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An atomistic model for the simulation of acoustic phonons, strain distribution, and Grüneisen coefficients in zinc-blende semiconductors

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Abstract

An accurate modeling of phonons, strain distributions, and Grüneisen coefficients is essential for the qualitative and quantitative design of modern nanoelectronic and nanooptoelectronic devices. The challenge is the development of a model that fits within an atomistic representation of the overall crystal yet remains computationally tractable. A simple model for introducing the anharmonicity of the interatomic potential into the Keating two-parameter valence-force-field model is developed. The new method is used for the calculation of acoustic phonon and strain effects in zinc-blende semiconductors. The model is fitted to the Grüneisen coefficients for long-wavelength acoustic phonons and reproduces the response to strain throughout the Brillouin zone in reasonable agreement with experiment.

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InAs/GaAs semiconductor heterostructures are the bases for many modern devices in nanoelectronics and optoelectronics. The large 7% lattice mismatch between GaAs and InAs makes it necessary to take into account the built-in strain in such structures, especially for the tailoring of the light emission spectrum in optical devices. Simple, easy-to-use continuum models are not able to explain many novel properties of nanostructures, since

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they do not resolve interface, disorder, and strain on an atomistic scale. The broader availability of computational power makes it possible to use atomistic-level models for the simulation of nanostructure properties without the use of supercomputing facilities.

To find the equilibrium strain distribution the total strain energy in the structure should be minimized. The most widely used atomistic-level model for the calculation of the strain energy in the harmonic approximation is the two-parameter valence-force-field (VFF) Keating model [1], later modified by Martin [2, 3]. However, this model is not able to adequately describe some strain effects; in particular it cannot reproduce the correct strain dependence of the phonon frequencies. The corresponding Grüneisen parameters have both the wrong magnitude and sign. To obtain those values correctly, Cerdeira et al. [4] introduced anharmonicity into the Keating model through strain dependent VFF constants. This model was designed to fit the optical branches of the phonon dispersion. However, to adequately describe the strain distribution the model should be fitted to the long-wavelength low-energy acoustic phonons, which represent the deformation waves appropriate for the spatial nanostructure scale. Since acoustic phonons are responsible for thermal conductivity in semiconductors, the proper description of lattice vibrations in the presence of strain is crucial for the modeling of heat removal from the active region of the device. Therefore a good description of Grüneisen coefficients, describing the shift of phonon modes as a function of strain, and their dependence upon strain is especially important.

Here the effect of anharmonicity is included into the interatomic potential within the Keating model as a step toward the accurate calculation of acoustic phonon dispersions and equilibrium atomic positions in III–V semiconductor nanostructures. The weakening of the interatomic potential with increasing interatomic separation is directly introduced into the Keating model in terms of the distance dependent VFF constants α and β [4]. We propose the following ansatz:

$$\alpha_{mn} = \alpha_0^{mn} \left[1 - A_{mn} \frac{(r_{mn}^2 - d_{mn}^2)}{d_{mn}^2} \right], \quad (1)$$

$$\beta_{mnk} = \beta_0^{nmk} \left[1 - B_{nmk} (\cos \theta^{nmk} - \cos \theta_0^{nmk}) \right] \\ \times \left[1 - C_{nmk} \frac{(r_{mn}r_{mk} - d_{mn}d_{mk})}{d_{mn}d_{mk}} \right], \quad (2)$$

where the constants $\beta_0^{nmk} \equiv \sqrt{\beta_0^{mn}\beta_0^{mk}}$, $B_{nmk} \equiv \sqrt{B_{mn}B_{mk}}$, and $C_{nmk} \equiv \sqrt{C_{mn}C_{mk}}$. The index m denotes an atom in the crystal, and its neighbors are denoted as n and k . r_{mn} is the distance between the m th atom and its n th neighbor; d_{mn} is the unstrained distance. θ^{nmk} and θ_0^{nmk} are the actual and the unstrained angles between mn and mk bonds, respectively. In homogeneous monatomic and binary compounds, all bonds are the same and the indices m , n , and k can be dropped. The anharmonicity correction coefficients A and C describe the dependence of bond-stretching and bond-bending forces on hydrostatic strain, while B is responsible for the change of the bond-bending term with the angle between bonds.

