Computer Simulation Study of the Strained Layer Superlattices by Tight-Binding Molecular Dynamics

Kinichi Masuda-Jindo[1] and Ryoichi Kikuchi[2]
[1]Tokyo Institute of Technology
Department of Materials Science and Engineering
Nagatuta 4259, Midori-ku
Yokohama 226-8503
Japan

[2]University of California
Materials Science and Mineral Engineering
Berkeley
Berkeley, CA 94720-1760

Recently, there has been great interest in the hetroepitaxial growth of highly mismatched semiconductor systems. However, there are certain serious problems concerning the heteroepitaxial growth; e.g., high density of generated dislocations and residual stresses. It is the purpose of the present study to investigate atomistic and thermodynamic properties of semiconductor heterostructures by using the density functional tight-binding and path probability methods in the statistical mechanics. The atomic diffusion in the semiconductor interface is investigated via vacancy mechanism of diffusion using the non-equilibrium irreversible statistical mechanical approach, path probability method (PPM). The effective pair interaction energies between the constituent atoms are derived by using the zero poles method takig into account the misfit strains at the interface. We study the atomistic properties of strain induced dislocations, both 60and 90types, in medium and highly mismatched semiconductor heterostructures like InGaAs/GaAs, GaAs/Si and InP/Si, and GeSi/Si systems. For InP/Si system, we also investigate the effects of GaAs buffer layer on residual stress and defect density. We estimate the critical layer thickness both for the generation of the 60 and 90type misfit dislocations and also calculate the electronic structures of the misfit dislocations in relation to the optical properties of the semiconductor heterostructures.