Direct enumeration of alloy configurations for semiconductor electronic structure properties

Sirichok Jungthawan, Sukit Limpijumnong

School of Physics, Suranaree University of Technology
Nakhon Ratchasima, Thailand

Peter A. Graf, Kwiseon Kim, Wesley B. Jones

National Renewable Energy Laboratory
Golden, CO, U.S.A.

Gus L. W. Hart

Department of Physics and Astronomy, Northern Arizona University
Flagstaff, AZ, U.S.A.

We present an approach to directly enumerating electronic structure properties of all possible zincblende-based alloy configurations whose unit cell contains up to a specified number of atoms. This method allows us to map the space of bandgaps and effective masses versus alloy composition and atomic configuration. We demonstrate for GaInP alloys that a large range of bandgaps and masses are available for a given composition. By decomposing the space of the possible atomic configurations into categories based on superlattice structure, we can identify trends in bandgap extrema. For example, bandgap maxima typically occur in [0 h k] superlattices where h is not equal to k, and minima typically occur in [1 1 1] superlattices. The configurations with large bandgap reduction have special ordering in that all the minority atoms are ordered in one plane. We focus on dilute GaInP and AlGaAs alloys where the minority composition is below 10 percent. The empirical pseudopotential method (EPM) and folded spectrum method (FSM) are used to solve the single particle Schrödinger equation. The results from the EPM are compared with first-principle calculations.