In the limit of a small deformation ($\mathbf{r} \simeq \mathbf{d}$) Eqs. (1) and (2) approach the corresponding expressions in [4]. However, here we use a multiplicative form of the strain dependence of β rather than the additive one, used in [4], where the emphasis was on the investigation of

Table 1

Grüneisen parameters for GaAs and InAs computed within the two-parameter Keating model (K) and including anharmonicity corrections (A) in comparison with experimental values from [6]. The relative error δ in per cent is shown where applicable. “F” indicates failure to reproduce the sign of the Grüneisen coefficient

	γ_K^{GaAs}	δ (%)	γ_A^{GaAs}	δ (%)	$\gamma_{\text{exp}}^{\text{GaAs}}$	γ_K^{InAs}	δ (%)	γ_A^{InAs}	δ (%)	$\gamma_{\text{exp}}^{\text{InAs}}$
γ_{TA}^Γ	-1.6591	F	0.5280	-0.5	0.531	-2.0610	F	0.1435	2.5	0.14
γ_{LA}^Γ	-0.9937	F	1.3031	0.008	1.303	-1.0264	F	1.3902	0.7	1.4
γ_{TA}^X	-1.4147	-13	0.7237	F	-1.62	-1.8484		0.3182		
γ_{LA}^X	-0.6576		1.6618			-0.6963		1.7569		
γ_{TO}^Γ	-0.6560	F	1.6965	88	0.9	-0.6992	F	1.7886	110	0.85
	-0.6560	F	1.6965	22	1.39					
γ_{LO}^Γ	-0.6560	F	1.6965	38	1.23	-0.6992		1.7886		
γ_{TO}^X	-0.5698	F	1.8344	6	1.73	-0.5862		1.9560		
γ_{LO}^X	-0.6563		1.6618			-0.6998		1.7527		

the shift of optical phonon energies with small deformations of bulk material. In contrast, we are interested in determining the strain distribution in semiconductor nanostructures. We therefore need to ensure the convergence of the minimization of the strain energy by truncating the VFF constants at large deformations, which is much easier for a two-parameter function when it is represented as a product of two simple one-parameter factors. Also, in contrast to [4], we have not assumed that $A = C$.

The valence-force-field constants α_0 and β_0 in *unstrained* materials are taken from [5]. The “shear deformation” anharmonicity corrections $B^{\text{GaAs}} = 7.62$ and $B^{\text{InAs}} = 4.78$ were found directly from the experimental shear deformation parameter [4], which describes the shift of the optical phonon energy in bulk crystal due to shear deformation. The choice of the “hydrostatic” anharmonicity parameters $A^{\text{GaAs}} = 7.2$, $A^{\text{InAs}} = 7.61$ and $C^{\text{GaAs}} = 6.4$, $C^{\text{InAs}} = 6.45$ was made by fitting to the experimental values [6] for the LA and the TA Grüneisen coefficients $\gamma_i = -(V/\omega_i) d\omega_i/dV$ near the center of the Brillouin zone. They describe the dependence of the frequency ω_i of the i th mode of lattice vibrations on the change of volume V . Note that the standard Keating model indeed fails to reproduce the correct sign for the Grüneisen coefficients. Our improved model fits the Γ acoustic phonons very well and reproduces the correct sign for almost all (known) coefficients (see Table 1).

Due to the anharmonicity of the interatomic potential, the Grüneisen coefficients depend on the strain itself. This effect was predicted theoretically by Soma et al. [7] for Ge and Si within the continuum approximation using a higher-order perturbation formalism and the Heine–Abarenkov model pseudopotential. Fig. 1 shows our model’s prediction for the dependence of the Grüneisen coefficients in the [100] crystallographic direction for long-wavelength acoustic phonons on the change of the volume due to hydrostatic strain for GaAs and InAs. The positive sign of the coefficients corresponds to a decrease of the sound velocity with hydrostatic expansion. The Grüneisen coefficients of the TA modes change sign at compressions of about 0.9617 (GaAs) and 0.9923 (InAs). The trend obtained within

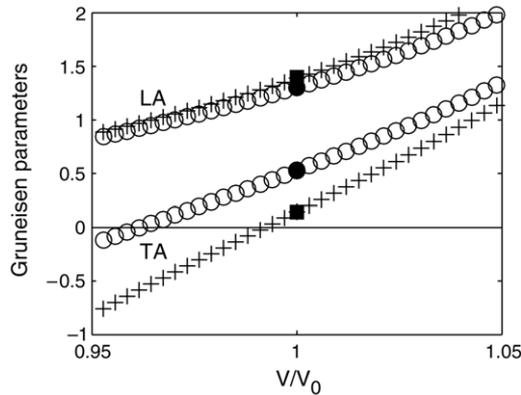


Fig. 1. Grüneisen parameters for acoustic modes near the center of the Brillouin zone in the [100] crystallographic direction as a function of hydrostatic strain. Open circles and crosses correspond to calculations within our model for GaAs and InAs, respectively. Filled circles and filled squares show the corresponding experimental values [6] used for fitting.

our atomistic model qualitatively agrees with that found by Soma et al. [7] within the continuum approximation for Ge and Si. We quote this as an additional indirect proof of the validity of our model.

In conclusion we have developed a simple model to introduce the anharmonicity of the interatomic potential into the two-parameter Keating valence-force-field model for the calculation of the acoustic phonon dispersion and strain effects in zinc-blende semiconductors. The model predicts the correct trend for the strain dependence of the Grüneisen coefficients and enables the simulation of the built-in strain distribution and lattice vibrations in nanostructures, which is essential for the design of many modern devices in nanoelectronics and optoelectronics.

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