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Thermal Conductivity of Boron and Some Boron Compounds*

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Thermal-conductivity measurements have been made on crystals of β-boron, $B_{12}P_2$, $B_{12}As_2$, and YB_{66} from 3 to 300 K. Phonons are the dominant carriers of heat, and their mean free paths range from 10^{-5} cm for temperatures near the Debye temperature to 10^{-1} cm near 4 K. A model in which only the phonons in the acoustic branches carry the heat is used. This model explains the large decreases observed in thermal conductivity as the crystal structure becomes more and more complex in the series $B_{12}As_2$, β-boron, YB_{66}. At the lowest temperatures the thermal conductivity of single crystals of YB_{66} behaves somewhat like that of a glass, presumably because of a substantial amount of frozen-in disorder in the melt-grown crystals.

I. INTRODUCTION

The element boron possesses several different complex crystalline structures[1] and forms numerous compounds which also have complex structures.[1] The simplest structure of boron is α-boron,[2] which is a slightly distorted face-centered-cubic packing of boron icosahedra or B_{12} units. The β-boron[3] structure is a distorted, fcc packing of B_{84} units, while the structure[4] of YB_{66} is a fcc packing of B_{156} units. Thus in this series of three structures we proceed from small molecular clusters of 12 atoms to large clusters of 156 atoms. The primitive unit cells of the crystals in this series contain, respectively, 12, 105, and 402 atoms. It has been shown[5] that the thermal conductivity of a solid depends critically on the molecular grouping of its atoms. Thus one would expect some rather distinct changes in thermal conductivity in the series α-boron, β-boron, YB_{66}. The present study shows these changes in the temperature range from 3 to 1000 K.

Since suitably large crystals of α-boron are very difficult to grow,[6,7] we have studied crystals of $B_{12}P_2$ and $B_{12}As_{12}$. These crystals, as well as $B_{12}C_3$, have a structure[1] very similar to that of α-boron. Hence we expect their thermal conductivity to be nearly the same as that of α-boron. All of the crystals mentioned are semiconductors with very small carrier concentrations. Hence the electronic component of the heat transport in all of them is insignificant. Phonons are the dominant carriers of the thermal energy. In addition there may be a small contribution from photons at high temperatures.

Previous studies of the thermal conductivity of β-boron have been published[5,8,9] as well as studies on boron carbide[10-13] $B_{12}C_3$, and boron subphosphide[14,15] $B_{12}P_2$. In only two of these studies[5,9] was any attention given to the effect of crystal structure on the thermal conductivity.

II. SAMPLES

The present measurements were all made on crystalline samples as listed in Table I. The samples were generally in the shape of rods with a rectangular cross section. The length of the sample as well as its effective diameter are given in Table I. This diameter is that of a circle whose area is equal to the cross-sectional area of the sample cut in a plane perpendicular to the heat flow. In most cases the cross sections were nearly square.

The pycnometric crystal density is also given in

TABLE I. Properties of the single–crystal samples.

Run No.	Crystal	Dimensions (mm) L	d	Density (g/cm^3) pycnometric	x ray	Heat-flow direction[a]
R145	$B_{12}As_2$	3.2	1.3	3.59 ± 0.05	3.583	Perpendicular to *c* axis
R147	$B_{12}P_2$	1.9	1.2	2.599 ±0.005	2.597	Oligocrystalline
R183	β-boron	12.4	2.6	2.329 ± .005	2.289	Parallel to *c* axis
R184	β-boron	2.5	2.1			Perpendicular to *c* axis
R187	YB_{66}	5.5	1.7	⋯	2.482	⋯
R202	YB_{66}[b]	8.5	2.4	2.568 ± .005		⋯

[a] The $B_{12}As_2$, $B_{12}P_2$, and β-boron have a rhombohedral crystal structure. This structure can be described by a hexagonal unit cell. The *c* axis is the long axis of this hexagonal cell.

