

Parameters for temperature dependence of mean-square displacements for B-, Bi- and Tl-containing binary III–V compounds

Marco Schowalter,^{a*} Andreas Rosenauer^a and Kerstin Volz^b

^aInstitut für Festkörperphysik, Universität Bremen, Otto-Hahn-Allee 1, 28359 Bremen, Germany, and ^bMaterials Science Centre and Faculty of Physics, Philipps Universität Marburg, Hans-Meerwein-Strasse, 35032 Marburg, Germany. Correspondence e-mail: schowalter@ifp.uni-bremen.de

Mean-square displacements were computed within the harmonic approximation from *ab initio* force constants for binary B-, Tl- and Bi-containing III–V compounds in sphalerite crystal structures in the temperature range from 0 to 1000 K in steps of 1 K. An Einstein model with a temperature-dependent characteristic frequency was used to model the temperature dependence of the mean-square displacements. A Gaussian was fitted to the temperature dependence of the characteristic frequency and parameters of the Gaussian are given. Phonon dispersion relations and densities of states derived during the computation of the mean-square displacements are also shown.

1. Introduction

In recent publications (Schowalter *et al.*, 2009 a,b) we have reported on the computation of mean-square displacements (MSDs) of various binary group II–VI, III–V and group IV semiconductors in sphalerite and wurtzite crystal structures. In these studies we restricted our work to semiconductors of technological importance. Hence, we computed MSDs for binary III–V semiconductors consisting of all possible combinations of group III and group V elements, besides B, Tl and Bi. Realizing that B-, Bi- and Tl-containing compounds are also considered for application in devices and that MSDs of these compounds are also required for (scanning) transmission electron microscopy [(S)TEM] image simulations, these data are computed in the present paper.

For example, (TlInGa)P quaternary material lattice-matched to InP was first successfully grown by Asahi *et al.* (1996). They suggested that this material may have application as a light emitter in the wavelength range from 0.9 to 10 μm . The material exhibits a temperature-independent band gap and therefore could be a candidate for laser diodes for wavelength division multiplexing optical fibre communication (Asahi *et al.*, 1996). An only slightly temperature-dependent band gap corresponding to approximately 1.3 μm was found for (TlGa)P/GaAs by Fushida *et al.* (1997). TIP, TIAs and TISb as well as the corresponding In-containing ternary compounds (InTl)P, (InTl)As and (InTl)Sb were grown by Antonell *et al.* (1998). The respective As- and Sb-containing materials can be crystallized in the sphalerite or CsCl crystal structures, respectively, whereas P-based compounds could not be synthesized by this group. Problems with incorporation of Tl in (TlGa)As (maximum 5% Tl) and (InTl)P as well as

(InGaTl)As on InP were reported by Lubyshev *et al.* (1998) and Wei *et al.* (1999), which could be connected to miscibility gaps reported for nearly all Tl-containing compounds (Chen & Piao, 2000). Most promising in this respect seemed to be InTIAs, which can be mixed up to 16% Tl content (Chen & Piao, 2000).

As for Bi-containing compounds, it was shown by Huang *et al.* (1994) that the band gap of In(AsSb) can be lowered to about 80 meV at 77 K by the addition of about 1.5% of Bi, suggesting a giant band-gap bowing due to the addition of small amounts of Bi (Zhang *et al.*, 2005), which appeared to be slightly smaller than in the dilute N systems (Yoshimoto *et al.*, 2006). This was also shown later for Ga(AsBi) by Young *et al.* (2007), for (InGa)(AsBi)/InP by Feng *et al.* (2006) and for (InGa)(NBi)/GaAs by Wei *et al.* (2004). Furthermore, a giant bowing of the spin–orbit splitting energy was found by Fluegel *et al.* (2006) resulting in the suppression of one Auger loss mechanism. The temperature dependence of the band gap is, as for the Tl-containing materials, expected to be very low (Oe, 2002). This makes dilute bismide-based III–V lasers interesting for high-temperature operation.

