Application of Continuous Displacement Treatment of Cluster Variation Method to Phase Transformation of Materials

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Cluster Variation Method (CVM) has been very successful in the computations of alloy phase diagrams as well as in many problems of the materials science related to the phase transitions. Originally, CVM was developed in the framework of the so-called rigid lattice approximation, but it has recently been extended to include continuous atomic displacements due to thermal lattice vibration and local atomic distortion due to size mismatch of the constituent atoms. In the present study, we focus our attention on the latter continuous displacement treatment of CVM. The continuous displacement (CD) formulation of the CVM is applied to study the phase stability of the binary alloys. The basic idea is to treat an atom which is displaced by r from its reference lattice point as a species designated by r. The effects of continuous atomic displacement on the thermodynamic quantities of binary alloy systems are investigated in detail using the tetrahedron cluster approximation. We also discuss the extension of the continuous displacement treatment of CVM to the calculations of liquid phases in conjunction with the gas-liquid phase transitions.