Structural Analysis of SiGeC Alloys by ab initio Total-Energy Calculations

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1. Introduction

SiGe alloys have been successfully applied to create heterojunction bipolar transistors (HBTs) [1-2] to open a new field in the Si-based device technologies, especially band gap engineering. However, epitaxial layers of SiGe grown on Si have unavoidable strain due to lattice mismatch, making the layer unstable with increasing thickness and Ge content.

To overcome this problem, SiGeC alloys have attracted much attentions because incorporation of C should reduce the lattice mismatch between SiGe and Si. Pseudomorphic SiGeC films have been grown on (100) Si substrates by several methods, such as chemical vapor deposition (CVD) [3] and molecular beam epitaxy (MBE) [4]. However, the incorporation of C has been typically limited up to 3% [5]. Furthermore, Kelires, in a recent work on Monte Carlo simulation of SiGeC alloys, reported that there is a strong repulsive interaction between Ge and C which leads to the absence of Ge-C bonds for low C fractions [6]. The reason is not clear and still opened for question. One can speculate that the large difference of ionic radii among these atoms is one of the origin of these phenomena.

In this study, we will estimate structural properties of SiGeC alloys by *ab initio* total-energy calculations and focus on the strain field around a C atom taking into account the atomic configurations.

2. Calculation method

The calculations are based on the density-functional method, including the conjugate gradient method and norm-conserving pseudopotential [7]. They were carried out with a cut off energy of 20 Ry in unit cells consisting of 32 atoms. For the calculation of stable structure of SiGe and SiGeC alloys, the atomic positions in the unit cell are relaxed until the calculated forces are smaller than 0.15 eV/Å.

3. Lattice constant of SiGeC alloys

First of all, the lattice constants of Si and Ge were estimated and we obtained the values of 5.40 Å and 5.62 Å, respectively. They are only 1 % smaller than the experimental values, 5.43 Å for Si and 5.66 Å for Ge, indicating the accuracy of our calculation. Then we calculated the lattice constant of SiGeC alloys.

The unit cell used for the calculation has 23 Si atoms, 8 Ge atoms and 1 C atom which corresponds to the alloy composition of $Si_{0.72}Ge_{0.25}C_{0.03}$. If Vegard's law applies, then the lattice constant of $Si_{0.72}Ge_{0.25}C_{0.03}$ should be equal to that of Si.

Figure 1 shows the dependence of the total energy on the volume of the unit cell. The results are then leastsquares-fitted to the empirical Murnaghan's equation of state which is indicated by the solid line in the figure. The calculated values show good agreement with the fitting. Thus the lattice constant is readily deduced from the fitted parameters in the equation and a calculated lattice constant of 5.39 Å was obtained. We also estimated the lattice constant with different atomic configurations, however, there was no difference in the values. The value is as same as the calculated lattice constant of Si (5.40 Å). It can be concluded from this result that Vegard's law is also valid in the SiGeC system whose C content is less than 3%.



Fig. 1 Dependence of the total energy on the volume of the unit cell.

4. Strain around the C atom

The most interest point in SiGeC system is the strain field around a C atom. Therefore, we calculated the total energy of $Si_{0.72}Ge_{0.25}C_{0.03}$ alloy by changing the number of Ge atoms around a C atom.

Figure 2 shows the dependence of the total energy on the number of Ge-C bond around a C atom. We carried out a few calculations with different atomic configurations and the final total energy showed some scattering. The error bar in the figure implies this scattering. The total energy increases with increasing the number of Ge-C bond. This result indicates that the most stable atomic configuration should be realized when the C atom is surrounded by four Si atoms instead of Ge atoms, which supports the prediction of a repulsive Ge-C interaction [6]. To clarify this point, we calculated Ge-C and Si-C bond length around a C atom and compared "ideal" bond length.



Fig. 2 Dependence of the total energy on the number of Ge-C bond around a C atom.

Table I summarizes the results. A virtual zincblende structure of SiC and GeC crystal was constructed for the calculation of "ideal" bond length and the lattice constant of the crystal was estimated by the same scheme for SiGeC alloys. The calculated "ideal" bond length of Si-C and Ge-C were 1.91 Å and 1.99 Å, respectively. We adopted these values as a reference and compared with those in SiGeC alloys. The third column in the table shows this distortion of the bond length. It is noticeable that the bond length around the C atom is lengthened in SiGeC alloys. Since the ionic radius of C atom is smaller than that of Si and Ge atom, the atom neighboring the C atom moves inward and relaxes the strain. However, the atom bonded with the C atom can't fully relax in SiGeC system because the atom is also bonded with other atoms, that is, the atom is in the SiGeC matrix. Furthermore, it is found from the table that the distortion of Ge-C bond length is larger than that of Si-C bond. The ionic radius of Ge atom is larger than that of Si, thus it is speculated that Ge atom can't easily move in SiGeC alloy compared with Si atom. Therefore, stain fields would be accumulated around the Ge-C bond, resulting in the increase of total energy with increasing the number of Ge-C bond. It is one of the cause of a repulsive Ge-C interaction predicted by Kelires [6].

Table I. Si-C and Ge-C bond length and its deviation from the "ideal" value in the SiGeC system.

5. Conclusions

We estimates structural properties of SiGeC alloys by *ab initio* total-energy calculations. It is found from the calculation that Vegard's law is valid in the SiGeC system whose C content is less than 3%. Furthermore, we calculate the total energy by varying the number of Ge-C bond around a C atom and find that the energy increases with increasing the number of Ge-C bond. One of the model of this phenomena is proposed by the hypothesis based on the difference of the bond-length distortion between Ge-C bond and Si-C bond in SiGeC alloys.

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