Boron-containing III–V materials are discussed for laser as well as solar cell applications. First of all, for Si-based dilute Ga(NAsP) laser structures, tensilely strained B-containing (BGa)(AsP) barrier and separate confinement layers are used for strain compensation as well as for current injection (Liebich *et al.*, 2011; Kunert *et al.*, 2008, 2011). Furthermore, B-containing III–V semiconductors are discussed as 1 eV or 1.7 eV band-gap material for quadruple junction solar cells on Ge substrates as well as for tandem solar cells on Si substrates, respectively (Geisz *et al.*, 2001). For both applications mainly the strain compensating action of B, which has a small covalent

Table 1

Table of lattice parameters of materials with the sphalerite crystal structure computed within the LDA and the GGA using *WIEN2k* and *VASP*.

For comparison, values found in the literature are given in the last column. It is also indicated whether the respective values were obtained by an experiment (EXP) or a DFT calculation using the LDA or the GGA.

Material	<i>Wien2k</i>		<i>VASP</i>		Literature value
	a_{LDA}	a_{GGA}	a_{LDA}	a_{GGA}	
BBi	5.419	5.529	5.413	5.528	5.529 (GGA) (Ferhat & Zaoui, 2006 <i>b</i>)
AlBi	6.306	6.438	6.299	6.435	6.46 (GGA) (Ferhat & Zaoui, 2006 <i>b</i>)
GaBi	6.260	6.450	6.262	6.446	6.33 (EXP) (Tixier <i>et al.</i> , 2003)
InBi	6.639	6.845	6.651	6.841	
TlBi	6.763	6.992	6.771	6.997	
TlSb	6.565	6.782	6.582	6.792	
TlAs	6.161	6.352	6.172	6.360	6.382 (GGA) (Ferhat & Zaoui, 2006 <i>a</i>)
TlP	5.976	6.138	5.959	6.120	6.124 (GGA) (Ferhat & Zaoui, 2006 <i>a</i>)
TlN	5.141	5.277	5.140	5.272	4.74 (EXP) (Zaoui, 2003)
BN	3.584	3.629	3.574	3.620	3.615 (EXP) (Wentorf, 1957)
BP	4.495	4.556	4.480	4.541	4.538 (EXP) (Perri <i>et al.</i> , 1958)
BA _s	4.736	4.816	4.725	4.804	4.777 (EXP) (Perri <i>et al.</i> , 1958)
BS _b	5.180	5.279	5.178	5.267	5.12 (LDA) (Ferhat <i>et al.</i> , 1998)

radius, is used, as B has only a very low influence on the band gap (Hossain *et al.*, 2011).

MSDs are important parameters in image simulations for the composition analysis from high-angle annular dark-field (HAADF) STEM images (Grillo *et al.*, 2008; Rosenauer *et al.*, 2009). The accuracy of the measured compositions depends on the accuracy of the values of the MSDs used in the simulations. In this article we present our results on the computations of MSDs for III–V compounds containing B, Tl and Bi in the sphalerite crystal structure. In §2 we briefly review how MSDs were computed and give parameters used within the computations. Values for MSDs for selected temperatures are presented in §3. An Einstein model with a temperature-dependent characteristic frequency has been used to fit the temperature dependence of the MSDs. Fit parameters are also listed in §3. Phonon dispersion relations and phonon density of states of the materials have been computed during the derivation of the MSDs and are depicted in Figs. 1–12.¹

2. Computation of mean-square displacements

For the computation of MSDs we use the direct method (Parlinski *et al.*, 1997). In this method, a series of supercells are generated and an inequivalent atom is displaced in each of the supercells in an inequivalent direction. Then forces due to the displacements on all atoms in the supercell are computed. From the forces and the modulus of the displacements force-constant matrices are derived that are transformed to dynamical matrices by Fourier transformation.

