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Boronizing structures of Si(1 1 3) surfaces

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Abstract

With the help of scanning tunneling microscopy observations and first-principles calculations, we demonstrate that B preferential occupation at self-interstitial sites of Si(1 1 3) induces 3×1:B surfaces made up of adatoms and interstitial pentamers. The B atoms may serve as adatoms, while the interstitial pentamers may be boronized with different numbers of B atoms owing to the self-interstitial effects of B atoms. Our findings indicate that a Si(1 1 3) surface may be doped with B to an extremely high level.

Keywords: Scanning tunneling microscopy; Ion implantation methods; Auger electron spectroscopy; Surface relaxation and reconstruction; High index single crystal surfaces; Boron; Silicon

1. Introduction

Efforts to prepare epitaxial nanostructures on Si substrates have given rise to special interest in Si high-index surfaces because of their various anisotropies. As a high-index surface, Si(1 1 3) is very stable during high-temperature annealing and a good substrate for epitaxial growth [1]. Compared with Si(1 0 0), Si(1 1 3) is more favorable for growth of Ge nanowires [2] and preparation of ultra-thin oxide films [3]. As for its atomic structures, Si(1 1 3) is peculiar among Si substrates in that it may contain self-interstitial atoms at its subsurface so that special surface structures may be induced [4–6]. This structural property seems to be attributed to the special orientation of the (1 1 3) surface, since the self-interstitial features have been also observed on Ge(1 1 3) [7] and Ge/Si(1 1 3) [8] surfaces. Therefore, an understanding of the self-interstitial effects is of basic importance to investigations of any atomic behavior on all (1 1 3) surfaces.

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As the bulk-truncated (1 1 3) surface consists of alternating rows of atoms terminated like (1 0 0) and (1 1 1) surface atoms, a Si(1 1 3) surface may reconstruct with three types of blocks, namely, adatoms, tetramers, and interstitial pentamers [4–8]. At room temperature these blocks are arranged in a 3×2 periodicity on the surface, while at a certain high temperature each tetramer may incorporate an interstitial atom at the subsurface and the surface appears in a 3×1 periodicity of adatoms and interstitial pentamers [7,9]. It has been demonstrated that the additional self-interstitial atoms of the 3×1 reconstruction raise the surface energy because they induce additional tensile strain [7]. Therefore, the self-interstitial sites could be favorable for doped foreign atoms whose radius is smaller than Si.

Boron (B) has been one of most important dopants in Si device fabrication for several decades, and its peculiar behavior in Si crystal or at Si surfaces has attracted much attention [10–15]. Particularly, it has been revealed that B atoms have a covalent radius smaller than that of the Si substrate atoms and therefore prefer to be incorporated into the subsurface of Si(1 1 1) [13–15] or Si(1 0 0) [16,17]. This indicates that B might be a suitable candidate for self-interstitial doping, which we checked experimentally and theoretically. In this paper, we demonstrate that B doping at Si(1 1 3) surfaces can greatly lower the surface energy, leading to the 3×1:B reconstruction at room temperature, which is indeed stabilized by B atoms at self-interstitial sites.

2. Experimental

We performed B^+ ion implantation on Si(1 1 3) samples (phosphorus doped, $1 - 10\,\Omega$cm) at energy of 40 keV to 1×10^{16} atoms/cm^2, which gave rise to an amorphous layer of Si and B atoms on the substrates [18,19]. Post-implantation annealing of the samples was performed in an ultrahigh vacuum system at 700 °C for 2 h for sample degassing, and actual recrystallization of the amorphous layer was carried out through a process called solid phase epitaxy [20]. At this temperature, amorphous Si and B should be incorporated into the Si substrate to the limit of B solubility in the Si crystal, and the overplus of B would be segregated at the final surface. In order to prepare atomically flat surfaces for scanning tunneling microscopy (STM) observations, all samples were then annealed at 1200 °C for different times and then cooled down from 700 °C to room temperature at a rate of about 1 °C/s. Surface concentrations of B were checked by Auger electron spectroscopy (AES), which indicated that after the 700 °C annealing the B concentration already reached maximum while the 1200 °C annealing lowered the B concentration slowly. Using the Si(1 1 1)-$\sqrt{3} \times \sqrt{3}$:B surface as studied in Refs. [13–15], we found a B density close to 1/3 ML at the surface after an initial 1200 °C annealing of about 20 s. Using STM, we observed a series of 3×1 surfaces with various features and studied B effects on the surface structures.

3. Results and discussion

At the initial stage of the 1200 °C annealing, we were able to observe the main features of the 3×1 surface in filled-state STM images, as shown in Fig. 1. Bright spot-like protrusions like the one indicated by arrow P appeared pronounced. There are also dark spot-like protrusions, which can be seen in high-resolution images in Fig. 1a and b (arrow Q). The measured height difference between the two types of the protrusions is about 0.5 Å. Surrounded by the protrusions are ring-like clusters (arrow R). There were some protrusions missing, leaving vacancies, as indicated by arrow V, but hardly any vacancies were found in the ring-like clusters. By comparing the arrangement of all features with the surface lattice, we determined that the spot-like protrusions correspond to rebonded adatoms and the ring-like clusters to pentamer blocks, which are arranged in a 3×1 periodicity. From these images, it is clear that number density of bright adatoms increased at the expense of the dark ones. Other filled-state STM images of the sample further annealed at 1200 °C just displayed dominant bright 3×1 adatoms.

Compared with the filled-state STM images, in which adatom features were dominant, empty-