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Debye-Waller Factor for Zinc-Blende-Type Crystals

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The Debye-Waller factors have been calculated for a number of zinc-blende-type crystals from the eigenfrequencies and eigenvectors of the phonon states as obtained from the modified-rigid-ion model of lattice dynamics. On the average the contribution from the acoustic-phonon states to the mean-square displacements of the constituent atoms was found to be more significant than that from the optical-phonon states. However, the relative optical-phonon-state contribution was found to be more significant in the lighter atom, and in fact in some cases at low temperatures, it was found to exceed the acoustic-phonon-state contribution. In all the cases studied, the mean-square displacements of the lighter atom were found to be larger. Lindeman's criterion for melting was tested by evaluating the ratio of the sum of the root-mean-square displacements of the constituent atoms to the nearest-neighbor distance. This ratio is approximately constant for the zinc-blende compounds. However, the average ratio for the II-VI compounds was found to be slightly larger than that for the III-V compounds. The calculated results are discussed in relation to available experimental data.

I. INTRODUCTION

The intensity of the scattered radiation from a crystal is observed to be temperature dependent and varies exponentially from its value at absolute zero. This temperature-dependent exponential factor is known as the Debye-Waller factor and is related to the mean-square displacements of the constituent atoms in the crystal.

Previous calculations of the Debye-Waller factor based on theoretical lattice-dynamical models have been primarily limited to crystals of the NaCl structure,[1-8] cubic metals,[9-13] rare-gas solids,[14] and a few crystals of the CsCl structure.[15] These calculations were motivated in part by the availability of experimental data and reliable lattice-dynamical models, especially in the case of the NaCl-type crystals and the cubic metals. A few experimental determinations of the Debye-Waller factor for zinc-blende crystals exist[16-22] in the literature, but, to date, no comprehensive calculation of this factor based on a consistent lattice-dynamical model has appeared.

The reliability of some of the available experimental measurements on the Debye-Waller factor for zinc-blende crystals is in fact questionable. In some of the previous experimental work no explicit correction to the x-ray Debye-Waller factor measurements due to thermal diffuse scattering intensity was made. The contribution due to this correction was indeed shown[1,23] to have a significant effect on the experimental results in some alkali-halide crystals. Furthermore, the existing experimental data are rather sparse and available only for a rather limited range of temperatures, and in some cases contradictory.[16,17] In view of the aforementioned points, a more reliable technique to obtain the Debye-Waller factor might be from the use of the eigenfrequencies and corresponding eigenvectors as calculated from a lattice-dynamical model. This, in fact, has been the procedure utilized in previous calculations on alkali halides, cubic metals, and rare-gas solids.

The purpose of this paper is to utilize the eigenfrequencies and eigenvectors of the phonon states as obtained by a lattice-dynamical model, found suitable for the zinc-blende-type crystals, in calculating the Debye-Waller factor for these crystals. The lattice-dynamical model used in this analysis is the modified-rigid-ion (MRI) model.[24] This model does not require extensive data on phonon dispersion, such as neutron scattering data for the determination of model parameters, but only the three elastic constants c_{11}, c_{12}, and c_{44} and the two long-wavelength optical-mode phonon frequencies ω_{LO} and ω_{TO} as input data. This model has yielded[24,25] reasonable agreement between calculated and experimental phonon dispersion for SiC and ZnS. The applicability of the MRI model to zinc-blende crystals has also been discussed[26] in terms of an invariance relation between the elastic constants and the long-wavelength optical mode phonon frequencies. The model has also predicted[27] reasonable agreement between the calculated and experimentally determined coefficient of thermal expansion for ZnTe. Recently, the model has been incorporated into the framework of a Green's-function technique to predict[28] the local-mode behavior in a large class of zinc-blende compounds with success. The present model has, however, cer-

TABLE I. Calculated mean-square displacements (in 10^{-16} cm^2) for various III–V zinc-blende compounds.