In order to take into account polarization effects [*i.e.* the LO–TO (longitudinal optical–transversal optical) phonon splitting at the Γ point] within the polar semiconductors, an additional non-analytical part is added to the dynamical matrix (Born & Huang, 1954). The non-analytical part

depends on the Born effective charge tensor and the dielectric matrix. Since in cubic material systems the three crystal basis vectors are symmetrically equivalent, the Born effective charge tensor and the dielectric matrix can be expressed as a scalar multiplied by the identity matrix. Therefore, the non-analytical part of the dynamical matrix is also diagonal and can be written as

$$D^{\text{NA}}(\mu, \nu; \mathbf{k}) = \frac{Z(\mu)Z(\nu)k^2}{\varepsilon_0\varepsilon_\infty\Omega_0(M_\mu M_\nu)^{1/2}}, \quad (1)$$

where μ and ν run over the atoms, $Z(\mu)$ and M_μ are the Born effective charge and the mass of atom μ , respectively, and ε_0 , ε_∞ and Ω_0 are the dielectric constant, the dielectric function at infinity frequency and the volume of the unit cell, respectively.

The phonon frequencies $\omega(\mathbf{k})$ and phonon polarization vectors are derived by diagonalization of the dynamical matrices. The phonon dispersion relation or generalized phonon density of states are then obtained from phonon frequencies and respective polarization vectors for certain \mathbf{k} vectors. MSDs $\langle u^2(\nu; T) \rangle$ for atom ν as a function of temperature T are derived from the generalized phonon density of states $g_\nu(\omega)$ by

$$\langle u^2(\nu; T) \rangle = \frac{\hbar}{2m_\nu} \int_0^\infty \frac{g_\nu(\omega)}{\omega} \coth\left(\frac{\hbar\omega}{2k_B T}\right) d\omega, \quad (2)$$

with \hbar being Planck's constant divided by 2π , k_B is Boltzmann's constant and m_ν is the mass of atom ν . A more detailed derivation of equation (2) can be found in Schowalter *et al.* (2009*a*).

3. Results

Forces are computed within the *WIEN2k* code (Blaha *et al.*, 2001). In this code, space is divided into spheres around the atom positions with radius R_{MT} and the interstitial region. Within the spheres atomic-like functions are used as basis functions, whereas in the interstitial region plane waves are used. The plane-wave cutoff is chosen such that $R_{\text{MT}}K_{\text{max}} = 7.0$ and 100 k points were used within the full Brillouin zone of the $2 \times 2 \times 2$ supercells. The supercells were generated starting from crystallographic unit cells having lattice parameters that have been found within the *WIEN2k* code. For that, the energy was computed for a series of crystallographic unit cells with different unit-cell sizes. The lattice parameters of the materials were found by fitting Murnaghan's equation of state to computed energies as a function of unit-cell volume. In Table 1 (columns 2–3) we list the derived lattice parameters computed within the local density approximation (LDA) (Ceperley & Alder, 1980) as well as in the generalized

¹ Figs. 1–12 are available from the IUCr electronic archives (Reference: TD5005). Services for accessing these data are described at the back of the journal.

Table 2

Born effective charges Z^* of the group III elements for $k = 0$ and macroscopic dielectric constants ϵ_∞ for materials with the sphalerite crystal structure.

Computations of ϵ_∞ for GaBi, InBi, TlSb and TIAs did not converge due to the fact that they appeared to be metallic in our calculations. ϵ_∞ is divergent for metals.

