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Method for Estimating the Lattice Thermal Conductivity of Metallic Alloys

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OF METALLIC ALLOYS

D. W. Yarbrough and R. K. Williams

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TABLE OF NOMENCLATURE

A	constant of proportionality, Eq. (9)
B	constant of proportionality, Eq. (10)
c	constant of proportionality, Eq. (11)
C	specific heat at constant volume
e	electron charge
h	Planck's constant, $h/2\pi$
I_i	integrals defined by Eqs. (4)–(6)
$\mathcal{I}_i$	modified transport integrals, Eq. (17)
J_i	transport integrals, Eq. (19)
k	Boltzmann's constant
m^*	effective mass of an electron
M	molecular weight, $\bar{M} = y_1 M_1 + y_2 M_2$
n	electron density
N	Avagadro's number
R	constant of proportionality in the Bloch-Grüneisen relation for ρ
T	temperature
V	atomic volume
v_s	velocity of sound (m/s)
W_{ep}	lattice thermal resistivity due to electron-phonon interactions
W_l	lattice thermal resistivity
W_{pp}	lattice thermal resistivity due to phonon-phonon and phonon-point defect interactions
W_{pp}^*	W_{pp} value for a pure material
W_{Th}	total thermal resistivity at the melting point
W_∞	high temperature limit of W_{ep}
x	dimensionless variable defined by Eq. (7)
x_0	the variable x evaluated at $\omega = \omega_0$
y	atomic fraction
α	the ratio τ_N^{-1}/τ_U^{-1}
α^*	proportionality constant, Eq. (29)
γ	Grüneisen constant

γ_e	electronic specific heat coefficient
Γ	distortion function defined by Eq. (15)
δ	cube root of the atomic volume, $\bar{\delta} = \gamma_1 \delta_1 + \gamma_2 \delta_2$
ϵ	lattice strain factor. Eq. (15)
θ_D	Debye temperature
λ	thermal conductivity
λ_L	lattice thermal conductivity
ρ	electrical resistivity
τ_C	composite relaxation time, Eq. (8)
τ_D	relaxation time for point defect scattering
τ_N	relaxation time for normal phonon scattering processes
τ_{pe}	relaxation time for phonon-electron scattering
τ_u	relaxation time for U-processes
ω	frequency

METHOD FOR ESTIMATING THE LATTICE THERMAL CONDUCTIVITY OF METALLIC ALLOYS

D. W. Yarbrough* and R. K. Williams

ABSTRACT

A method is described for calculating the lattice thermal conductivity of alloys as a function of temperature and composition for temperatures above $\theta_D/2$ using readily available information about the atomic species present in the alloy. The calculation takes into account phonon interactions with point defects, electrons and other phonons. Comparisons between experimental thermal conductivities (resistivities) and calculated values are discussed for binary alloys of semiconductors, alkali halides and metals. A discussion of the theoretical background is followed by sufficient numerical work to facilitate the calculation of lattice thermal conductivity of an alloy for which no conductivity data exist.

INTRODUCTION

This report describes a method for estimating the lattice thermal conductivity of metallic alloys using readily available property data for the alloy components. The goal of the research was to produce a model for making plausible estimates for metallic systems where the lattice thermal conductivity or its reciprocal, lattice thermal resistivity, is unknown. The calculational procedure that resulted takes into account thermal resistivity due to phonon scattering by other phonons, electrons and point defects. Phonon-phonon and phonon-point defect interactions enter the calculation through the relaxation time approach while the phonon-electron contribution to lattice thermal resistivity is estimated from a heuristic correlation of experimental data. The report is organized into sections which outline the development of the various parts of the mathematical model followed by comparisons of experimental with calculated lattice thermal resistivities.

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The theory of the lattice thermal conductivity of nonmetals has been discussed in the literature by a number of authors.¹⁻⁶ A major fraction of the effort has been directed toward simplifications of the Boltzmann equation that make use of relaxation times for the various phonon scattering processes. The relaxation time approach to lattice thermal conductivity calculations has been explored and extended in papers by Callaway,¹⁻³ Holland⁷ and Sharma et al.⁸ Calculation of lattice thermal conductivities using relaxation times requires specification of the temperature dependence of the relaxation times and invariably involves integrals that cannot be evaluated in closed form.