[b] A typical mass-spectrograph impurity analysis of YB_{66} shows the following impurity concentrations in units of 10^{18} atoms/cm^3: C = 6, O = 2, N = 1, Gd = 1, Ti = 0.8, Fe = 0.7, Cu = 0.4, and all others < 0.6.

Table I because stoichiometry is often uncertain in these boron compounds. For densities between 2.2 and 2.9 g/cm^3 the densities were determined by floating the crystals is a mixture of 1.2-dibromoethane and 1, 1, 2, 2-tetrabromoethane at 25 C. The liquid density at the floatation point equals the crystal density. In the simpler crystal structure cases, $B_{12}As_2$ and $B_{12}P_2$, the measured density equals the x-ray density. This indicates that the 12-to-2 stoichiometry assigned is the actual value. For β-boron and especially for YB_{66} the pycnometri density is significantly larger than the x-ray value. This seems to indicate some extra B or Y atoms included in the rather open crystal structure. The measured density of β-boron corresponds to 107 atoms in the unit cell; that of YB_{66} corresponds more nearly to a boron-to-yttrium ratio of 69 instead of 66, but still with 24 Y atoms in a unit cell.

The crystals of β-boron were cut from a boule obtained commercially from Wacker-Chemie,[16] which was grown by a floating-zone technique. Samples R183 and R184 were both cut from the same single-crystal boule, but had different crystallographic orientations. Samples R187 and R202 of YB_{66} were grown[17] in this laboratory by the Czochralski technique. For R187 the melt was contained in a boron nitride crucible, for sample R202 the melt was suspended by radio-frequency induction levitation over a water-cooled copper boat in order to avoid possible nitrogen contamination. The impurity concentration in the β-boron was less than 5×10^{18} cm^{-3} and was mainly carbon. The impurities in the YB_{66} are listed in Table I.

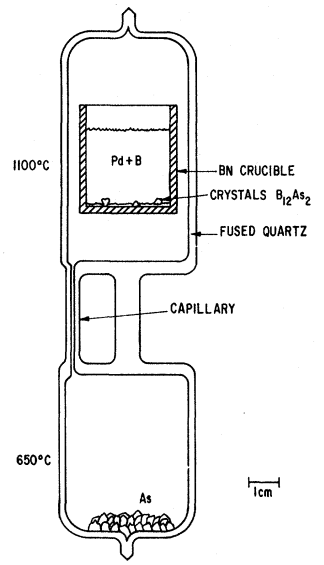

FIG. 1. Fused-quartz reaction vessel used for growing single crystals of $B_{12}P_2$ or $B_{12}As_2$. The liquid palladium-boron melt is held in the boron nitride crucible in the upper part of the vessel, the elemental phosphorus or arsenic is in the lower part. The whole vessel is evacuated at room temperature and sealed.

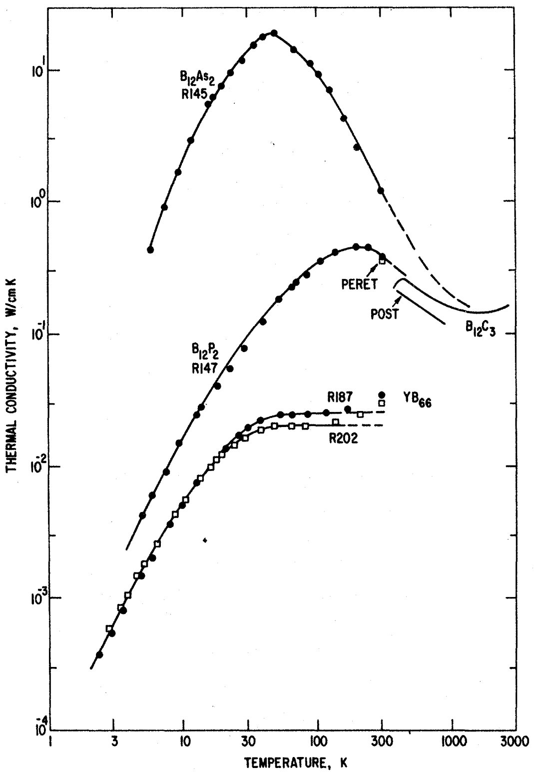

FIG. 2. Thermal conductivity vs temperature for $B_{12}As_2$, $B_{12}P_2$, $B_{12}C_3$, and YB_{66}. The $B_{12}C_3$ data are from the literature. The point given by Peret is probably for $B_{12}P_{1.85}$. The curve from Post is for $B_{12}P_{1.88}$. The dashed lines for YB_{66} show the probable trend of the curves when radiation losses are corrected for.