Material	Z^*		ϵ_∞	
	LDA	GGA	LDA	GGA
BBi	-1.27	-1.06	16.0	23.2
AlBi	1.81	1.86	19.7	23.3
GaBi	1.75	1.94		
InBi	2.43	2.64		
TlSb	2.92	2.99		
TIAs	3.35	3.71		
TlP	3.24	3.49	28.1†	30.6†
TlN	4.30	4.21	35.4†	36.2†
BN	1.87	1.91	4.5	4.6
BP	-0.64	-0.46	9.1	9.1
BAAs	-0.56	-0.39	9.6	10.1
BSb	-1.34	-1.22	10.9	11.4

† TIP and TIN according to our calculations are semiconductors with a very tiny (<0.1 eV) band gap and therefore also converged very slowly. For these materials $\Re\{\epsilon(0)\}$ was taken instead.

gradient approximation (GGA) (Perdew *et al.*, 1996). It is commonly known that the LDA is overbinding and therefore leads to underestimated lattice parameters, whereas the GGA is underbinding and therefore leads to overestimated lattice parameters.

For comparison, values found in the literature are given in the last column. It is also indicated whether the respective values were obtained by an experiment (EXP) or a density functional theory (DFT) calculation using the LDA or the GGA. The presented values fit quite nicely to the values from the literature with the exception of TIN, where our values lie significantly above the values of Zaoui (2003). However, the lattice parameter of Zaoui for TIN (4.74 Å) lies in between the experimental values for InN (5.042 Å) and GaN (4.5 Å), whereas our value (5.2 Å) follows the trend that the lattice parameter increases as the atomic number of the group III element increases.

In order to take into account the splitting of LO and TO phonon frequencies close to the Γ point, a non-analytical term can be added to the dynamical matrix. For this Born effective charges (BECs) $Z^*(\nu)$ and the macroscopic dielectric constant ϵ_∞ are required (Schowalter *et al.*, 2009a). BECs and dielectric constants were computed within density functional perturbation theory as implemented (Gajdos *et al.*, 2006) in the *Vienna Ab Initio Simulation Program (VASP)* (Kresse & Furthmüller, 1996). Using lattice parameters computed within *VASP* (given in columns 4–5 in Table 1) BECs and the macroscopic dielectric constant were computed within the LDA and the GGA, respectively. The results are shown in Table 2. Computations of macroscopic dielectric constants ϵ_∞ for GaBi, InBi, TlSb and TIAs did not converge with respect to the number of k points due to the fact that these materials appeared to be metallic in the sphalerite crystal structure according to our calculations (ϵ_∞ diverges for metals and

Table 3

MSDs in Å² computed within the LDA at selected temperatures.

Material	Element	0.005 K	100 K	300 K	600 K	900 K
BN	B	1.94e-03	1.96e-03	2.21e-03	3.06e-03	4.13e-03
	N	1.61e-03	1.63e-03	1.89e-03	2.68e-03	3.65e-03
AlBi	Al	3.26e-03	6.54e-03	1.64e-02	3.21e-02	4.80e-02
	Bi	1.48e-03	4.98e-03	1.45e-02	2.88e-02	4.32e-02
BAAs	B	2.74e-03	2.97e-03	4.24e-03	6.92e-03	9.89e-03
	As	1.12e-03	1.41e-03	3.04e-03	5.81e-03	8.64e-03
BBi	B	3.31e-03	4.05e-03	6.79e-03	1.19e-02	1.74e-02
	Bi	8.92e-04	1.86e-03	5.10e-03	1.01e-02	1.51e-02
BP	B	2.62e-03	2.74e-03	3.68e-03	5.84e-03	8.27e-03
	P	1.58e-03	1.71e-03	2.81e-03	5.03e-03	7.37e-03
BSb	B	3.04e-03	3.48e-03	5.39e-03	9.16e-03	1.32e-02
	Sb	1.02e-03	1.59e-03	3.97e-03	7.77e-03	1.16e-02
GaBi	Ga	2.40e-03	6.86e-03	1.92e-02	3.81e-02	5.70e-02
	Bi	1.50e-03	5.57e-03	1.62e-02	3.23e-02	4.85e-02
InBi	In	2.33e-03	9.71e-03	2.82e-02	5.63e-02	8.44e-02
	Bi	1.71e-03	7.95e-03	2.33e-02	4.66e-02	6.99e-02
TIAs	Tl	1.84e-03	7.95e-03	2.33e-02	4.66e-02	6.99e-02
	As	2.09e-03	6.34e-03	1.77e-02	3.52e-02	5.27e-02
TlN	Tl	1.09e-03	2.61e-03	7.33e-03	1.46e-02	2.18e-02
	N	2.99e-03	3.95e-03	7.29e-03	1.33e-02	1.95e-02
TlP	Tl	1.60e-03	5.57e-03	1.62e-02	3.23e-02	4.85e-02
	P	2.60e-03	5.13e-03	1.27e-02	2.47e-02	3.69e-02
TlSb	Tl	2.04e-03	1.07e-02	3.15e-02	6.28e-02	9.42e-02
	Sb	1.98e-03	8.37e-03	2.43e-02	4.84e-02	7.25e-02

