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Origin of enhanced Ge interdiffusion at the initial stage of Ge deposition on Si(5 5 12)-2×1: Tensile stress induced by substrate chain structures

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ABSTRACT

By combined investigation of STM and synchrotron PES on Ge/Si(5 5 12)-2×1 at 530 °C, it has been found that, in addition to the upward-relaxed surface Si atoms, a subsurface Si atom is also readily replaced by an arriving Ge atom at the initial adsorption stage. Such enhanced interdiffusion is due to a unique character of one-dimensional chain structures of the reconstructed substrate, such as π-bonded and honeycomb chains not existing on other low-index Si surfaces such as Si(001)-*c*(4×2) and Si(111)-7×7, applying a tensile surface stress to the neighbouring subsurface atoms. Interdiffusion of Ge having lower surface energy induces adsorption of the displaced Si atoms on the surface to form sawtooth-like facets composed of (113)/(335) and (113)/(112) with arriving Ge atoms until the surface is filled with those facets. Such displacive adsorption is the origin of high Si concentration of formed facets.

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1. Introduction

Strain-induced self-assembled nanometre-scale structures such as Ge nanowires or Ge nanodots on Si substrates have attracted much research interest due to their interesting physical properties and potential applications in nanoscale optoelectronic devices [1]. Since Ge and Si are isoelectronic, they are completely miscible at any concentration in the identical diamond crystal structure [2]. In addition, due to their lattice mismatch of 4.2%, it is expected that a compressive surface stress is applied to Ge structures formed on Si substrates while a compensating tensile surface stress is applied to the Si substrate. Therefore, in such a Ge/Si system, stress relaxation and interdiffusion are closely related and crucial for controlled fabrication of Ge nanostructures on Si substrates.

Generally, Ge preferentially adsorbs on the surface, since the Ge dangling-bond energy is lower than that of Si [3,4]. However, it is expected theoretically that the tensile stress induced by reconstruction (and/or nanostructures) makes Ge atoms diffuse into the subsurface and even into the bulk [5]. So, evolution of crystallographic facets of strained Ge structures as well as Ge diffusion into the Si substrate sensitively depends on the kind of the substrate [6]. On the Si(001)-*c*(4×2) surface, deposited Ge atoms preferentially substitute the upward-relaxed Si atoms of dimers and then the downward-relaxed Si atoms of dimers; however, only a small number of Ge atoms diffuse into the subsurface (or the bulk) at submonolayer Ge coverage [3–5,7,8]. After forming a 3–4 monolayer (ML) wetting layer, with increasing Ge coverage, the initial shape of shallow pyramids with {105} facets evolves into that of steep domes with {105}, {113} and {15 3 23} facets [9]. The dome contains a Si-rich core covered by a Ge-rich shell [10]. On the Si(111)-7×7 surface, the Si adatoms are preferentially substituted by deposited Ge atoms [2], since an adatom pulls three surface atoms closer together, inducing a large tensile stress on the adatom [11].

On the other hand, on the Si(5 5 12)-2×1 surface, one of the stable high-index surfaces [12], only the structural evolution during Ge deposition was obtained by scanning tunnelling microscopy (STM) [13]. However, since Ge and Si are isoelectronic elements whose chemical compositions are not easily discerned by STM, it was difficult to find out which sites deposited Ge atoms occupy and how much they are diffused into the subsurface or the bulk. Therefore, in the present study, based upon the knowledge on the atomic structure of Si(5 5 12)-2×1, the synchrotron photoemission spectroscopy (PES) has been employed in order to get chemical information at each evolving stages. Especially, at the initial stage of submonolayer Ge coverage, it has been tried to identify the hierarchy of Ge substitution expecting that it might give an answer to the question: which is the determining factor of such reconstruction, the surface energy or the surface stress?

