STRUCTURAL AND THERMODYNAMIC PROPERTIES OF QUATERNARY SEMICONDUCTOR ALLOYS

Abstract

by

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The local structural properties of quaternary semiconductor alloys of the type $A_{1-x}B_xC_{1-y}D_y$ where the cations (A,B) occupy one face centered cubic sublattice and the anions (C,D) occupy the other sublattice are determined by minimizing the strain energy of the system using the conjugate gradient method. Among four systems considered, $Ga_{1-x}In_xP_{1-y}Sb_y$ has the highest strain energy. Four different types of bonds, AC, AD, BC, and BD exist in the quaternary alloy $A_{1-x}B_xC_{1-y}D_y$. The bond lengths calculated tend to preserve their bond lengths in the binary compounds in agreement with the EXAFS results. Also the thermodynamic properties of quaternary alloys are studied using the Monte Carlo method. In alloys with the lattice mismatch, there is strain energy in addition to the chemical bonding energy. The numerical simulation becomes computationally intense because the effects of strain are long ranged. The phase separation directions of two alloys $Ga_{1-x}In_xP_{1-y}As_y$ and $Zn_{1-x}Cd_xSe_{1-y}Te_y$ are determined. While the relative number of bonds AC and BC in the ternary $A_{1-x}B_xC$ is simply 1-x and x, the relative number of bonds in the quaternary alloy $A_{1-x}B_xC_{1-y}D_y$ has to be determined by minimizing the free energy
of the system. The deviation of the relative number of bonds from that in the random alloy is also calculated and the degree of deviation is represented by a single short range ordering parameter $\Delta$. 