The crystals of $B_{12}P_2$ and $B_{12}As_2$ were grown from a liquid palladium-boron melt containing 4–9 wt% of boron held in a boron nitride crucible at 1100 °C (for $B_{12}As_2$) or 1300 °C (for $B_{12}P_2$) for 350 h. The arsenic or phosphorus vapor was slowly admitted to the surface of the molten alloy in the apparatus shown in Fig. 1. The 0.2-mm-diam fused-quartz capillary controlled the rate of vapor admission to the growing chamber. The crystal-growth rate was about 1 μ/h, and several crystals, with some as large as 0.4 cm in diameter, were grown in one run. The vapor pressure of the As or P was controlled by the temperature of the lower fused-quartz bulb. Bulb temperatures of 650 °C gave $B_{12}As_2$, while temperatures of 250-450 °C were used to make $B_{12}P_2$ or BP crystals. The BP crystals grew at the higher[18] phosphorus pressures. The impurity concentrations in the $B_{12}P_2$ and $B_{12}As_2$ are unknown, but the major impurities are probably Pd, Si, N, or O at concentrations less than 10^{21}/cm^3.

TABLE II. Representative values of thermal conductivity.

T (K)	κ (W/cm K) $B_{12}As_2$	 $B_{12}P_2$ ($\times 10^{-2}$)	 YB_{66}[a] ($\times 10^{-3}$)	 β-boron[b]
3	...	...	0.62	0.081
6	0.50	0.62	2.3	0.39
10	2.00	1.7	5.2	0.86
20	7.8	5.2	12.5	1.86
30	13.2	9.3	17	2.62
45	19.0	15	20	3.13
60	15.8	21	20	3.23
100	9.3	33	20	2.00
200	2.7	44	~20	0.55
300	1.2	38	~20	0.26

[a] Sample R202.

[b] This is an average value, $\bar{\kappa}$, given by $\bar{\kappa} = (\kappa_{\parallel} + 2\kappa_{\perp})/3$. The peak value of $\bar{\kappa}$ is 3.28 W/cm K at 50 K.

III. EXPERIMENTAL TECHNIQUE

The thermal-conductivity measurements were made using an apparatus described previously.[19]

IV. EXPERIMENTAL RESULTS

The thermal-conductivity (κ)-vs-temperature (T) curves for $B_{12}As_2$, $B_{12}P_2$, and YB_{66} are shown in Fig. 2. The other data in Fig. 2 for $B_{12}C_3$ and $B_{13}P_2$ are taken from the literature.[10–15] The κ values at 300 K range from 1.2 W/cm K for $B_{12}As_2$ to 0.02 W/cm K for YB_{66}. Some κ values at selected temperatures are given in Table II. Note that the curves for YB_{66} are drawn as dashed lines above 150 K. The upward trend of the data points from 150 to 300 K is believed to be caused by uncompensated thermal-radiation losses from the sample and heater. The true κ is probably close to the dashed lines as shown.

