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Relationship between strain and electronic structure of Ge nanoislands on a Si(111)-7×7 surface

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Introduction

Germanium quantum dots formed on the Si substrate have been attracted for their potential applications as Si-based quantum electronic and photo electronic devices. In such a hetero-epitaxial system, a key phenomenon is the change in the electronic structure due to the strain caused by the lattice mismatch between Si and Ge. To control the property, it is very important to understand the relation between the strain and the electronic structure for the system, synthetically.

In this report, we show a relation between the electronic structure and the the relaxation structure of Ge nanoislands on a Si(111)-7×7 surface[1]. Since the relaxation structure depends on the size of Ge nanoislands, we fabricated the Ge nanoislands a uniform size on the Si(111) substrate and investigate the electronic structure by the angle resolved ultraviolet photoelectron spectroscopy (ARUPS).

Energy calculation

We also calculated electronic structure for the adatom on the Ge island. To simplify the calculation, we chose a cluster forming a T_4 site as shown in Fig. 1(a). In the calculation, we fixed the first-layer atoms at the ideal sites of the Si crystal to reproduce the situation on the Si substrate. The energies of the electronic states were calculated for a Si and a Ge cluster with an adatom at various heights in the range of 0.08–0.26 nm from the first layer. The energy calculations were performed based on the density functional method within the generalized gradient approximation using the Becke3LYP functional [2,3] and the 6-311G basis functions by Gaussian 03[4]. The relations between the height of the adatom and the energy of the DB state for the Si and Ge cluster are shown in Fig. 1(b).

For the whole adatom height range, the calculated electron density of the highest occupied molecular orbital (HOMO) was preferentially distributed around the adatom. Therefore, the HOMO state is the DB state at the adatom. The energy of the HOMO state decreases with the adatom height almost linearly at the rate of −9.4 eV/nm for the Si cluster and −8.2 eV/nm for the Ge cluster while their total energies reach their minimums at 0.185 nm for the Si and 0.193 nm for the Ge from the first layer, respectively.

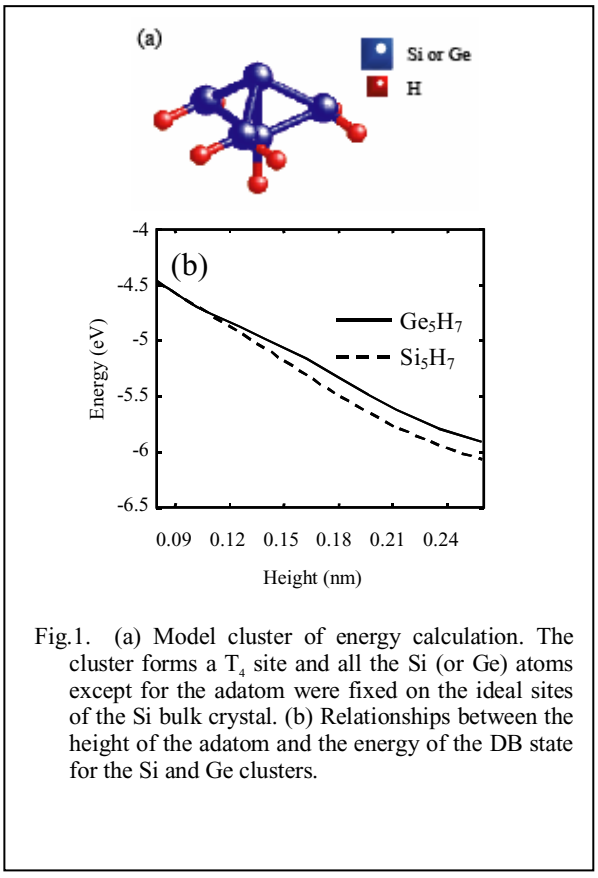

Fig.1. (a) Model cluster of energy calculation. The cluster forms a T_4 site and all the Si (or Ge) atoms except for the adatom were fixed on the ideal sites of the Si bulk crystal. (b) Relationships between the height of the adatom and the energy of the DB state for the Si and Ge clusters.

Experiment

The STM measurements were performed in an ultrahigh-vacuum STM chamber (base pressure: 2×10^{-8} Pa) equipped with reflection high-energy electron diffraction (RHEED) and an electron beam evaporation source. STM images were observed with an STM. The ARUPS measurements were performed by using synchrotron radiation on the beam line BL-7B. The experimental chamber, whose base pressure is about 6×10^{-8} Pa, is equipped with an angle-resolved photoelectron spectrometer, an evaporation source, a quartz crystal thickness monitor and a sample manipulator with a cryostat.