

Effect of Anharmonicity of Interatomic Potential on Strain Distribution in Semiconductor Nanostructures

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Experiments and theory have shown that the energy spectrum of nanostructures is extremely sensitive to the built-in strain. Knowledge of the strain distribution is therefore of utmost importance for the design of optical devices with prescribed light emission spectrum. The widely used Valence-Force-Field (VFF) model developed by Keating and later Martin relies on a parabolic expansion of the inter-atomic potential. However, for the lattice mismatches present in Ge/Si and InAs/GaAs heterostructures (4% of the equilibrium bond length in Ge/Si and 7% in InAs/GaAs), which are materials widely used in the design of optical and electronic devices, anharmonic terms are expected to play an important role.

We have developed a simple extension of the Martin-Keating two-parameter VFF model to take into account anharmonicity in the inter-atomic potential. VFF constants also determine the phonon frequencies in the crystal. We have chosen a set of anharmonicity parameters by fitting the experimental strain dependence of the phonon spectra (expressed in terms of a set of Grueneisen parameters) in GaAs, InAs, Si, and Ge. We have found that anharmonic corrections reduce the computed hydrostatic compressive strain in quantum dots by up to 20%. To further test the impact of our model, the electronic eigen-energies of an InAs/GaAs QD array have been computed within an empirical spds* tight binding approximation, where the Hamiltonian matrix elements are dependent on the atomic positions. The modification of the strain distribution due to anharmonicity results in a shift of the lowest quantized states by up to 45 meV in the conductance band and up to 30 meV in the valence band. A valuable advantage of our simple model is that the computational cost is nearly unchanged.

This work was performed while one of the authors (OLL) held a National Research Council Research Associateship Award at the Jet Propulsion Laboratory.

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