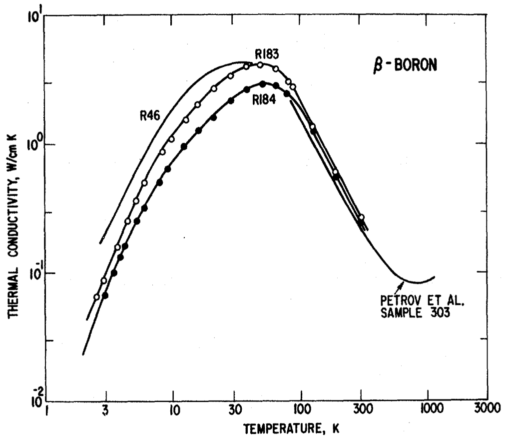

FIG. 3. Thermal conductivity of two single crystals of β-boron. For R183 the heat flow is parallel to the c axis. For R184 it is perpendicular to the c axis. The results for sample R46 and those of Petrov *et al.* are for polycrystalline samples.

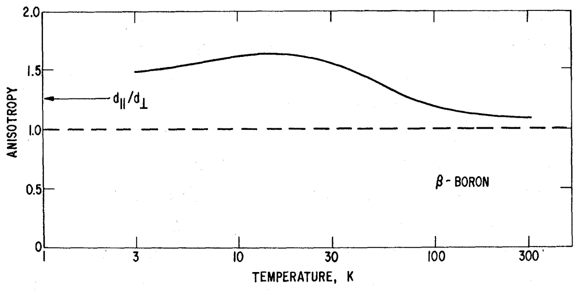

FIG. 4. Arnistropy $k_{\parallel}/\kappa_{\perp}$ of the thermal conductivity of β-boron. The ratio of the diameters of the samples R181 and R184 is $d_{\parallel}/d_{\perp}$.

The κ results for β-boron are given in Fig. 3 for the two different crystal orientations. These results are somewhat higher than those of Petrov *et al.*[9] for their sample 303 which had the highest κ values. The curve for sample R46 of polycrystalline boron from Ref. 5 is also shown. For $T > 100$ K the results for sample R46 fall between those of R183 and R184. For $T < 40$ K the κ of R46 is higher than the present results, presumably because the sample diameter (0.6 cm) was larger although the crystallite size (0.1 mm) was smaller.

Because β-boron has a rhombohedral crystal structure it possesses two principal values of thermal conductivity. If we use the hexagonal-cell description of the structure, the principal values of κ are those parallel to and perpendicular to the c axis of this hexagonal cell, i.e., $\kappa_{\parallel}$ and $\kappa_{\perp}$. Our results show that $\kappa_{\parallel} > \kappa_{\perp}$ over the whole temperature range studied. Figure 4 shows a plot of the ratio $\kappa_{\parallel}/\kappa_{\perp}$. We expect that at 2 K the anisotropy will include the sample diameter ratio $d_{\parallel}/d_{\perp} = 1.24$ from Table I if κ is limited by boundary scattering. This will be shown later to be the case. Thus the intrinsic crystal anisotropy should be less than the observed curve in Fig. 4. The intrinsic anisotropy for β-boron appears to lie between

$$1.3 \geq \kappa_{\parallel}/\kappa_{\perp} \geq 1.1 \qquad (1)$$

over the temperature range from 3 to 300 K.

V. ANALYSIS OF RESULTS

A. Debye Temperature

The analysis of the κ-vs-T curves depends on a knowledge of the phonon spectrum of the crystals, since the heat is carried primarily by phonons. The Debye temperature Θ is a convenient quantity to use in discussing the phonon spectrum.

The Θ values[5] for β-boron and $B_{12}C_3$ are both close to 1300 K, based on specific-heat-capacity measurements. We are using the Θ_E values from Ref. 5, which agree with the values calculated from the elastic constants. The sound velocities at 10^7 Hz in a YB_{66} crystal have been measured for a [100] propagation direction at 300 K. They are 12.1×10^5 cm/sec for a longitudinal wave and 7.9×10^5 cm/sec for a transverse wave. These give a calculated value of $\Theta = (1300 \pm 50)$ K. Thus β-boron, $B_{12}C_3$, and YB_{66} all have a Θ value of 1300 K. In order to estimate Θ for α-boron, $B_{12}P_2$, and $B_{12}As_2$, we use a scaling law devised by Steigmeier[20] which says that for a series of similar solids

$$\Theta = b(\bar{M}\delta^3)^{-1/2}, \tag{2}$$

where b is some constant, $\bar{M}$ is the average mass of an atom of the crystal, and δ^3 is the average volume occupied by one atom. From the value of $\Theta = 1300$ K for YB_{66} and the $\bar{M}$ and δ values in Table III we have estimated the Θ values of 1430, 1160, and 940 K for α-boron, $B_{12}P_2$, and $B_{12}As_2$, respectively. These are listed in Table III.