Compound	Temperature (°K)	Acoustic[a] $\langle u^2\rangle_A$	$\langle u^2\rangle_B$	Optical[a] $\langle u^2\rangle_A$	$\langle u^2\rangle_B$	Total[a] $\langle u^2\rangle_A$	$\langle u^2\rangle_B$
GaP	10	0.0039	0.0024	0.0004	0.0036	0.0043	0.0060
	30	0.0040	0.0025	0.0004	0.0036	0.0044	0.0061
	50	0.0042	0.0027	0.0004	0.0036	0.0046	0.0063
	70	0.0047	0.0031	0.0004	0.0036	0.0051	0.0067
	100	0.0056	0.0038	0.0004	0.0036	0.0060	0.0074
	150	0.0074	0.0051	0.0004	0.0038	0.0078	0.0089
	200	0.0093	0.0066	0.0004	0.0041	0.0097	0.0107
	250	0.0113	0.0080	0.0005	0.0045	0.0118	0.0125
	300	0.0134	0.0096	0.0005	0.0050	0.0139	0.0146
	600	0.0261	0.0187	0.0009	0.0086	0.0270	0.0273
GaAs	10	0.0029	0.0031	0.0015	0.0012	0.0044	0.0043
	30	0.0030	0.0033	0.0015	0.0012	0.0046	0.0044
	50	0.0034	0.0037	0.0015	0.0012	0.0050	0.0049
	70	0.0040	0.0043	0.0015	0.0012	0.0056	0.0055
	100	0.0050	0.0053	0.0016	0.0012	0.0066	0.0065
	150	0.0069	0.0073	0.0018	0.0014	0.0088	0.0087
	200	0.0090	0.0094	0.0021	0.0016	0.0111	0.0110
	250	0.0110	0.0116	0.0024	0.0018	0.0135	0.0134
	300	0.0131	0.0138	0.0028	0.0021	0.0159	0.0159
	600	0.0259	0.0272	0.0051	0.0038	0.0310	0.0310
	1511	0.0650	0.0682	0.0126	0.0093	0.0775	0.0775
GaSb	10	0.0024	0.0033	0.0024	0.0005	0.0048	0.0038
	30	0.0027	0.0036	0.0024	0.0005	0.0051	0.0041
	50	0.0033	0.0043	0.0024	0.0005	0.0057	0.0048
	70	0.0041	0.0053	0.0024	0.0005	0.0065	0.0058
	100	0.0054	0.0068	0.0026	0.0005	0.0080	0.0073
	150	0.0078	0.0097	0.0030	0.0006	0.0108	0.0103
	200	0.0101	0.0126	0.0036	0.0007	0.0137	0.0133
	250	0.0126	0.0156	0.0042	0.0008	0.0168	0.0164
	300	0.0150	0.0186	0.0049	0.0010	0.0199	0.0196
	600	0.0298	0.0369	0.0092	0.0018	0.0390	0.0397
	979	0.0486	0.0601	0.0147	0.0292	0.0633	0.0630
InP	10	0.0038	0.0022	0.0002	0.0044	0.0040	0.0067
	30	0.0040	0.0025	0.0002	0.0044	0.0042	0.0069
	50	0.0047	0.0030	0.0002	0.0044	0.0048	0.0074
	70	0.0055	0.0036	0.0002	0.0045	0.0057	0.0081
	100	0.0070	0.0048	0.0002	0.0045	0.0072	0.0093
	150	0.0099	0.0068	0.0002	0.0049	0.0101	0.0117
	200	0.0128	0.0089	0.0002	0.0054	0.0130	0.0143
	250	0.0158	0.0110	0.0002	0.0061	0.0160	0.0171
	300	0.0188	0.0131	0.0003	0.0069	0.0191	0.0200
	600	0.0372	0.0260	0.0005	0.0121	0.0377	0.0381
	1343	0.0830	0.0582	0.0010	0.0260	0.0840	0.0842
InAs	10	0.0035	0.0026	0.0006	0.0022	0.0041	0.0048
	30	0.0039	0.0030	0.0006	0.0022	0.0045	0.0052
	50	0.0047	0.0037	0.0006	0.0022	0.0053	0.0059
	70	0.0057	0.0046	0.0006	0.0023	0.0063	0.0069
	100	0.0074	0.0062	0.0007	0.0024	0.0081	0.0086
	150	0.0106	0.0089	0.0008	0.0028	0.0114	0.0117
	200	0.0139	0.0117	0.0009	0.0034	0.0148	0.0151
	250	0.0171	0.0145	0.0011	0.0040	0.0182	0.0185
	300	0.0205	0.0173	0.0013	0.0046	0.0218	0.0219
	600	0.0406	0.0343	0.0024	0.0088	0.0430	0.0431
	1215	0.0820	0.0694	0.0048	0.0174	0.0868	0.0868
InSb	10	0.0030	0.0032	0.0013	0.0011	0.0043	0.0042
	30	0.0036	0.0037	0.0013	0.0011	0.0049	0.0048
	50	0.0046	0.0048	0.0014	0.0011	0.0060	0.0059
	70	0.0059	0.0061	0.0014	0.0011	0.0073	0.0072