Abeles⁹ used the high temperature limits of the integrals that appear in the relaxation time formulation and published equations that have proven useful for estimating the lattice thermal resistivity of alloys of materials such as silicon and germanium. Kudman¹⁰ has extended this analysis to data for III-V compound semiconductor solid solutions. Ackerman et al.¹¹ have shown that the relaxation time approach can be used to calculate lattice thermal conductivities without the high temperature approximations imposed by Abeles if one is willing to undertake numerical evaluation of modified transport integrals. Calculations of the lattice thermal conductivities of alloys of electrical insulators include consideration of phonon-phonon interactions and phonon-point defect interactions. The symbol W_{pp} is used in the following discussion to denote lattice thermal resistivity resulting from both of the preceding scattering mechanisms.

In metals and alloys conduction electrons scatter phonons and limit the lattice thermal conductivity. This is particularly true in the transition metals at low and intermediate temperatures. Some theoretical calculations of the electron-phonon relaxation time have been published¹² but in our present treatment the electron-phonon resistance, W_{ep} , is evaluated using an empirical correlation. The total phonon resistance, W_l , is then assumed to be given by the sum of two terms.

$$W_l = W_{pp} + W_{ep} \quad (1)$$

The detailed evaluation of the terms in Eq. (1) is presented in the following sections.

THERMAL RESISTIVITY DUE TO PHONON-PHONON AND PHONON-POINT DEFECT INTERACTIONS

The pioneer papers of Callaway¹⁻³ and Klemens⁶ deal with the development of equations for W_{pp} that include point-defect scattering, normal three-phonon processes, U-processes and boundary scattering and form the framework for the present work. Parrott⁴ has summarized much of the earlier work of Callaway and Klemens and has extended Callaway's model to the high temperature region. No attempt has been made in this work to use Parrott's suggestion based on a study of the thermal conductivity of Si-Ge alloys that the ratio of U-process relaxation time to N-process relaxation time be a function of the frequency of the lattice waves, ω . Equation (2) which is the same as Callaway's Eq. (19) is the starting point for the evaluation of W_{pp} .

$$W_{pp}^{-1} = \frac{k}{2\pi^2 v_s} \left(\frac{kT}{h}\right)^3 (I_1 + I_2^2/I_3) \quad (2)$$

The integrals; I_1 , I_2 , and I_3 ; appearing in Eq. (2) are expressed in terms of relaxation times for L-processes, τ_N , U-processes, τ_U , and point-defect scattering, τ_D . Experimental values for the velocity of sound, v_s , are available for many materials. In order, however, to make the calculation accessible with a minimum amount of input information, v_s is calculated in the Debye approximation. This means, of course, that polarization of the acoustical velocity is not taken into account.

$$v_s = 3.977 \theta_D \quad (3)$$

The integrals appearing in Eq. (2) are defined by Eqs. (4-8).

$$I_1 = \int_0^{\theta_D/T} \tau_c x^4 e^x (e^x - 1)^{-2} dx \quad (4)$$

$$I_2 = \int_0^{\theta_D/T} (\tau_c/\tau_N) x^4 e^x (e^x - 1)^{-2} dx \quad (5)$$

$$I_3 = \int_0^{\theta_D/T} (\tau_N)^{-1} (1 - \tau_c \tau_N^{-1}) x^4 e^x (e^x - 1)^{-2} dx \quad (6)$$

$$x = \omega \hbar / kT \quad (7)$$

$$\tau_c^{-1} = \tau_N^{-1} + \tau_U^{-1} + \tau_D^{-1} \quad (8)$$

Equations (2-8) describe the theoretical model for the calculation of W_{pp} . Quantitative results can be obtained if the relaxation times are expressed as functions of temperatures, T , and the vibrational frequencies, ω , in the crystalline solid. Assignments for the temperature and frequency dependencies used for the relaxation times at high temperatures are the same as those used by Klemens.⁶

$$\tau_N^{-1} = A T \omega^2 \quad (9)$$

$$\tau_U^{-1} = B T \omega^2 \quad (10)$$

$$\tau_D^{-1} = C \omega^4 \quad (11)$$

Changes in the temperature dependencies of τ_N^{-1} and τ_U^{-1} at low temperature have not been taken into account in the present work thus limiting the discussion to temperatures above approximately $\theta_D/2$. The constants A and C are specified in terms of a new set of symbols by Eqs. (12-14)¹¹ primarily for mathematical convenience.