B. Phonon Cutoff Energy

Following the same type of arguments as given in the discussion of the thermal conductivity of garnets[21] we are interested in finding the highest-energy acoustic phonons that are present in the various crystals. These phonons have an energy[21] in wave numbers called $\bar{\nu}_C$, where the C means cutoff. From a knowledge of the average sound velocity v and the lattice constant a_0 of YB_{66}, we can calculate[21] $\bar{\nu}_C$ from

$$\bar{\nu}_C = 2v/\pi a_0 c_0, \tag{3}$$

where c_0 is the velocity of light in a vacuum. Equation (3) is valid for either bcc or fcc lattices, and YB_{66} is fcc. We find for YB_{66} that $\bar{\nu}_C = 80\ \text{cm}^{-1}$.

The problem of estimating $\bar{\nu}_C$ for the other crystals is more difficult because they do not possess a cubic crystal structure. They have a rhombohedral structure[1] where the rhombohedral angle α varies from 58° to 72°. If we distort this angle to exactly 60° without changing the crystal density, then the crystals become fcc with an equivalent lattice constant,[22] s. The calculated values of s are given in Table III. Note that for YB_{66} we have $s = a_0$. With these values of s and a value of v estimated from Θ, we have calculated the $\bar{\nu}_C$ in Table III. These values of $\bar{\nu}_C$ are much less than the energy given by $k\Theta$, where k is Boltzmann's constant. For example, $\Theta = 1300$ K is equivalent to an energy in wave numbers of $\bar{\nu}_D = 904\ \text{cm}^{-1}$, where the subscript D stands for Debye. The ratios $(\bar{\nu}_C/\bar{\nu}_D)$ are given in Table IV. This ratio indicates what fraction of the total range of phonon energies actually lies within the acoustic branch, and hence takes part in the thermal transport. It is assumed[21] that no heat is transported by phonons in any of the optical branches. For those crystals[1] with the α-boron structure this acoustic fraction ranges from 26 to 30%, for the β-boron structure it is 14%, while for the most complex YB_{66} structure it drops to only 9%. We believe that it is this feature of the crystal structure that is responsible for determining the magnitude of the thermal conductivity in the temperature range from, say, 100 K to the melting point. This will be evaluated quantitatively later. There is some experimental confirmation of the $\bar{\nu}_C$ value for β-boron. Far-infrared optical-absorption studies[23] show that the lowest-energy strong-absorption peak is at $\bar{\nu} = 139\ \text{cm}^{-1}$ at 4.2 K. This lowest infrared-active optical branch is expected to occur at an energy slightly above the acoustic-branch energy at the zone boundary which is calculated to be 130 cm^{-1} (see Table III).

C. Phonon Mean Free Path

A first approximation to the mean free path l of the phonons can be calculated from

$$\kappa = \tfrac{1}{3} v\, C_{\text{tot}}\, l, \tag{4}$$

where C_{tot} is the heat capacity per unit volume and v is the average sound velocity. We have used

TABLE III. Some physical constants of boron and boron compounds.

Crystal	$\bar{M}$ (g)	δ (10^{-8} cm)	N_c [a]	N_b [b]	Θ (K)	s (10^{-8} cm)	$\bar{\nu}_c$ (cm^{-1})
α-boron	10.811	1.94	12	12	1430	7.04	300
β-boron	10.811	1.99	105	84	1300	14.88	130
$B_{12}C_3$	11.051	1.94	15	12	1300	7.60	240
$B_{12}P_2$	13.691	2.06	14	12	1160	7.88	220
$B_{12}As_2$	19.970	2.10	14	12	940	8.03	170
YB_{66}	11.977	2.00	402	156	1300	23.44	80

[a] N_c is the number of atoms per primitive crystallographic unit cell.