Table 4

MSDs in Å² computed within the GGA at selected temperatures.

Material	Element	0.005 K	100 K	300 K	600 K	900 K
BN	B	2.00e-03	2.02e-03	2.31e-03	3.21e-03	4.35e-03
	N	1.65e-03	1.68e-03	1.95e-03	2.79e-03	3.81e-03
AlBi	Al	3.40e-03	6.96e-03	1.76e-02	3.45e-02	5.16e-02
	Bi	1.52e-03	5.26e-03	1.53e-02	3.05e-02	4.57e-02
BAAs	B	2.85e-03	3.09e-03	4.44e-03	7.30e-03	1.05e-02
	As	1.15e-03	1.46e-03	3.16e-03	6.07e-03	9.03e-03
BBi	B	3.55e-03	4.38e-03	7.48e-03	1.33e-02	1.94e-02
	Bi	9.32e-04	2.02e-03	5.58e-03	1.11e-02	1.66e-02
BP	B	2.70e-03	2.82e-03	3.80e-03	6.06e-03	8.60e-03
	P	1.60e-03	1.74e-03	2.87e-03	5.15e-03	7.54e-03
BSb	B	3.16e-03	3.61e-03	5.65e-03	9.68e-03	1.40e-02
	Sb	1.05e-03	1.65e-03	4.14e-03	8.11e-03	1.21e-02
GaBi	Ga	2.60e-03	7.73e-03	2.17e-02	4.32e-02	6.47e-02
	Bi	1.58e-03	6.09e-03	1.78e-02	3.55e-02	5.32e-02
InBi	In	2.49e-03	1.07e-02	3.13e-02	6.25e-02	9.37e-02
	Bi	1.78e-03	8.51e-03	2.50e-02	5.00e-02	7.49e-02
TIAs	Tl	1.93e-03	8.60e-03	2.53e-02	5.05e-02	7.57e-02
	As	2.19e-03	6.63e-03	1.86e-02	3.69e-02	5.53e-02
TlN	Tl	1.15e-03	2.84e-03	8.00e-03	1.59e-02	2.38e-02
	N	3.19e-03	4.16e-03	7.66e-03	1.40e-02	2.06e-02
TlP	Tl	1.66e-03	5.93e-03	1.73e-02	3.45e-02	5.17e-02
	P	2.74e-03	5.33e-03	1.32e-02	2.57e-02	3.84e-02
TlSb	Tl	2.09e-03	1.07e-02	3.16e-02	6.31e-02	9.46e-02
	Sb	2.04e-03	8.25e-03	2.39e-02	4.77e-02	7.15e-02

therefore the LO–TO phonon splitting will be zero). TIP and TIN exhibit very small (<0.1 eV) band gaps and therefore the computation was also difficult to converge. For these materials we used the following technique: we computed the real part of the frequency-dependent dielectric function $\epsilon(\omega)$. $\Re\{\epsilon(0)\}$ can be approximated by ϵ_∞ according to Gajdos *et al.* (2006). We checked that for BN in the LDA: we got $\Re\{\epsilon(0)\} = 4.6$ and $\epsilon_\infty = 4.5$. Both values agree within the convergence with respect to the number of bands (100), number of k points [$16 \times 16 \times 16$ Monkhorst–Pack grid (Monkhorst & Pack, 1976)] and the