The temperature independent parameter α is the ratio of τ_N^{-1}/τ_U^{-1} and is a measure of the relative importance of the two scattering mechanisms.

$$\tau_N^{-1} = \alpha \tau_U^{-1} \quad (12)$$

$$C = \delta^3 \Gamma / 4 \pi v_s^3 \quad (13)$$

$$\tau_D^{-1} = \tau_U^{-1} @ \omega = \omega_0 \quad (14)$$

The calculations completed in this study include the assumption that α is independent of temperature and the assignment $\alpha = 1.8$, which produce a set of formulas containing a single adjustable parameter. Abeles⁹ has treated α as an adjustable parameter and found that $\alpha = 2.5$ results in good agreement between theoretical calculations and measurements of the thermal resistivity of Si-Ge alloys. Kudman¹⁰ obtains $\alpha = 1.5$ from an analysis of data for alloys of III-V semiconductors. The assignment $\alpha = 1.8$ appears to be in the range of the empirically determined values and carries with it a vague aura of theoretical respectability.⁹

The quantity Γ which is a measure of the distortion of the lattice due to impurities or alloying elements can be written in terms of atomic mass and atomic volume differences between the components of the mixture and determines the magnitude of point defect scattering. Calculations in this work were completed using the Abeles expression for Γ , Eq. (15).

$$\Gamma(y) = y(1-y) [(\Delta M/\bar{M})^2 + \epsilon(\Delta\delta/\bar{\delta})^2] \quad (15)$$

The lattice strain term, ϵ , is associated with the introduction of alloying atoms into the lattice and is treated as an adjustable parameter in the present work. Abeles⁹ obtained $\epsilon = 39$ from a theoretical model evaluated using physical properties of silicon and obtained $\epsilon = 45$ from a numerical analysis of the thermal conductivity data for Ga_{1-x}In_xAs. An alternative formulation for Γ given by Ackerman et al.¹¹ was also evaluated.

Equations (2-14) are rearranged to obtain an expression for W_{pp} in terms of modified transport integrals which are defined in Eq. (17).

$$W_{pp}^{-1} = \frac{k^2}{2\pi^2 v_s \hbar B(1+\alpha)} \{ \mathfrak{S}_2(\theta_D/T, x_0) + \alpha \mathfrak{S}_4^2(\theta_D/T, x_0) / \quad (16)$$

$$(\mathfrak{S}_6(\theta_D/T, x_0) + \mathfrak{S}_8(\theta_D/T, x_0) x_0^{-2}) \}$$

$$\mathfrak{S}_n(\theta_D/T) = \int_0^{\theta_D/T} x^n e^x / ((1+x^2/((1+\alpha)x_0^2))(e^x-1)) dx \quad (17)$$

The quantity x_0 which is obtained by combining Eqs. (8-14) is consistent with the equation for x_0 given by Ackerman.¹¹

$$x_0 = (\hbar/k) (4\pi v_s^3 B / 5^3 \Gamma T)^{1/2} \quad (18)$$

The objective at this point in the discussion is to obtain an expression for B that can be evaluated readily. The constant B depends only on phonon-phonon scattering and can, therefore, be obtained from W_{pp}^{-1} for the pure material, W_{pp}^{*-1} , in the high temperature limit.

$$B = \frac{k^2 W_{pp}^*}{2\pi^2 v_s^3 \hbar (1+\alpha)} \{J_2(\theta_D/T) + \alpha J_4^2(\theta_D/T) / J_6(\theta_D/T)\} \quad (19)$$

$$J_n(\theta_D/T) = \int_0^{\theta_D/T} x^n e^x / (e^x - 1) dx \quad (20)$$

A high temperature approximation, the Leibfried and Schlömann Equation (LS) as modified by Julian,¹³ was used in conjunction with a correction factor to be described in a later section to calculate W_{pp}^* . With α defined as 1.8 the bracketed quantity in Eq. (19) approaches $2\theta_D/T$ at high temperature and the specification of B is complete.

$$W_{pp}^{*-1} = 3.343 \times 10^{-8} M \theta^3 / T \gamma^2 \quad (21)$$

All of the quantities required for the calculation of W_{pp}^{-1} using Eq. (16) have been identified. It should be noted that the point-defect scattering enters the calculation via x_0 . The quantity B which is a measure of the three-phonon U-scattering is evaluated using the properties of a "virtual crystal" having the same composition as the alloy of interest. The virtual crystal is a hypothetical, unalloyed material having an appropriately averaged θ_D , γ , atomic mass and volume.

