Reciprocal-Space Methods for the Statistical Thermodynamics of Alloys with Atomic Size-Mismatch

Volodymyr Bugaev
Max-Planck-Institut für Metallforschung, Stuttgart
vbugaev@mail.ru

A statistical-thermodynamic successive corrections technique will be presented for calculations of the Fourier components of atomic short-range-order (SRO) parameters and thermodynamic potential for binary alloy. The lattice distortions caused by the atomic size-mismatch are considered by means of the lattice statics method taking into account the statistical coupling between local lattice displacements and atomic SRO. As an example, the diffuse scattering of the system $Cu_{83}Mn_{17}$ is described in detail using only a few physical (energy and force) parameters. The resulting diffuse scattering intensity is non-analytic at q=0 due to the strains caused by atomic size-mismatch. Inverse Monte Carlo data on the real-space atomic interaction energy parameters can not be used to describe this non-analyticity.