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Local strains in SiGe alloys for the strained silicon

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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 bond lengths for different types of neighbor atom pairs (Ge-Ge, Ge-Si and Si-Si bond) by the ab-initio electronic structure calculations for the comparison with the experimental investigations of extended X-ray absorption fine structure(XAFS)[1] in bulk SiGe alloy crystals in the entire composition range. Four different models of SiGe lattice structures [2] have been calculated under the full relaxation 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 most stable energies on the different Ge compositions show the dependency as shown in Fig.1. The energies of three models are located on the average of the constituent pure lattices. The local bond lengths for different types of neighbor atom pairs shows the similar dependency. The model of 75% Ge, however, shows the large deviation from the linear dependency of energy. The origin of this deviation is investigated from the local coordination environment.

References:

[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.

[2] Marcel H. F. Sluiter, and Yoshiyuki Kawazoe, "Bond lengths and phase stability of silicon-germanium alloys under pressure," Materials Trans., **42** No.11, (2001), pp.2201-2205.

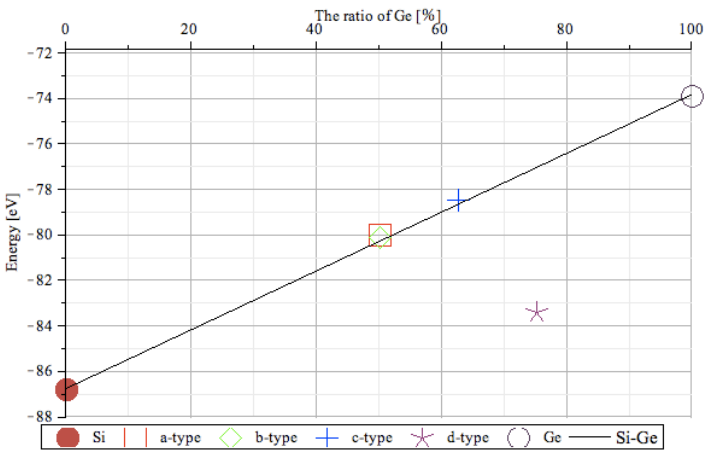

Fig.1 Total energy dependency on Ge composition.