2. Experimental

The experiments were carried out under ultrahigh vacuum (UHV) at a base pressure of 2×10^{-10} Torr using a sample cut from a P-doped *n*-type

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Si(5 5 12) wafer. After outgassing the sample at 700 °C under UHV, the native oxide was removed through resistive flashing at 1170 °C. Then, the surface was reconstructed by cooling it slowly (~1 °C/s) from 900 °C to room temperature (RT). In the whole processes the pressure was kept less than 3.0×10^{-10} Torr. Ge atoms from an effusion cell were thermally evaporated on the reconstructed surface held at 530 °C at a rate of 0.1 ML/min, where one ML is defined as 6.8×10^{14} atoms/cm^2. When the substrate temperature was 480 °C, an ordered structure was not formed. Temperature was checked by optical pyrometers. Topographic STM images were obtained using constant current mode ($I_{\text{tunneling}}=0.5$ nA) at RT. Under the identical condition, the Si 2*p* and Ge 3*d* core levels were also obtained at the 7B1 bending magnet beam line of the Pohang Accelerator Laboratory (PAL) in Korea equipped with a PHOIBOS 150 hemispherical analyzer with charge-coupled device (CCD) detector made by SPECS [14]. All of the Si 2*p* (Ge 3*d*) raw data were analysed by a standard least-squares fitting procedure using Voigt functions with a Lorentzian width of 0.10 eV (0.12 eV) and a Gaussian width of 0.41 eV (0.40 eV) after subtracting the Shirley-type background. The branching ratio was 1/2 (2/3) and the spin-orbit splitting energy was 0.60 eV (0.59 eV) for Si 2*p* (Ge 3*d*).

3. Results and discussion

Based on the morphology changes of Ge/Si(5 5 12)-2×1 obtained by STM, the corresponding photoemission spectra were obtained from the reproduced surfaces.

3.1. Preferential adsorption and faceting of Ge/Si(5 5 12)-2×1: STM observation

From the upper-left area of Fig. 1(a) obtained after 0.15 ML of Ge deposition, the remaining area of the clean Si(5 5 12)-2×1 has been found. Its periodic unit along the [66$\bar{5}$] direction is composed of one (225) subunit and two kinds of (337) subunits [15]. Fig. 1(e) shows the side- and top-view atomic structural models of the clean Si(5 5 12)-2×1. The (225) subunit designated by a white bar in Fig. 1(a) is composed of a honeycomb (H) chain, a dimer-adatom (D-A) row and a tetramer (T) row. One (337) subunit designated by a grey bar is the T(337) subunit composed of a *π*-bonded (*π*) chain and a T row. The other (337) subunit designated by a black bar is the D(337) subunit composed of an H chain and a D-A row. Part of these D-A rows has additionally adsorbed species, i.e., addimers (ADs). As a result of charge transfer, the surface orbitals are rehybridized from sp^3 toward downward-relaxed (down) sp^2-like and upward-relaxed (up) s^2p^3-like configurations [16].

After depositing 0.15-ML Ge on Si(5 5 12)-2×1 at 530 °C, a new *π* chain grows along the row on the D-A sites of a (225) subunit as marked by a red arrow in Fig. 1(a). Such an observation is quite similar to indirect Si deposition at the initial stage of Sb adsorption on Si(5 5 12)-2×1 at 600 °C [17]. Due to this new chain, the original D(337), (225) and T(337) subunits have been converted to (225), T(337) and D(337) subunits. Such a subunit exchange provides a seed of nanofaceting [13]. Differently from homoepitaxy [18], the conversion from the T(337) subunit to a D(337) subunit advances the formation of the newly-grown *π* chain by ~3 nm along the [1$\bar{1}$0] direction as marked by a red dotted line. The conversion from T(337) to D(337) occurs under tensile stress induced by the newly-grown *π* chain [18]. In Fig. 1(a), such advanced conversion is due to an additional tensile stress induced by Ge atoms diffused into the sites under the (225) subunit of the clean surface, meaning that the new *π* chain is mixed with deposited Ge atoms and displaced Si atoms. During Ge deposition, Si atoms can be displaced from the surface as well as the subsurface and migrate to the D-A row in the (225) subunit.