Table 5

Table of parameters A , B and σ of the Gaussian describing the temperature dependence of the characteristic frequency for computations within the LDA (parameters are given in Hz, Hz and K, respectively).

Material	Element	A	B	σ
BN	B	1.467717e+14	1.324178e+14	2.526991e+02
	N	1.371529e+14	1.235466e+14	2.365031e+02
AlBi	Al	3.614082e+13	2.408509e+13	4.439379e+01
	Bi	1.026777e+13	9.108768e+12	2.103261e+01
BAs	B	1.070945e+14	8.546188e+13	1.486077e+02
	As	3.774802e+13	3.411766e+13	6.997375e+01
BBi	B	8.867670e+13	6.385159e+13	1.026586e+02
	Bi	1.704233e+13	1.539339e+13	3.162126e+01
BP	B	1.119407e+14	9.382721e+13	1.755874e+02
	P	6.486315e+13	5.783204e+13	1.190842e+02
BSb	B	9.648295e+13	7.343069e+13	1.229865e+02
	Sb	2.552331e+13	2.304549e+13	4.736935e+01
GaBi	Ga	1.899643e+13	1.372894e+13	2.909575e+01
	Bi	1.011272e+13	8.595942e+12	2.078585e+01
InBi	In	1.188625e+13	8.788692e+12	1.998516e+01
	Bi	8.902331e+12	7.160114e+12	1.721351e+01
TlAs	Tl	8.460070e+12	7.240114e+12	1.836347e+01
	As	2.032722e+13	1.377235e+13	2.804594e+01
TiN	Ti	1.429506e+13	1.296287e+13	2.932818e+01
	N	7.581964e+13	5.274753e+13	8.631213e+01
TiP	Ti	9.710197e+12	8.694132e+12	2.122464e+01
	P	3.940553e+13	2.564470e+13	4.594784e+01
TiSb	Ti	7.612909e+12	6.235259e+12	1.554100e+01
	Sb	1.314125e+13	9.208657e+12	1.996929e+01

Table 6

Table of parameters A , B and σ of the Gaussian describing the temperature dependence of the characteristic frequency for computations within the GGA (parameters are given in Hz, Hz and K, respectively).

Material	Element	A	B	σ
BN	B	1.425278e+13	1.325423e+14	2.534653e+02
	N	1.350219e+13	1.236731e+14	2.372797e+02
AlBi	Al	3.458991e+13	2.322878e+13	4.267901e+01
	Bi	1.001993e+13	8.854952e+12	1.994927e+01
BAs	B	1.032368e+14	8.297777e+13	1.441663e+02
	As	3.690987e+13	3.337495e+13	6.811860e+01
BBi	B	8.274162e+13	6.031009e+13	9.700560e+01
	Bi	1.630137e+13	1.471567e+13	3.000549e+01
BP	B	1.088490e+14	9.190769e+13	1.715502e+02
	P	6.400386e+13	5.714859e+13	1.169089e+02
BSb	B	9.308999e+13	7.132592e+13	1.196533e+02
	Sb	2.493103e+13	2.255158e+13	4.625588e+01
GaBi	Ga	1.751027e+13	1.288291e+13	2.737245e+01
	Bi	9.600904e+12	8.208464e+12	1.972531e+01
InBi	In	1.110756e+13	8.342946e+12	1.905768e+01
	Bi	8.528503e+12	6.915025e+12	1.658485e+01
TlAs	Tl	8.047052e+12	6.957975e+12	1.758195e+01
	As	1.935831e+13	1.344951e+13	2.712059e+01
TiN	Ti	1.352907e+13	1.239935e+13	2.822190e+01
	N	7.102059e+13	5.130764e+13	8.367263e+01
TiP	Ti	9.341648e+12	8.419029e+12	2.042467e+01
	P	3.738966e+13	2.512906e+13	4.469119e+01
TiSb	Ti	7.444484e+12	6.223054e+12	1.548464e+01
	Sb	1.278037e+13	9.276636e+12	1.993282e+01