TABLE I. (*Continued*)

Compound	Temperature (° K)	Acoustic[a] $\langle u^2\rangle_A$	Acoustic[a] $\langle u^2\rangle_B$	Optical[a] $\langle u^2\rangle_A$	Optical[a] $\langle u^2\rangle_B$	Total[a] $\langle u^2\rangle_A$	Total[a] $\langle u^2\rangle_B$
InSb	100	0.0080	0.0082	0.0016	0.0013	0.0096	0.0095
	150	0.0116	0.0120	0.0020	0.0016	0.0136	0.0136
	200	0.0153	0.0158	0.0024	0.0019	0.0177	0.0177
	250	0.0190	0.0196	0.0029	0.0023	0.0219	0.0219
	300	0.0227	0.0234	0.0034	0.0027	0.0261	0.0261
	600	0.0453	0.0466	0.0065	0.0052	0.0518	0.0518
	803	0.0605	0.0623	0.0086	0.0069	0.0692	0.0692
AlSb	10	0.0022	0.0039	0.0051	0.0001	0.0073	0.0040
	30	0.0025	0.0041	0.0051	0.0001	0.0076	0.0043
	50	0.0030	0.0048	0.0051	0.0001	0.0081	0.0049
	70	0.0037	0.0058	0.0051	0.0001	0.0088	0.0059
	100	0.0049	0.0074	0.0052	0.0001	0.0101	0.0075
	150	0.0070	0.0104	0.0056	0.0001	0.0126	0.0105
	200	0.0091	0.0136	0.0062	0.0001	0.0153	0.0137
	250	0.0113	0.0168	0.0069	0.0002	0.0182	0.0169
	300	0.0135	0.0200	0.0078	0.0002	0.0213	0.0202
	600	0.0268	0.0395	0.0136	0.0003	0.0404	0.0398
	1338	0.0596	0.0879	0.0293	0.0007	0.0889	0.0886

[a] *AB* represents the zinc-blende compound of interest.

tain drawbacks. Whenever experimental data have been available, the present model predicts the phonon dispersion for the TA branch to be somewhat higher near the Brillouin-zone boundary.

It is hoped that making available extensive data on the Debye-Waller factor of zinc-blende compounds will serve a useful purpose. In the case of the interpretation of neutron and x-ray scattering and in the Mössbauer effect, the calculated results can be used when experimental data are either unreliable or nonexistent. Very recently there has been interest[17,22,29] in calculating the temperature dependence of the energy gap of zinc-blende-type crystals, in particular, HgTe and GaP. A knowledge of the Debye-Waller factor is necessary in order to interpret the effect of the electron-phonon interactions on the temperature dependence of the energy gap. Further, the knowledge of the root-mean-square displacements of the constituent ions in a crystal at temperatures approaching the melting point might enable one to gain insight into the melting process.

Explicit calculations for the temperature dependence of the Debye-Waller factor have been performed for GaP, GaAs, GaSb, InP, InAs, InSb, AlSb, ZnS, ZnSe, ZnTe, CdTe, HgTe, and SiC. These results are then compared to existing experimental data. Also, the sum of the root-mean-square displacements of the constituent atoms is compared to their nearest-neighbor distance at the melting temperature.

II. THEORY

The temperature variation of the scattering amplitude from a particle K in a crystal is incorporated in the term

$$e^{-W_K(T)}, \tag{1}$$

where the factor $W_K(T)$ is known as the Debye-Waller factor.