[b] N_b is the number of boron atoms in the fundamental boron unit from which the lattice is built.

TABLE IV. Comparison of observed and computed thermal conductivity values for $T = \Theta$.

Crystal	κ_Θ (W/cm K)	κ'_Θ (W/cm K)	G	$\bar{v}_C/\bar{v}_D$	$\kappa'_\Theta(\bar{v}_C/\bar{v}_D)$ (W/cm K)
α-boron	⋯	0.61	⋯	0.302	0.18
β-boron	0.08	0.59	0.14	0.144	0.085
$B_{12}C_3$	0.14	0.52	0.27	0.265	0.14
$B_{12}P_2$	~0.16	0.54	~0.30	0.273	0.15
$B_{12}As_2$	0.20	0.53	0.38	0.260	0.14
YB_{66}	~0.02	0.58	~0.04	0.089	0.05

the Θ values in Table III to compute C_{tot} and v, and then have used the κ results in Figs. 2 and 3 to compute l as a function of temperature. We are assuming, for the time being, that C_{tot} is the total heat capacity of all of the phonon branches. This means, in the nomenclature of Ref. 5, that we are treating the crystals as monatomic solids. The resultant l-vs-T curves are shown in Fig. 5. For β-boron we have used $\bar{\kappa}$ to calculate l (see Table II). For both $B_{12}As_2$ and β-boron the results below 10 K extrapolate at 1 K to the d values given in Table I. This means that the phonons are undergoing primarily boundary scattering from the sample walls at the lowest temperatures. This is not the case for either crystal of YB_{66}. At 2 K the phonon mean free path is about 7×10^{-4} cm, which is much less than the sample diameter. From the impurity analysis in Table I it does not appear that any of these impurities is present in sufficient concentration to be responsible for the small mean free path. In the analysis of the crystal structure[4] it was found that the location of the Y atoms as well as of the 36- and 48-atom boron groups in the unit cell were random. Thus the lattice is disordered to this extent and looks something like a glass. Indeed, the κ-vs-T curve for YB_{66} resembles that for fused quartz[24] in both its magnitude and temperature dependence. This random structure for YB_{66} may have been frozen in at the high temperature, i.e., about 2100 °C, at which these crystals were grown from the melt. It would be interesting to grow YB_{66} at a lower temperature by using a suitable flux to see if this disorder is still present. Further disorder in a boron sample could probably be found in glassy boron as prepared by Talley *et al.*[25] They report a thermal conductivity of 3.2×10^{-2} W/cm K at 335 K, a value close to that which we find in YB_{66}.

From Fig. 2 the κ values for $B_{12}P_2$, sample R147, below 10 K indicate that the phonon mean path for this crystal is approaching 2×10^{-3} cm, a value much less than the sample diameter. Indeed the κ of $B_{12}P_2$ is much less than that of $B_{12}As_2$ over the whole temperature range studied. It is believed that this low κ is caused either by the fact that the sample was oligocrystalline as determined by x rays or by some unknown impurities in the $B_{12}P_2$, or by both. The close agreement of pycnometric and x-ray density rules out a large phosphorus deficiency[1] from the stoichiometric composition. The crystal growth temperature of 1300 °C rules out the possibility of much disorder such as that found in YB_{66}.

