DFT study of the hole states charge density in Ge/Si structures

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1. Introduction

Recently, more and more attention has been paid to quantum computing, which has already proven effective in solving specialized problems, which cannot be produced by classical computing machines. Various systems are being studied to produce quantum dots used as qubits. Recent studies have shown that holes in semiconductors have a spin-orbit interaction, so not only the filled states of the conduction band, but also the vacant states of the valence band are promising for the implementation of spin qubits [2]. We pay special attention to structures based on germanium, which has the highest hole mobility at room temperature among all semiconductors. Among such systems the most promising are germanium nanowires (HW) produced on the surface of silicon (001) by molecular beam epitaxy, having a triangular cross-section with planes (105), bounded from above also by a silicon layer [3].

2. Model

Supercells representing an interface of alternating Si/Ge/Si layers, each of which contained the same number of atoms (in the ratio 1/3 : 1/3 : 1/3), were considered. Two types of interfaces were simulated, which correspond to the crystallographic planes (001) and (105), respectively. The latter, according to the experimental data [2], plays a key role in the formation of hole states. As a result of relaxation calculations the change in the volume of cell (001) was less than 1%, cell (105) - 25%, there was a significant compression (parameters are given in Table I, structures are shown in Figure 1).

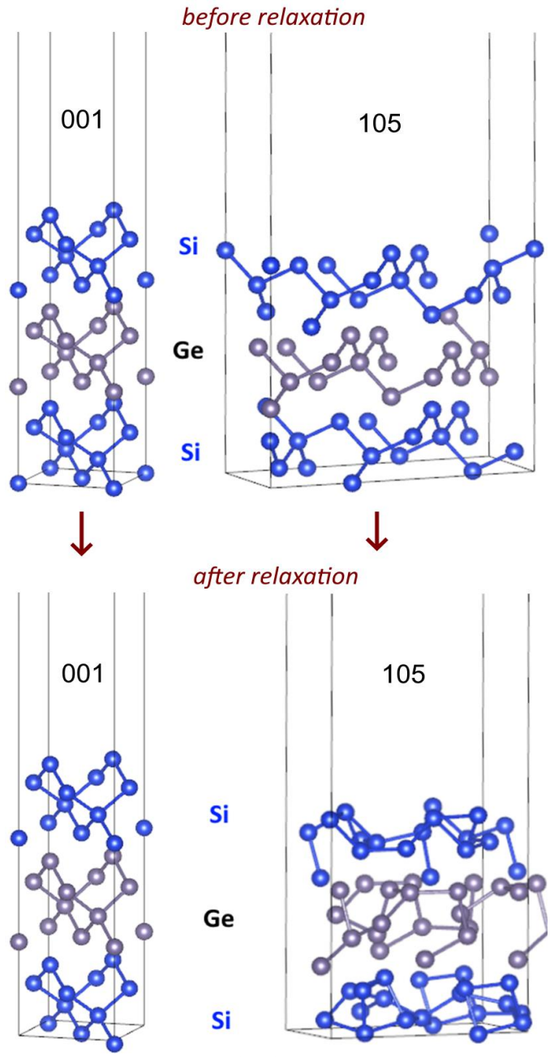

Fig. 1. *Structures of Si/Ge/Si supercells with vacuum in (001) and (105) planes before and after relaxation.*

3. Results and discussions

Hole states were simulated for the following interfaces: Si/Ge/Si (001) included 96 atoms placed in a cell with the 10.886 × 10.886 × 31.932 Å^3 volume and Si/Ge/Si (105) included 168 atoms in a cell with the 21.566 × 11.420 × 26.653 Å^3 volume. The electronic density in the structures was calculated by introducing an excess positive charge corresponding to the presence of one hole. The density of the neutral structure was then subtracted from the obtained distributions. During calculation of the Si/Ge/Si system electronic density, for the (001) plane model we used a special 4 × 4 × 1 k-points set, for the (105) plane model – 2 × 4 × 1 k-points set. Cut-off energy of plane waves was set to 680 eV in both cases

Charge density distribution of hole states in Si/Ge/Si, interfaces are shown in Figure 2. The analysis of the hole electron density distribution in the Ge layer showed that the hole formation probability for the Ge (105) orientation is at least one order of magnitude higher than for Ge (001).

The specific atomic energies of the structures were also determined, with values of -4.12 eV for Si/Ge/Si (001) interface and -4.08 eV for Si/Ge/Si (105) interface.

4. Conclusions

The proposed model agrees with the experimental data [4] and will make it possible to analyze the change in the distribution of hole states in the Ge/Si structure under the action of the applied electric field. It will also allow us to reveal the regularity of the magnetic moment change due to the presence of holes in Ge.

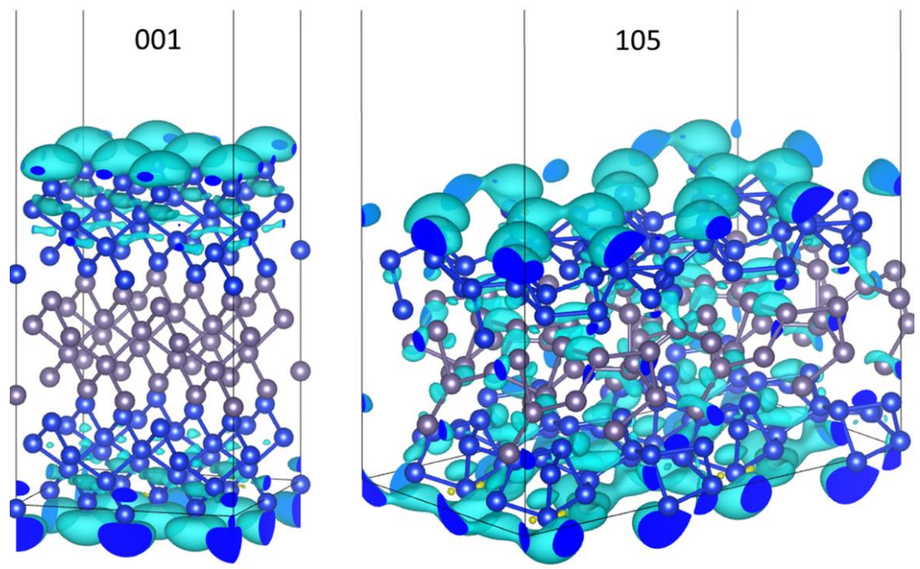

Fig. 2. *Charge density distribution of hole states in Si/Ge/Si (001) and (105) interfaces*

Table I. *Evolution of Si/Ge/Si structures parameters as a result of relaxation*

Structure	a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)
(001) before	5.431	5.431	31.93	90.0	90.0	90.0
(001) after	5.443	5.443	31.93	90.0	90.0	88.6
(105) before	14.499	5.687	26.65	90.0	90.0	90.0
(105) after	10.783	5.710	26.65	90.0	90.0	90.7

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