The U-scattering usually is the dominant resistance term at high temperatures, and some caution must be exercised in applying Eq. (21). Extensive tests of this formula have shown that it gives good (~50%) results for inert gas solids¹⁴ and FCC alkali halides that have mass

ratios close to unity.¹⁵ However, the LS formula is much less satisfactory for Si and Ge¹⁵ and results on CsI indicate that it underestimates the lattice resistance of the BCC compound by a factor of about 2. This formula also does not account for all of the temperature dependence of W_{pp}^* .¹¹

The mass-ratio dependence is another complication, which is important in some alloys. Data for insulating compounds show that for large mass-ratios ($m_2/m_1 > 3$ as in the case of InP, AlSb, CsCl) the LS equation underestimates W_{pp}^* by a factor of about 3, while at lower mass-ratios the calculations can be either better or worse.¹⁵ These difficulties with bonding type or crystal structure and mass-ratio probably become especially important at higher temperatures and in concentrated alloys of elements having greatly different masses. Overall, the tests show that the W_{pp}^* estimates should be best for FCC alloys of nearly equal mass (Cu-Ni, Ag-Pd) and may yield estimates which at most could be low by a factor of about 3 for BCC alloys having large mass ratios.

THERMAL RESISTIVITY DUE TO ELECTRON-PHONON INTERACTIONS

Theoretical Background

The purpose of this section is to describe a correlation which can be used to estimate W_{ep} . The electron-phonon interaction severely limits the phonon conductivity of metals at low temperatures, but the resistance, W_{ep} , decreases with temperature, initially as T^{-2} , and should approach a constant value of high temperatures.¹⁶ One theory¹² yields an expression for the high temperature limit of W_{ep} .

$$W_{ep} < \frac{\rho}{T} \left(\frac{e}{k}\right)^2 n^2 \left(\frac{3Nk}{c}\right)^2. \quad (22)$$

The expression for W_{ep} contains the appropriate T dependence, but the magnitude is not defined. This limitation also applied to other more specific formulas, since they are either based on over simplified models¹²

or involve the use of experimental data to describe the electron-phonon interaction.¹⁶

Since the inequality gives the correct T dependence, it is convenient to convert it to an equation for treating experimental data. Then assuming that the Bloch-Grüneisen and Debye formulas hold for the resistivity ρ and the specific heat, c :

$$\rho = \frac{4R}{\theta_D} T \frac{J_5}{(\theta_D/T)^4} \quad (23)$$

$$c = 9Nk J_4 / (\theta_D/T)^3 \quad (24)$$

$$W_{ep} T^2 = \frac{4}{9} R \theta_D \left(\frac{e}{k}\right)^2 n^2 \frac{J_5}{J_4^2} \quad (25)$$

Utilizing the high temperature limit of $9/4$ for $(J_5/(\theta_D/T)^4)/(J_4/(\theta_D/T)^3)^2$, the quantity W_{ep} is written in terms of its high temperature limit, W_∞ :

$$W_{ep} T^2 = \frac{4}{9} \theta_D^2 W_\infty \frac{J_5}{J_4^2} \quad (26)$$

The low temperature limit for $(4/9)(J_5/J_4^2)$ is 0.08196 and Eq. (27) follows.

$$W_{ep} T^2 = 8.196 \times 10^{-2} \theta_D^2 W_\infty \quad (27)$$

This formulation can then be used with appropriate θ_D values and experimental data to express all of the results in terms of the W_∞ parameter. The ratio of transport integrals in Eq. (26) have been evaluated and are tabulated in Appendix A3 for $0.4 \leq \theta_D/T \leq 2.5$. The thermal conductivity calculations that appear later in this report make use of Eq. (26) for the determination of W_{ep} .

Summary of Experimental Information

A set of experimental results are summarized and converted to a common basis in this section and the results are shown in Table 1. The