number of frequency intervals to sample the density of states (2000). Values for TiP and TiN (indicated by † in Table 2) are therefore derived from $\Re\{\epsilon(0)\}$.

For the numerical derivation of the phonon density of states, phonon frequencies have been computed for about

400 000 k points and grouped into bins of width 0.05 THz using the *PHONON* software of Parlinski *et al.* (1997). Computed phonon dispersion relations as well as phonon densities of states are depicted in Figs. 1–12. This was sufficient to converge the MSDs to three digits, which have been computed using equation (2). MSDs at selected temperatures computed within the LDA and the GGA are given in Tables 3 and 4, respectively.

Comparing the values in these tables shows that the MSDs computed within the LDA are slightly smaller than those computed within the GGA. This can be attributed to the tendency of the LDA to overbind and the GGA to underbind (Vila *et al.*, 2007). This can also be observed for the lattice parameters shown in Table 1, for which it is more commonly known.

In order to provide MSDs at an arbitrary temperature, we fitted the MSDs as a function of temperature using the following scheme: we transform equation (2) using the mean-value theorem into an equation with a temperature-dependent characteristic frequency:

$$\langle u^2(v, T) \rangle = \frac{\hbar}{2M_v} \frac{\coth[\hbar\omega_c(v; T)/2k_B T]}{\omega_c(v, T)}. \quad (3)$$

This allows us to transform the temperature-dependent MSDs to temperature-dependent characteristic frequencies. Then a Gaussian,

$$\omega_c(v; T) = A_v \exp(-T^2/\sigma_v^2) + B_v, \quad (4)$$

is fitted to the temperature dependence of the characteristic frequency (Schowalter *et al.*, 2009a). The parameters A , B and σ for the LDA and the GGA are given in Tables 5 and 6, respectively. MSDs can then easily be derived by

$$\langle u^2(v, T) \rangle = \frac{\hbar}{2M_v} \frac{\coth\{\hbar[A_v \exp(-T^2/\sigma_v^2) + B_v]/2k_B T\}}{[A_v \exp(-T^2/\sigma_v^2) + B_v]}. \quad (5)$$

Note that the presented parameterization is optimized for the calculation of MSDs and not of the characteristic frequency.

We finish with a short note on definitions of Debye parameters and Debye–Waller factors, which can be important for applications of the presented data. The relation between the Debye parameters $B(v, T)$ and MSDs $\langle u^2(v, T) \rangle$ follows from the definition of the Debye–Waller factor. For the case of a definition such as $\exp[-(1/4)B(v; T)g^2]$

$$B(v; T) = 8\pi^2 \langle u^2(v; T) \rangle, \quad (6)$$

with a definition of $|g| = 1/d$, where d is the respective lattice plane distance in real space. For a definition of $|g| = 2\pi/d$ we would get

$$B(v; T) = 2\langle u^2(v; T) \rangle. \quad (7)$$

4. Summary

In summary, we have computed the temperature dependence of the MSDs of B-, Bi- and Tl-containing III–V compounds with the sphalerite crystal structure. The temperature dependence of the MSDs was fitted using the solution for an

Einstein model with a temperature-dependent characteristic frequency fitted using Gaussians. The parameters of the Gaussians for the derivation of MSDs at any temperature are tabulated and phonon dispersion relations as well as densities of states are shown in the supplementary material.

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