In the case of zinc-blende crystals, which are cubic, the Debye-Waller factor is related to the total mean-square displacement of the Kth particle, $\langle u^2\rangle_K$, as follows:

$$W_K(T)=\frac{8\pi^2}{3}\left(\frac{\sin\theta}{\lambda}\right)^2\langle u^2\rangle_K\ . \tag{2}$$

λ is the wavelength of the incident radiation and 2θ is the corresponding scattering angle. The mean-square displacement of the Kth particle is temperature dependent and can be expressed in terms of the eigenfrequencies and eigenvectors of the phonon states of the crystal lattice as[30]

$$\langle u^2\rangle_K=\frac{\hbar}{Nm_k}\sum_{\vec{k}}\sum_{j}\frac{|\vec{\sigma}\,(K\,|\,{}^{\vec{k}}_{j})|^2\,[n\,(\omega_j(\vec{k}))+\tfrac{1}{2}]}{\omega_j(\vec{k})}\ . \tag{3}$$

$\omega_j(\vec{k})$ is the eigenfrequency for the jth phonon branch corresponding to the wave vector $\vec{k}$ and $\vec{\sigma}(K\,|\,{}^{\vec{k}}_{j})$ is the corresponding eigenvector of the Kth particle with mass m_K. The quantity $n(\omega_j(\vec{k}))$ is the phonon occupation number defined as

$$n\,(\omega_j(\vec{k}))=(e^{\hbar\omega_j(\vec{k})/k_BT}-1)^{-1}. \tag{4}$$

The sum over $\vec{k}$ in Eq. (3) is performed over an equidistant mesh of N wave-vector points in the first Brillouin zone.

The MRI model[24] is used to obtain the eigenfrequencies and eigenvectors of the phonon states

TABLE II. Calculated mean-square displacements (in 10^{-16} cm^2) for various II-VI zinc-blende compounds and SiC.

Compound	Temperature (° K)	Acoustic^a		Optical^a		Total^a	
		$\langle u^2\rangle_A$	$\langle u^2\rangle_B$	$\langle u^2\rangle_A$	$\langle u^2\rangle_B$	$\langle u^2\rangle_A$	$\langle u^2\rangle_B$
ZnS	10	0.0048	0.0031	0.0006	0.0042	0.0054	0.0073
	30	0.0051	0.0033	0.0006	0.0042	0.0057	0.0075
	50	0.0057	0.0038	0.0006	0.0042	0.0062	0.0080
	70	0.0065	0.0045	0.0006	0.0042	0.0071	0.0087
	100	0.0081	0.0058	0.0006	0.0043	0.0086	0.0101
	150	0.0110	0.0081	0.0006	0.0047	0.0116	0.0127
	200	0.0141	0.0105	0.0007	0.0052	0.0148	0.0157
	250	0.0174	0.0129	0.0008	0.0060	0.0182	0.0189
	300	0.0206	0.0154	0.0009	0.0068	0.0215	0.0222
	600	0.0405	0.0304	0.0016	0.0121	0.0422	0.0425
	1923	0.1292	0.0970	0.0051	0.0374	0.1343	0.1344
ZnSe	10	0.0033	0.0040	0.0022	0.0011	0.0055	0.0051
	30	0.0036	0.0043	0.0022	0.0011	0.0058	0.0054
	50	0.0044	0.0051	0.0022	0.0011	0.0066	0.0062
	70	0.0053	0.0061	0.0023	0.0012	0.0076	0.0073
	100	0.0069	0.0078	0.0025	0.0013	0.0094	0.0091
	150	0.0098	0.0110	0.0029	0.0015	0.0127	0.0125
	200	0.0128	0.0144	0.0035	0.0018	0.0163	0.0162
	250	0.0159	0.0178	0.0041	0.0021	0.0200	0.0199
	300	0.0190	0.0212	0.0047	0.0024	0.0237	0.0236
	600	0.0376	0.0419	0.0089	0.0046	0.0465	0.0465
	1373	0.0859	0.0956	0.0200	0.0103	0.1059	0.1059
ZnTe	10	0.0026	0.0040	0.0032	0.0005	0.0058	0.0045
	30	0.0032	0.0045	0.0032	0.0005	0.0064	0.0050
	50	0.0041	0.0057	0.0032	0.0005	0.0073	0.0062
	70	0.0052	0.0071	0.0033	0.0005	0.0086	0.0076
	100	0.0071	0.0094	0.0037	0.0006	0.0108	0.0100
	150	0.0103	0.0135	0.0045	0.0007	0.0148	0.0142
	200	0.0136	0.0178	0.0054	0.0008	0.0190	0.0186
	250	0.0169	0.0220	0.0065	0.0010	0.0234	0.0230
	300	0.0202	0.0263	0.0076	0.0011	0.0278	0.0275
	600	0.0401	0.0523	0.0145	0.0022	0.0546	0.0545
	1511	0.1009	0.1315	0.0361	0.0054	0.1370	0.1369
CdTe	10	0.0035	0.0039	0.0018	0.0012	0.0053	0.0051
	30	0.0046	0.0050	0.0018	0.0012	0.0064	0.0062
	50	0.0064	0.0069	0.0019	0.0012	0.0083	0.0081
	70	0.0084	0.0089	0.0020	0.0013	0.0104	0.0102
	100	0.0115	0.0122	0.0023	0.0015	0.0138	0.0137
	150	0.0169	0.0179	0.0030	0.0019	0.0199	0.0198
	200	0.0224	0.0237	0.0038	0.0024	0.0261	0.0261
	250	0.0278	0.0294	0.0046	0.0029	0.0324	0.0324
	300	0.0334	0.0353	0.0054	0.0035	0.0388	0.0388
	600	0.0665	0.0702	0.0105	0.0067	0.0770	0.0770
	1371	0.1517	0.1603	0.0239	0.0153	0.1756	0.1756
HgTe	10	0.0036	0.0027	0.0006	0.0023	0.0043	0.0050
	30	0.0049	0.0040	0.0006	0.0023	0.0055	0.0063
	50	0.0070	0.0057	0.0006	0.0024	0.0076	0.0082
	70	0.0092	0.0077	0.0007	0.0027	0.0099	0.0104
	100	0.0127	0.0107	0.0009	0.0032	0.0136	0.0139
	150	0.0188	0.0158	0.0011	0.0043	0.0199	0.0201
	200	0.0249	0.0210	0.0015	0.0055	0.0263	0.0265
	250	0.0310	0.0262	0.0018	0.0067	0.0328	0.0329
	300	0.0371	0.0314	0.0021	0.0080	0.0392	0.0394
	600	0.0740	0.0626	0.0041	0.0156	0.0782	0.0782
	943	0.1163	0.0983	0.0065	0.0245	0.1128	0.1228