Table 1. Summary of Numerical Electron-Phonon Thermal Resistance Values

Element	Electronic Specific Heat Coefficient (j/kg at. wt. deg ²)	Debye Temperature (K)	Method Used in Obtaining Data	W_{∞} Value from Eq. (26) (deg m/watt)	Best Current Estimate of W_{∞} (deg m/watt)	Minimum Uncertainty (deg m/watt)
Cu	.693	342	A	.057 E-2	.057 E-2	—
Ag	.659	228	A	.10-.12 E-2	.11 E-2	.02 E-2
Au	.748	165	A	.12-.17 E-2	.15 E-2	.05 E-2
Be	.223	1160	A	.045 E-2 .034 E-2	.04 E-2	.01 E-2
Al	1.36	423	A	.79 E-2	.79 E-2	—
Ga	.598	317	A	.22 E-2	.2 E-2	.02 E-2
		317	B	.18 E-2		
In	1.70	109	A	1.9 E-2	1.9 E-2	—
Sn	1.78	140	A	6.5 E-2	3.7 E-2	2.8 E-2
			B	.81 E-2		
		see text				
Ta	5.84	225	C	12.4 E-2	12.4 E-2	5.6 E-2
Mo	2.10	377	C	3.4 E-2	3.4 E-2	1.3 E-2
W	1.22	388	B	.16 E-2		
		312	C	.88 E-2	.54 E-2	.4 E-2
		312	D	.24 E-2		
Fe	4.98	373	C	2.9 E-2	2.9 E-2	.8 E-2
Pd	10.0	283	A	4.9 E-2	4.9 E-2	1.2 E-2
Pt	6.68	234	A	1.8 E-2	1.8 E-2	1.1 E-2
Sb	.109	150	A	0.16 E-2	0.16 E-2	—

(A) Low (<20 K) temperature data on alloys.

(B) Low (<20 K) temperature magnetoresistance data.

(C) Intermediate (80-100 K) temperature data on alloys.

(D) Intermediate (80-100 K) temperature magnetoresistance data.

literature search was rather cursory, and much of the older work was located through a review article by Klemens.¹⁶ Wherever possible, the discussion includes attempts to define the uncertainties involved in the determination of W_{∞} .

Copper, Silver and Gold

The low temperature alloy studies have been summarized by White et al.¹⁷ and by Kemp and Klemens.¹⁸ W_{ep} values for concentrated alloys tend to be high, and a cusp-like W_{ep} minimum was found by varying the Pd and Cd concentration in Ag.¹⁸ Annealing reduced, but did not eliminate the effect. Therefore, the most appropriate values for elements are obtained from very dilute alloys or extrapolation of values for a series of alloys. For Cu, the data are from a Cu-Fe alloy,¹⁷ for Ag the average of values for Ag-Sn,¹⁷ Ag-Pd and Ag-Cd¹⁸ were used, and for Au the data for Fe,¹⁷ Pt and Cr solutions¹⁹ were extrapolated and averaged to yield the value for W_{∞} shown in Table 1. Debye temperatures from low temperature specific heat measurements²⁰ were used throughout the calculation. The W_{∞} value for Ag seems to be fairly well defined by the data, and a tentative uncertainty of $\pm 15\%$ is based on experimental scatter and a ± 10 K variation in θ_D . On a similar basis, the W_{∞} for Au is uncertain by about $\pm 30\%$, and there is no basis for making an estimate for Cu.

Van Witzenberg and Laubitz²¹ also have reported magnetoresistance measurements which could be used to derive W_{ep} values for Cu, Ag and Au at intermediate temperatures. Unfortunately, calculations involving the modified Wiedemann-Franz Law produce λ_L values which are 2 to 3 times larger than the Leibfried-Schlömann estimate²² so W_{ep} values cannot be obtained from these results. It should be noted that the LS equation usually overestimates the conductivity,²² and thus in this case the magnetic method seems to give a lattice resistance which is too low.

Tungsten

Results on this element can also be used to compare the magnetic and alloying techniques for lattice conductivity determination. The alloy results, obtained using W-Re and W-Ta alloys²³ indicate that the total lattice resistance is about 0.021 deg m/watt at 90 K, and using the LS equation to correct for phonon scattering ($\sim 30\%$) yields a W_{ep} value of about 0.014 at 90 K. This base temperature was chosen because

W_{ep} decreases in importance at higher T . For tungsten, θ_D varies significantly with T and the high T values are lower than those obtained from low T experiments.²⁴ Using a high-temperature θ_D value²⁰ and Eq. (26) produces a W_∞ value of about 0.009 deg m/watt. It is difficult to assess the uncertainties associated with the W_∞ values determined in this fashion. Some obvious difficulties include experimental uncertainties associated with the phonon-phonon resistance correction, failure of the Bloch-Grüneisen model²⁵ and the observation that the W_∞ values derived for transition metals do not strictly follow the theoretical formula. In this case, the first and second sources of uncertainty lead to a band of about $\pm 40\%$ for the W_∞ value, but this is only a lower limit. The estimated uncertainty shown in Table 1 includes a $\pm 7\%$ contribution from the θ_D value.

