First principles calculations of the copper silicide precipitates

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Very recently, the authors have reported the experimental observation of the precipitates of Cu_3Si in a heavily copper doped Si. In this research, the energetic assessment of this precipitation behavior has been investigated by the first principles calculations.

We adopted two atomistic structure models of Cu_3Si based on the Zintl phases [1]; one is a bcc based structure ($D0_3$ type), and the other is a fcc based structure ($L1_2$ type). The reported stable intermetallic structure of Cu_7Si_2 (the η phase) is also calculated. The energy calculations with the outer and inner relaxes of atomistic structures are performed by the VASP(Vienna Ab-initio Simulation Package) code.

Figure 1 shows that two Cu_3Si phases are both more stable than the segregation limit of pure Cu and Si. Although the experimentally observed precipitates show the very close structure with the $D0_3$ model, the $L1_2$ model is more stable than the $D0_3$ model. Both models of Cu_3Si show no band gap, which indicates that the phases are conductor.

The other phase of Cu_7Si_2 is also more stable than the segregation limit. The tie line between pure Cu and Cu_7Si_2 drawn by the dashed line indicates that the $D0_3$ model is metastable to Cu + Cu_7Si_2, and the $L1_2$ model is most stable. Because the $D0_3$ model shows the good lattice coherency with pure Si, it would appear as the structure of the precipitates.

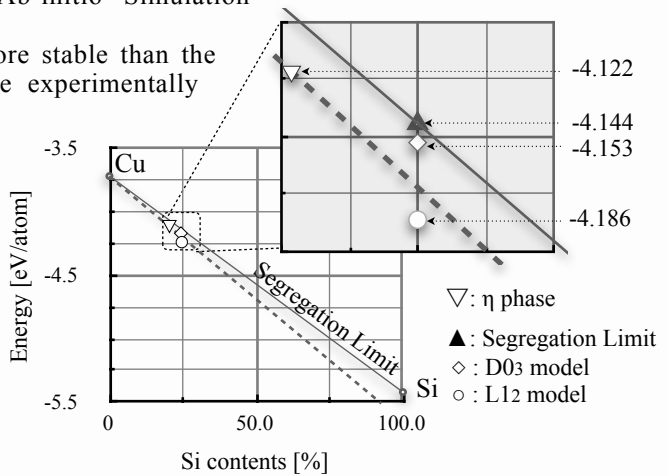

Fig.1 Energy composition diagram of Cu-Si system.

Reference :
[1] N. E. Christensen., PHYSICAL REVIEW., **32** No.1, (1985), pp.209-210.