TABLE II. (*Continued*)

Compound	Temperature (°K)	Acoustic[a]		Optical[a]		Total[a]	
		$\langle u^2\rangle_A$	$\langle u^2\rangle_B$	$\langle u^2\rangle_A$	$\langle u^2\rangle_B$	$\langle u^2\rangle_A$	$\langle u^2\rangle_B$
SiC	10	0.0041	0.0022	0.0004	0.0042	0.0044	0.0064
	30	0.0041	0.0022	0.0004	0.0042	0.0045	0.0064
	50	0.0041	0.0022	0.0004	0.0042	0.0045	0.0065
	70	0.0042	0.0023	0.0004	0.0042	0.0045	0.0065
	100	0.0043	0.0024	0.0004	0.0042	0.0047	0.0066
	150	0.0047	0.0027	0.0004	0.0043	0.0051	0.0070
	200	0.0053	0.0031	0.0004	0.0043	0.0056	0.0074
	250	0.0059	0.0036	0.0004	0.0043	0.0063	0.0079
	300	0.0067	0.0041	0.0004	0.0044	0.0070	0.0085
	400	0.0083	0.0052	0.0004	0.0047	0.0086	0.0099
	500	0.0099	0.0063	0.0004	0.0051	0.0103	0.0114
	600	0.0117	0.0074	0.0005	0.0056	0.0121	0.0130
	2973	0.0550	0.0355	0.0018	0.0215	0.0568	0.0570

[a] *AB* represents the zinc-blende compound of interest.

of the zinc-blende compounds. This model incorporates short-range noncentral nearest-neighbor interactions, equal central interactions for second-nearest neighbors, and long-range Coulomb interactions among ions of appropriate effective ionic charge. There are consequently, essentially four model parameters, three short-range force constants, and the effective ionic charge as parameters in the model. The model parameters are determined by relating them to the three cubic elastic constants and the long-wavelength optical mode phonon frequencies. Reliable data on these exist for the majority of zinc-blende cyrstals.