The magnetoresistance data of von Witeenburg and Laubitz,²¹ which were also obtained at 90 K, can be analyzed along similar lines and yield a W_∞ of 0.0024 deg m/watt. This value is somewhat higher than the W_∞ of 0.0016 which was derived from the low temperature magnetoresistance data of Wagner²⁶ by using a low temperature θ_D of 388 K. Better agreement would be obtained if a consistent θ_D value was used. The situation for tungsten is thus very similar to the results for the noble metals, with the alloy approach yielding higher values for W_{ep} . In this case, since both sets of values are at least plausible, the W_∞ chosen for tungsten was an average, and the range gives a rough measure of the uncertainty.

Platinum and Palladium

Fletcher and Greig have reported²⁷ low T lattice conductivity values derived from data on Pt-Au, Pt-Ir and Pd-Ag alloys. Buhl and Giauque¹⁹ have also determined a W_L value for a Pt-9% W alloy, but this result was not used in the analysis because there is no basis for correcting to infinite solute dilution. The Pd-Ag data are consistent with earlier results²⁹ and indicate that W_∞ is large for this element. Difficulties arise because the W_L values do not exactly show the expected T dependence and the values shown in Table 1 are averaged over the 10-20 K range. This variation also gives a rough lower limit for the uncertainty in the

W_{∞} values, and it should also be noted that the W_{ep} values for Pd-Ag alloys do not show the solute composition dependence noted for Pt, W and the noble metals. The total minimum uncertainty estimate also includes a contribution from the θ_D value.

Molybdenum

The W_{∞} value is based on unpublished data²⁹ on Nb and Zr alloys and a previously reported²³ value for Mo-0.5% Ti is consistent with the later results. The results were analyzed using the method employed for the tungsten alloy data and at 90 K the phonon-phonon resistance correction amounted to about 10%. The derived W_l values do not show consistent trends with composition, and the best value was taken to be an average determined at 90 K. The total minimum uncertainty estimate shown in Table 1 contains contributions from the scatter in the derived W_l values, phonon-phonon resistance correction and the θ_D choice.

Tantalum

Data for Ta-6% W and Ta-12% W alloys were used to define W_{∞} (ref. 30). Data at 80 K were extrapolated to infinite dilution to yield a W_l value of 0.188 deg m/watt and a 9% correction was applied for phonon-phonon scattering. The W_{∞} value found for this element, 0.124 deg m/watt is the highest yet determined, and must be rather uncertain because the λ_p is necessarily small relative to the total λ and thus cannot be determined with much accuracy. The W_{∞} uncertainty estimate shown in Table 1 is based on the calculated uncertainty in the derived W_l values. This error calculation is from a conventional analysis of the errors involved in deriving the W_l from two λ and two ρ measurements.

Iron

Results for three Fe-Cr and one Fe-Cr-Ni alloy were used to determine W_l at 100 K (refs. 31, 32). The data for all four alloys yield W_l values with a range of only 11% so this seems to be a case in which W_l is fairly well defined. A calculated²² phonon-phonon resistance correction amounting to 26% was applied and the room temperature specific heat value for θ_D was used in obtaining W_l . The uncertainty estimate for this element was obtained with the procedure used for Mo and W.

Beryllium

Kohler¹⁶ analyzed magnetoconductivity data obtained near 20 K to obtain an estimate of the lattice conductivity of Be between 12 and 17 W/m K. Assuming that this is within the T^2 - W_{ep} range and using the low temperature specific heat ϵ_D yields an average W_{∞} value of 0.0003 deg m/watt. This value is only about 30% less than the W_{∞} value derived from White and Woods³³ data on a sintered Be specimen, and the two values have been averaged for use in this analysis. The range of these W_{∞} values, plus a contribution due to the uncertainty in ϵ_D , was used to establish the uncertainty estimate shown in Table 1.

Indium

The data of Hulm³⁴ on the isoelectronic alloy In-10% Tl can be analyzed in the conventional way¹⁷ to yield a W_{∞} estimate for In. This was done by using the normal-state data at 4 K for In with the residual resistivity and the Sommerfeld Lorenz number to estimate the electronic conductivity of the alloy. The phonon conductivity, which is presumed to vary as T^2 is obtained by subtraction and combined with the low temperature specific heat ϵ_D to yield a W_{∞} value of 0.019 deg m/watt. This result is somewhat lower than that originally suggested by the author.

Antimony

This element is an anisotropic semimetal, and the results on it are included for the sake of completeness. The data of Rosenberg³⁵ on extruded, polycrystalline Sb at 5 K were corrected for electronic conduction¹⁷ and combined with the low temperature specific heat ϵ_D (ref. 20) to yield the W_{∞} value shown in Table 1. This W_{∞} is comparable to the results on the noble metals, a result which would not be expected if only conduction electron scattering were effective.³⁵ There does not seem to be a good basis for establishing the uncertainty in the W_{∞} values for In and Sb, but they must be at least as large as those found for Ag and Au.