The phonon mean-free-path values at high temperatures are quite informative. If we extrapolate the $B_{12}As_2$ curve in Fig. 2 as shown to 1300 K, we see that the isomorphous compounds $B_{12}As_2$, $B_{12}P_2$, and $B_{12}C_3$ all have comparable values of κ at high temperatures. At a temperature of $T = \Theta$ they have a value of κ equal to

$$\kappa_\Theta \simeq 0.14\text{–}0.20 \text{ W/cm K}.$$

This corresponds to a mean free path at $T = \Theta$ of

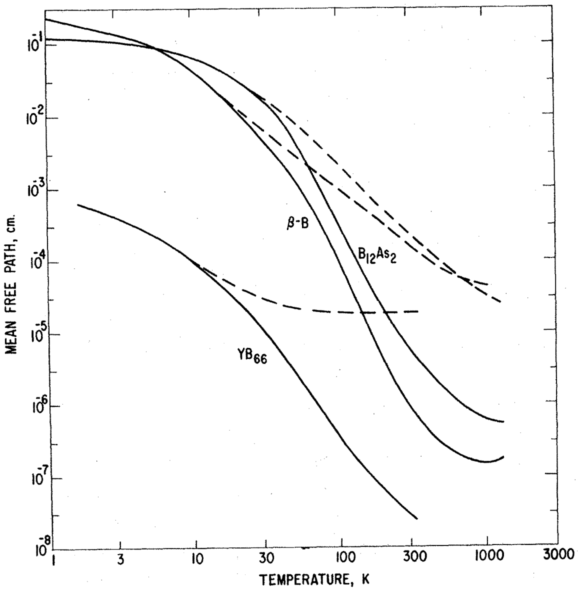

FIG. 5. Phonon mean free path for three different crystals as a function of temperature. The solid lines are computed from the heat capacity of all of the phonon branches. The dashed lines represent the behavior of the acoustic phonons only and correspond to the mean free path of the actual carriers of the thermal energy.

$$l(\Theta) \simeq 6\times 10^{-7}\ \text{cm}$$

and thus

$$l(\Theta)/s \simeq 8 \quad \text{for } B_{12}As_2,\ B_{12}P_2,\ \text{and } B_{12}C_3\ .$$

This same ratio is about 1 for β-boron and about 0.05 for YB_{66}. Now s is a measure of the fundamental repeat distance of the crystal lattice, and hence there are no phonons with wavelengths less than s. The concept of a phonon with a mean free path l of 5% of its wavelength is meaningless. However, we must be careful here because we have calculated the l-vs-T curves in Fig. 5 by assuming that all of the phonons had the same average propagation velocity in Eq. (5). At low temperatures, i.e., below, say, 10 K, all of the phonons that are excited do have the same velocity, which is just the sound velocity. Hence Fig. 5 is valid for $T \leq 10$ K. For $T \sim \Theta$ it is incorrect. At $T \sim \Theta$ almost all of the optical-phonon modes are excited, but these have essentially zero group velocity. The acoustic phonons that have $v > 0$ and are the carriers of thermal energy actually have mean free paths larger than s. Let us define $l_C(T)$ as the mean free path calculated from Eq. (4) using the measured $\kappa(T)$ and the heat capacity C_c associated only with the acoustic branch. This C_C is less than the C_{tot} by

$$\frac{C_C}{C_{\text{tot}}} = \left(\frac{\Theta_C}{\Theta}\right)^3 \frac{f(\Theta_C/T)}{f(\Theta/T)}\ , \tag{5}$$

where f is the Debye function, Θ is the Debye temperature of the crystal, $\Theta_C = hv\bar{\nu}_C/k$, and h and k are Planck's and Boltzmann's constants, respectively. We can take the $l(T)$ curves in Fig. 5 and convert them to $l_C(T)$ curves by using

$$l_C(T)/l(T) = C_{\text{tot}}/C_C\ . \tag{6}$$

Now the results for YB_{66} at 300 K become

$$l_C(300) = 660\, l(300) = 1.8\times 10^{-5}\ \text{cm}\ .$$

This value is much larger than s of YB_{66}. The concept of phonons now makes some sense. If we convert all of the $l(T)$ curves in Fig. 5 to $l_C(T)$ curves, we obtain the dashed lines as shown in Fig. 5. At high temperatures when $T \geq \Theta$, all of the phonons that are carrying heat have a mean free path of about 2×10^{-5} cm. In this respect all of the boron-containing compounds are the same. At low temperatures near 1 K the mean free path, $l_C(T)$, becomes equal to $l(T)$ and approaches the boundary-scattering limit for $B_{12}As_2$ and β-boron but not for YB_{66}. So we conclude that YB_{66} behaves normally at high temperatures near $T = \Theta$ where phonon-phonon scattering is dominant but shows disorder scattering at low temperatures.