The eigenfrequencies and corresponding eigenvectors were calculated for a mesh of 4096 wave-vector points in the first Brillouin zone. Due to the symmetry properties of the Brillouin zone, the eigenfrequencies and eigenvectors of the phonon states were determined at the nonequivalent points in $\vec{k}$ space, defined as

$$\vec{k} = \frac{\pi}{8a}\,(q_x,\,q_y,\,q_z)\;, \tag{5}$$

where

$$16 \geqslant q_x \geqslant q_y \geqslant q_z \geqslant 0\;,$$

$$q_x + q_y + q_z \geqslant 24\;,$$

and a is the lattice constant such that the unit cell volume equals $\frac{1}{4}a^3$.

A divergence occurs for the $\vec{k} = 0$ acoustic-mode phonons in the sum over the wave-vector mesh in Eq. (3). The contribution to the mean-square displacement owing to the $\vec{k} = 0$ acoustic-mode phonon frequencies was therefore calculated by converting the summation to an integral and assuming a Debye distribution over the volume of integration which was assumed to be $\frac{1}{4096}$th of the total Brillouin-zone volume.

III. RESULTS AND DISCUSSION

A. Mean-Square Amplitudes

Utilizing the eigenfrequencies and the corresponding eigenvectors as determined by the MRI model, Eq. (3) was solved for the mean-square displacements of the constituent atoms in GaP, GaAs, GaSb, InP, InAs, InSb, AlSb, ZnS, ZnSe, ZnTe, CdTe, HgTe, and SiC. The contribution due to the $\vec{k} = 0$ acoustic-mode phonons was found to be small for all zinc-blende compounds considered. In fact at temperatures near the melting point, where this contribution was the most significant, it was found to be less than 0.4% of the total mean-square displacement of any constituent atom.

The mean-square displacements of both of the constituent atoms for the aforementioned zinc-blende compounds at different temperatures are presented in Tables I–III. With the exception of GaP, the highest temperature represents the melting point of the compound of interest. The separate contributions to the mean-square displacements from the acoustic and optical phonons are also summarized in these tables. The temperature dependence of the mean-square displacement of the constituent atoms is linear from 300 °K to the melting point of the compound with the exception of SiC where linearity begins around 500 °K. This is not surprising, since the Debye temperature of SiC is considerably higher than that of the other compounds considered.

B. Acoustic- and Optical-Phonon Contributions

The separate listing of the acoustic- and optical-phonon contributions to the total mean-square displacements enables some interesting observations to be made. The contribution of the acoustic phonons to the mean-square displacement is more temperature dependent than the corresponding optical-mode contribution. For the heavier atom, the contribution to the mean-square displacement from the acoustic phonons is greater than that from the optical phonons at all temperatures. For the lighter atom, the contributions from the acoustic and optical phonons are comparable at low tem-

TABLE III. Comparison of calculated and experimental values of root-mean-square displacements (in 10^{-8} cm) for various zinc-blende compounds.

Compound	Temperature (°K)	$\langle u^2\rangle_A^{1/2}$ [a]		$\langle u^2\rangle_B^{1/2}$ [a]		$\langle u^2\rangle_{AB}^{1/2}$ [a]		Reference for expt. data
		Calc	Expt	Calc	Expt	Calc	Expt	
GaP	100	0.077	0.076	0.086	0.063			17, 16
	200	0.099	0.1068	0.103	0.088			17, 16
	293	0.117	0.129	0.120	0.107			17, 16
			0.203		0.130			
GaAs	184					0.102	0.105	18
	345					0.135	0.123	18
	380					0.141	0.127	18
	425					0.149	0.131	18
	434					0.150	0.132	18
	485					0.158	0.137	18
GaSb	332	0.148	0.191	0.148	0.121			19
	370	0.156	0.277	0.156	0.225			19
	410	0.164	0.311	0.163	0.260			19
InP	250	0.127	0.274	0.131	0.272			16
	380	0.155	0.291	0.157	0.288			16
	450	0.168	0.308	0.170	0.305			16
	525	0.181	0.331	0.184	0.325			16
InAs	184					0.138	0.116	18
	386					0.167	0.181	18
	432					0.176	0.200	18
	482					0.186	0.220	18
	528					0.195	0.220	18
	578					0.204	0.258	18
InSb	332	0.169	0.191	0.169	0.147			19
	370	0.179	0.320	0.179	0.242			19
	410	0.188	0.416	0.188	0.294			19
ZnSe	296					0.153	0.214	20
ZnTe	359	0.182	0.230	0.181	0.155	0.182	0.192	21
	440	0.201	0.263	0.200	0.212	0.201	0.231	21
	503	0.214	0.298	0.214	0.255	0.214	0.276	21
CdTe	242	0.177	0.233	0.177	0.212			21
	296					0.196	0.236	20
	306	0.199	0.277	0.199	0.259			21
	359	0.215	0.307	0.215	0.290			21
HgTe	80	0.106	0.098	0.107	0.083			22
	100	0.116	0.110	0.118	0.092			22
	200	0.162	0.155	0.163	0.130			22
	300	0.198	0.190	0.198	0.160			22