Aluminum

Klaaffky et al.³⁶ obtained data on a series of annealed Al-Mg alloys and derived values for the lattice conductivity of pure, defect free Al in the appropriate (< 20 K) temperature range. This result,

$$W_{ep} T^2 = 1.16 \times 10^2 \quad (\text{deg m/watt})$$

was used in this study.

Gallium

Gorter and Noordermeer³⁷ have presented alloy and magnetoconductivity results on this anisotropic element, and the magnetoconductivity data were used to derive λ_p values along the three principal axes. These results show a maximum anisotropy ratio of 1.6 and the alloy method gave a lattice resistance which was about 15% higher than the magnetoconductivity value for the a axis. The approximate value used in this work was obtained by averaging the three principal conductivities and increasing the mean $W_{ep} T^2$ by 8% to include the alloy value.

Tin

Pernicone and Schroedner³⁸ have published magnetoconductivity data for this element and compared the λ_p results with the alloy data of Karamargin et al.³⁹ The magnetoconductivity data show an anisotropy ratio of about 2.2 and the basal plane λ_p values are about 8 times higher than the results from the alloy work. The discrepancy between the two methods is thus similar to the results for W. Pernicone and Schroeder³⁸ also noted a departure from the usual T^2 dependence and suggested that this was due to the rapid variation of θ_D with T. This variation, the anisotropy, and the disagreement between the two methods were all considered in arriving at the final W_{∞} value shown in Table 1. The θ_D variation was included by using the tabulated λ_p -T values with the appropriate θ_D to calculate individual W_{∞} values at a series of temperatures for both principal axes and averaging these results to get mean values for both principal axes. The anisotropy ratio from magnetoconductivity was used to estimate an (001) alloy λ_p value from the (100) measurement and mean W_{∞} values for both experimental methods were then obtained from the averaging formula¹⁴ for polycrystalline conversions.

Rhodium

The magnetoconductivity data of Natarajan and Chari,⁴⁰ which were obtained on a specimen with a residual resistivity ratio of about 200 by using fields up to only two tesla were also considered and are not

included in the analysis because they indicate a W_{∞} value about an order of magnitude (4×10^{-3} deg m/watt) smaller than the minimum value shown in Table 1. Some of the difficulties associated with this study can be seen by comparing it with the Pernicone and Schroder work in fields up to 10 tesla on specimens with residual resistivity ratio values of 3×10^4 .

Discussion and Correlation of Results for W_{∞}

The resistance values shown in Table 1 range from a low of 0.0004 deg m/watt for Be to 0.124 found for Ta. This variation, which amounts to a factor of 300, is more than 10 times larger than the electrical or thermal conductivity variations for these elements.^{41,42} The enhanced sensitivity probably is due to interactions between phonons and low mobility electrons.²⁷ This indicates that studies of W_{ep} may provide a fairly sensitive probe of the electron-phonon interaction in metals.

Theory^{12,16,43} indicates that the electron-phonon resistance depends on a product of terms, one involving band structure and the other scattering; and this was used as a guide in developing a correlation equation. The theory contains the temperature dependence of ρ , and this can be re-expressed in the usual form:

$$\frac{\rho}{T} = \frac{m^*}{n e^2 \tau_{pe} T} \quad (28)$$

Then, since τ_{pe} is roughly inversely proportional to T at high temperature and the proportionality constant, α^* , is a measure of strength of the scattering:

$$\frac{\rho}{T} = \frac{\alpha^* m^*}{n e^2} \quad (29)$$

This shows that the W_{∞} values should vary as:

$$W_{\infty} \propto \alpha^* n m^* \quad (30)$$

The effective mass is related to the electronic specific heat coefficient, γ_e ; and, since α^* may also depend on the density of states,²⁵ an obvious correlation possibility is suggested. This correlation, which is also contained in Wilson's formula,¹² is shown in Fig. 1. The γ_e values were taken from the literature.^{20,44} Except for Sb, most of the W_m values

Fig. 1. W_m for Pure Metals as a Function of the Electronic Specific Heat Coefficient.

