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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.

Figure 1 shows two atomistic structure models of Cu_3Si based on the Zintl phases [1]; one is the $D0_3$ type structure called 'twisted', and the other is arranged on the position of Si sites called 'parallel'. The reported stable intermetallic structure of Cu_7Si_2 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 2 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 Cu_3Si twisted model, the parallel Cu_3Si is more stable than the twisted one. The outer shape of the parallel model, however, is very irregular, and its c-axis is 41.2% larger than the a-axis. 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 twisted model of Cu_3Si is metastable to Cu + Cu_7Si_2, and the parallel model of Cu_3Si is most stable. Because the twisted Cu_3Si shows cubic shape and the good lattice coherency with Si, it would appear as the structure of the precipitates.

[1] N. E. Christensen, Phys. Rev. B, 32 No.1, (1985), pp.209-228.

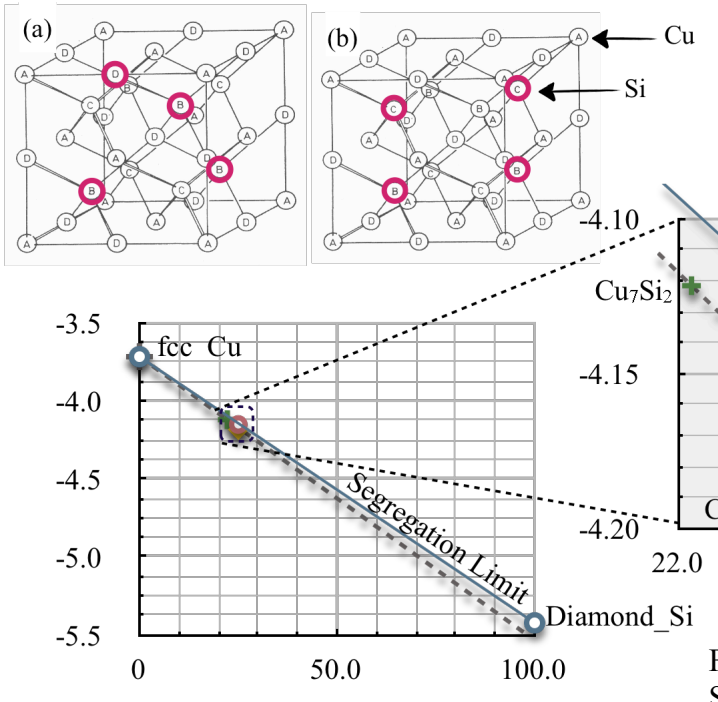

Fig.1 (a) twisted and (b) parallel atomistic structure models of Cu_3Si.

Fig.2 Energy composition diagram of Cu-Si system.