First principles calculations on local strains of SiGe alloys

R. Taniguchi*, Y. Yamamoto, S. R. Nishitani, and I. Yonenaga[1)]
Department of Information, Kwansei Gakuin University, Gakuen 2-1, Sanda, 669-1337 Japan. (email:tcqh74129@kwansei.ac.jp)
[1)] *Institute for Materials Research, Tohoku University, Katahira 2-1-1, Aoba-ku Sendai, 980-8577 Japan.*

Silicon germanium (SiGe) is one of the most important semiconductors, due to the starting materials or substrates of the strained silicon, whose transistors switch 35% faster than the normal Si. SiGe is a complete solid solution alloy with the cubic diamond structure. The electronic and thermodynamical properties are strongly affected by the 4.2% difference in the lattice constants of the constituents Ge and Si. Thus, the accurate knowledge of the atomistic bonding structure with the local strain relaxation is essential and crucial to clarify the origins of such properties and to utilize the device potential of SiGe.

In this paper, we have investigated the composition dependency of the atomistic bonding structure by the ab-initio electronic structure calculations. Six different models of SiGe lattice structures have been calculated under the internal and external relaxations of the local coordinations with the constrained outer shapes. The energies, lattice and volume changes and bond length differences have been investigated in detail.

The bond lengths for different types of neighbor atom pairs (Ge- Ge, Si-Ge and Si-Si bond) are different on each Si composition, and show the linear dependency as shown in Fig.1. The result is good agreement with the experimental investigations of extended X-ray absorption fine structure (XAFS)[(1)] in bulk SiGe alloy crystals in the entire composition range. The model of 25% Si, however, shows the large deviation from the linear dependency. The origin of this deviation is investigated from the local coordination environment.

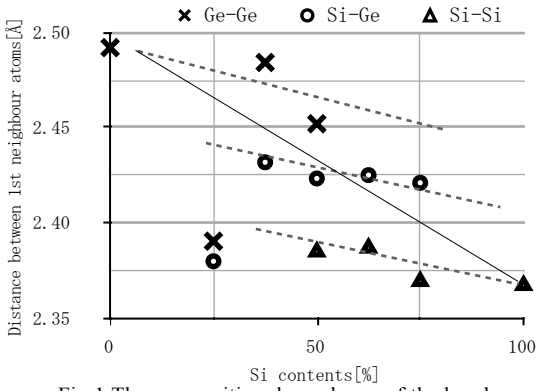

Fig.1 The composition dependency of the bond lengths for different types of neighbor atom pairs (Ge- Ge, Si-Ge and Si-Si bond)

Reference :
(1) I. Yonenaga, M. Sakurai, M. H. F. Sluiter, Y. Kawazoe, and S. Muto, "Atomic structure and strain relaxation in Czochralski-grown Si_xGe_{1-x} bulk alloys," Journal of Materials Science, **16** (2005), pp.429-432.