1.05, to 1.04, and to 1.01 eV, while the full width at half maximum (FWHM) increases from 0.23 to 0.25, to 0.27, and to 0.30 eV. As for the intensity, it drops continuously. That is, the closer to the edge of modulated strip, the lesser the intensity of LUQWS, and the smaller the energy of LUQWS. And the change accelerates with the points getting closer to the strip edge where the surface consisted by outward stretched atoms along the $[01\bar{1}]$ - β -Sn direction is most strained.

According to Bohr–Sommerfeld phase accumulation model, the condition to form QWS in two-dimensional quantum well system is

$$2k_z d + \Phi_B + \Phi_C = 2\pi n, \quad (1)$$

where k_z is a normal component of the wave vector, d is the QW thickness, whereas Φ_B is the phase shift associated with the metal-vacuum interface which is determined by the local surface chemical potential and dependent on the local surface structure^{8,9} and Φ_C is the phase shift associated with the semiconductor-metal interface. Since the surface structure is inhomogeneous at the nanometer scale, the phase shift associated with the metal-vacuum interface becomes a function of lateral position, $\Phi_B = \Phi_B(x)$, where x is the position with respect to the modulated strip along the $[01\bar{1}]$ - β -Sn direction. Provided that the phase shift associated with the semiconductor-metal interface Φ_C is constant, as a result of the derivation of Eq. (1),

$$\delta k_z \approx -\frac{1}{2d} \left[\delta \Phi_B(x) + \frac{4\pi\delta d}{\lambda_F} \right], \quad (2)$$

where λ_F is the Fermi wavelength which is 3.88 Å for the β -Sn crystal.¹⁰ For the first order approximation, the energy shift of QWSs is

$$\begin{aligned} \delta E(x) &\approx \hbar v_f \delta k_z = -\frac{\pi \hbar v_f}{2d} \left[\frac{\delta \Phi_B(x)}{\pi} + \frac{4\delta d}{\lambda_F} \right] \\ &= -\frac{\Delta}{2} \left[\frac{\delta \Phi_B(x)}{\pi} + \frac{4\delta d}{\lambda_F} \right], \end{aligned} \quad (3)$$

where v_f is the Fermi velocity and $\Delta = \pi \hbar v_f / d$ is the well-known expression for the energy separation between the QWSs. Consequently, with Eq. (3) and taking $\Delta = 1.75$ eV [refer to the bottom spectrum in Fig. 5(b) in Ref. 3], $\delta d = 0.2$ Å [refer to the line profile below Fig. 1(a)] and $\delta E(x) = -50$ meV, the phase shift $\delta \Phi_B(x)$, as from A to D, is -27° . Namely, the strain could locally mediate surface chemical potential¹¹ and thus induce a 27° phase shift in a lateral distance of 2 nm.

Furthermore, the result that the FWHM exhibits maximum at the strip edge suggests the local strain suppresses the formation of QWSs. This is reasonable since the edge of strip is where is most uneven. It is important to note that the native electronic structures do not change with the temperature decreased from 80 to 4.6 K as the dI/dV - V spectra acquired at these temperatures are primarily identical, which further verifies the previous statement that the atomic up-down movement in the temperature range of 3.2–14.2 K is induced by elastic relaxation.

In conclusion, we present experimental evidence for the atomic scale strain in Sn islands on Si(111)-Sn($2\sqrt{3} \times 2\sqrt{3}$) $R30^\circ$ substrate. The overall modulated strip structure consisting in the distortion of surface structures and the periodic apparent height variation results from the strain relaxation in Sn islands. The position-dependent LUQWS indicates the effect of the strain relaxation on the electronic property.

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