[a] AB represents the zinc-blende compound of interest.

peratures and in fact in some cases the optical-phonon contribution may be even larger. The contribution from the acoustic phonons, however, predominates at higher temperatures. The relative contribution from the acoustic phonons is more predominant in the heavy atom while the relative contribution from the optical phonons predominates for the lighter atom. At any particular temperature the value of the mean-square displacement is greater for the lighter atom. This difference in mean-square displacement becomes even more pronounced when the mass difference of the constituent atoms is quite large, e.g., AlSb. The present analysis shows that the contribution from the optical-phonon states does in fact have a significant contribution to the mean-square displacements, especially in the case of the lighter atom.

C. Comparison with Experiment

The available experimental data for the root-mean-square displacements are compared to the calculated results in Table III. The agreement between the calculated and experimental values is excellent in the case of GaP, GaAs, and HgTe, and tolerably good for InAs, ZnTe, and CdTe. However, it is decidedly poor for GaSb, InP, and InSb. There is a possibility that the reliability of some of the experimental data may be questionable.

TABLE IV. Ratio of the sum of the root-mean-square displacements (in 10^{-8} cm) to the nearest-neighbor distance (in 10^{-8} cm) at the melting temperature for various zinc-blende compounds.

Compound	Melting temperature (°K)	$\langle u^2\rangle_A^{1/2\,a} + \langle u^2\rangle_B^{1/2\,a}$	Nearest-neighbor distance	Ratio
InP	1232	0.5801	2.541	0.2283
GaAs	1511	0.5568	2.440	0.2282
InAs	1215	0.5892	2.615	0.2253
AlSb	1338	0.5958	2.654	0.2245
GaSb	979	0.5027	2.649	0.1898
InSb	803	0.5260	2.793	0.1883
ZnS	1923	0.7330	2.350	0.3117
CdTe	1371	0.8382	2.776	0.3020
ZnTe	1511	0.7402	2.628	0.2816
ZnSe	1373	0.6508	2.454	0.2652
HgTe	943	0.7008	2.754	0.2545
SiC	2973	0.4770	1.883	0.2533

[a] *AB* represents the zinc-blende compound of interest.

For example, proper correction for the thermal diffuse scattering was not made in interpreting many, if not all, of the experimental data. The discrepancy in some of the reported data, e.g., GaP, also leads one to further question the reliability of some of the experimental work. A further source of error comes from the fact that the model used consistently predicts slightly higher TA-mode frequencies, which in turn affect the Debye-Waller factor.

D. Melting and Vibrational Amplitudes

It was originally proposed by Lindeman[31] that the melting process occurs when the root-mean-square amplitude of vibration reaches a critical fraction, presumed to be the same for all crystalline solids, of the nearest-neighbor distance. It was later shown[8,32–34] that in various cubic metals and alkali halides this fraction was indeed not constant but might in fact be a function of the crystal structure and location of the constituent atom or atoms in the periodic table of elements. This ratio has been calculated for the zinc-blende compounds and is tabulated in Table IV. The present calculation shows that the ratio is a constant for the II-VI and III-V compounds, although the average ratio for the II-VI compounds is slightly larger than the corresponding ratio of the III-V compounds. For SiC the ratio seems to be closer to that characteristic of the II-VI compounds. A more thorough lattice-dynamical treatment including anharmonic effects, which are more predominant at higher temperatures, might give further insight into the melting process.

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