D. Computation of κ for T near Θ

Rather than compute a weighted-average mean free path for the whole spectrum of acoustic phonons from the experimental κ data as we did in Sec. V C, we can use the theory of phonon-phonon interactions and their energy dependence to estimate κ itself. This has been done by Leibfried and Schlömann.[26] They find that at $T = \Theta$ the calculated value of κ, which we call κ'_Θ, is given by

$$\kappa'_\Theta = 5.72\times 10^{-8}\, \bar{M}\Theta^2\delta\gamma^{-2}\ \text{W/cm K}\ , \tag{7}$$

where γ is an effective Grüneisen constant which we assume equals two for want of a better value, $\bar{M}$ is the average atomic mass in grams, Θ is the Debye temperature in degrees Kelvin, and δ^3 is the average volume per atom in units of 10^{-24} cm^3. The theoretical model used for deriving[26] Eq. (7) assumed that the crystal was a simple monatomic cubic solid where the phonon cutoff energy is just $\bar{\nu}_D$. For complex crystals where the phonon cutoff energy is $\bar{\nu}_c$ the computed κ should be less[21] by a factor of

$$\kappa_C/\kappa_D = (\bar{\nu}_C/\bar{\nu}_D)^m,\quad 1 \leq m \leq 2\ . \tag{8}$$

Let us define the crystal complexity factor[27] G as

$$G = \kappa_\Theta/\kappa'_\Theta, \tag{9}$$

where κ_Θ is the experimental value of κ at $T = \Theta$, and κ'_Θ is the value of κ_Θ from Eq. (7). From the above arguments we expect that

$$\kappa_\Theta \cong \kappa'_\Theta (\bar{\nu}_C/\bar{\nu}_D)^m\ . \tag{10}$$

From Table IV it can be seen that Eq. (10) fits the experimental data fairly well for $m = 1$. So this calculation also shows that the model we are using, where only the acoustic phonons carry thermal energy, is in reasonably good agreement with the data.

The predicted value of κ of α-boron at $T = \Theta$ is 0.18 W/cm K. If we extrapolate this value back to 300 K by assuming that the κ-vs-T curves for α-boron and $B_{12}As_2$ are similar, we get $\kappa(300\ \text{K}) \simeq 2$ W/cm K for α-boron. This means that this polymorph of boron, with the simplest known crystal structure, is a good conductor of heat at room temperature. Its thermal conductivity is predicted to be about $\frac{1}{2}$ that of copper.

VI. CONCLUSIONS

We have measured the thermal conductivity of crystals of $B_{12}As_2$, $B_{12}P_2$, β-boron, and YB_{66} from 3 to 300 K. We believe that these results can be explained by assuming that heat is carried in these crystals primarily by the acoustic phonons. The mean free path of these phonons is about 2×10^{-5} cm in all the crystals for temperatures near

$T = \Theta$, and increases as T decreases. For $B_{12}As_2$ and β-boron it increases to become equal to the sample diameter at $T \sim 3$ K. For $B_{12}P_2$ and YB_{66} it falls much below this limit at 3 K. Impurity and crystallite scattering is suggested as the cause of this small mean free path in $B_{12}P_2$, whereas randomness of boron- and yttrium-atom positions in the lattice is believed to be the cause in YB_{66}.

The anisotropy in the κ of β-boron was measured and was found to be $1.3 \geq \kappa_{\parallel}/\kappa_{\perp} \geq 1.1$ over the whole temperature range studied.

The κ of α-boron is predicted to be about 2 W/cm K at 300 K. All other polymorphs of boron are expected to have lower values of κ.

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