Extended Ge deposition on Si(5 5 12)-2×1 at 530 °C induces 1D nanofacets grown from these *π*-chain seeds, as shown in Fig. 1(b) obtained from the 0.7-ML Ge-deposited Si(5 5 12)-2×1 surface. The lower-right corner shows the initial faceting stage, where the (113) facet is composed of alternating T and D-A rows and the (112) facet

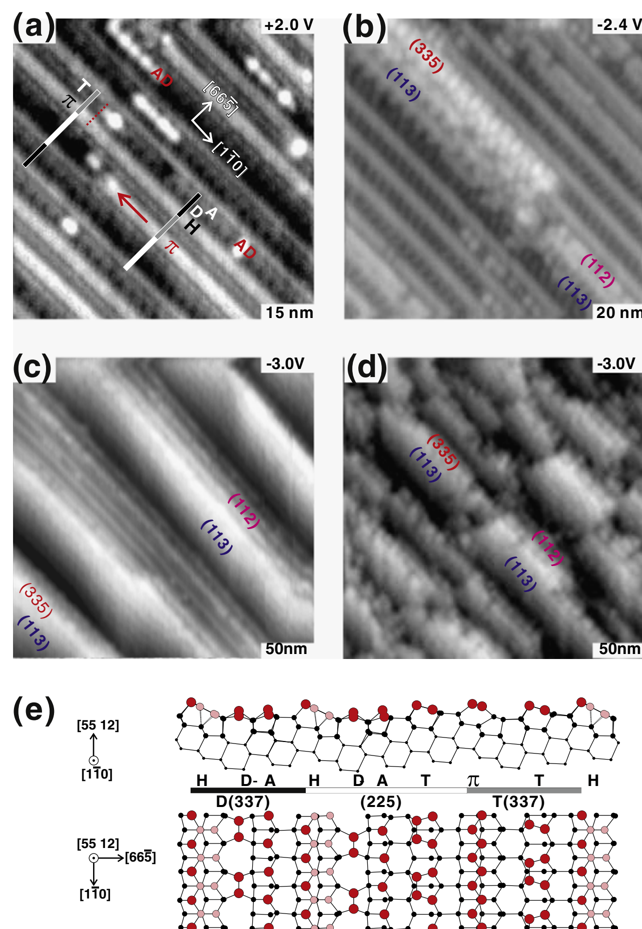

Fig. 1. Topographic STM images of nanostructures grown on Si(5 5 12)-2×1 at 530 °C by deposition of (a) 0.15-ML, (b) 0.7-ML, (c) 1.5-ML and (d) 3-ML Ge. In the upper-right (lower-right) corner of each image, the sample bias voltage (the scan size) is designated. (e) Side- and top-view structural models of the clean Si(5 5 12)-2×1 surface [15]. Letters H, *π*, D-A, T and AD, in (a) and (e), represent a honeycomb chain, a *π*-bonded chain, a dimer-adatom row, a tetramer row and an addimer, respectively.

is composed of *π* and H chains. At the next faceting stage appearing in the upper-left area in Fig. 1(b), the structures of the (113) and (112) facets are transformed to (113)-3×2 and (335)-5×1 facets. Such a (113)-3×2 structure is typical on the Si(113) surface at RT [19], while the pure Ge(113) surface has the structure mixed with 3×2 and 3×1 [20]. As shown in Fig. 1(c) obtained from the 1.5 ML Ge-deposited surface, such isolated sawtooth-like facets composed of (113)/(112) [or (113)/(335)] planes cover the whole Si(5 5 12) surface.

In Fig. 1(d), a filled-state STM image obtained from 3-ML Ge/Si(5 5 12)-2×1 at 530 °C, 1D nanostructures are broken irregularly along the [66$\bar{5}$] direction and lose 1D symmetry along the [1$\bar{1}$0] direction. Such a breaking lowers the surface stress along the [1$\bar{1}$0] direction caused by the 4.2% lattice mismatch between Ge and Si.

3.2. Synchrotron photoemission results of Ge/Si(5 5 12)-2×1

In Fig. 2, surface-sensitive Si 2*p* (Ge 3*d*) core-level spectra obtained at normal emission angle from Ge/Si(5 5 12)-2×1 using $h\nu=130$ eV ($h\nu=65$ eV) photons are shown in the left (right) panel. The corresponding fitting results are listed in Table 1.

In Fig. 2(a) obtained from the clean Si(5 5 12)-2×1, two major surface-related peaks, S1 and S2 and the bulk peak, B, can be decomposed. Surface core-level shifts (SCLSs) of S1 and S2 relative to the bulk

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