show the expected trend and seem to vary roughly as $\gamma_e^{1.5}$, while the Wilson formula would predict a γ_e^2 dependence. Since the electrical resistivity should also depend on the scattering, it seems logical to include this by introducing the experimental high temperature thermal resistivity or the temperature coefficient of ρ . Except for the Fe data, the correlation shown in Fig. 2 was developed by using total thermal resistivity values for the solid elements at their melting points,⁴² W_{Th} , to define the electronic thermal resistance. The W_{Th} value for Fe was derived from $d\rho/dt$ of paramagnetic Fe⁴⁵ and the Sommerfeld Lorenz number, and this approach was adopted in an attempt

Fig. 2. W_e/W_{Th} for Pure Metals as a Function of the Electronic Specific Heat Coefficient.

to compensate for the additional spin-disorder thermal resistance. This modification of the correlation improves the description of the Sb results, reduces the scatter somewhat, and decreases the dependence of W_∞ on γ_e to about $\gamma_e^{1.3}$. The overall correlation equation

$$\frac{W_\infty}{W_{Th}} = 0.49 \gamma_e^{1.3} \quad (31)$$

overestimates the value for Pt by nearly a factor of 2, but most of the predictions are considerably better than this. Similar correlations can be developed by using the temperature coefficient of ρ (R/θ_D) or introducing the electron-phonon mass enhancement factor.⁴⁶ The R/θ_D correlation:

$$W_\infty = 20 \gamma_e^{1.1} (R/\theta_D) \quad (32)$$

is probably more useful at this time because experimental mass enhancement values are not always available.

These correlations seem to represent a reasonable balance between mathematical complexity (low) and experimental uncertainties (high). A conduction electron concentration dependence is implied, but this is really not a true concentration term and studies²³ show that, with the possible exception of Sb,³⁵ n would not be expected to vary by a large amount. Also, more detailed numerical band structure calculations might be helpful for identifying the band structure and scattering contributions and explaining the deviations from the simple correlations.

Application of these correlations to alloys requires some additional data and analysis. The γ_e values are frequently available for binary solid solution alloys, and of course the scattering corrections, W_{Th} or R/θ_D must be adjusted for the impurity contribution. The general formula can be evaluated at any temperature using tabulated transport integrals.⁴⁷ Because of compensating errors the first two terms of the high temperature series expansion give a good description down to a R/θ_D of about 0.25. Actual applications should probably be limited

to temperatures above the calculated W_i minimum because the data indicate that most of the W_{∞} values are consistently lower than the experimental alloy values.

EVALUATION OF THE MODIFIED TRANSPORT INTEGRALS

Calculation of W_{pp} and W_{ep} using the equations discussed in the preceding paragraphs requires numerical evaluation of several integrals and arithmetic combinations of integrals. The bracketed term in Eq. (16) containing the integrals J_2 , J_4 , J_6 and J_8 has been evaluated for $\alpha = 1.8$ and a range of θ_D/T using 40-point Gauss-Legendre Quadrature. The combination of transport integrals in Eqs. (16) and (18) have also been evaluated for $\alpha = 1.8$ using gaussian quadrature. Tables of the three integral combinations of interest have been prepared and are included as an appendix. Weight factors and base points required for the gaussian quadrature were extracted from Abramowitz and Setgun.⁴⁸ Powell and Rogers⁴⁷ have evaluated the J integrals and have published tables of values that provide a convenient standard for comparison. Comparisons shown in Table 2 between integral evaluations completed as part of this work with values calculated using the Powell and Rogers transport integral tabulations show agreement to at least four significant digits.

Table 2. Comparison of $J_2 + 1.8 J_4^2/J_6$ Values from Two Sources

θ_D/T	Powell & Rogers	This Work
.1	0.19993	0.19993
.5	0.99153	0.99154
1.0	1.93386	1.93386
2.0	3.51644	3.51644
4.0	5.14655	5.14653

LATTICE CONDUCTIVITY OF BINARY SEMICONDUCTOR ALLOYS

Published experimental data for the thermal conductivity of undoped semiconductor alloys provides a convenient test of the model for W_{pp} since the electronic component of the thermal conductivity for these materials is negligible. In order to calculate W_{pp} using Eq. (16) a value for the strain factor, ϵ , must be specified if the Abeles expression for Γ is used.⁹ In this work the strain factor has been treated as an adjustable parameter. The thermal conductivity data selected to test the W_{pp} model and establish an ϵ value for the semiconductor alloys were those of Kudman,¹⁰ Abeles,⁹ Abrahams et al.⁴⁹ and Kudman and Steigmeier.⁵⁰

Kudman has calculated lattice thermal conductivities for the systems GaAs-InAs, GaSb-GaAs, GaSb-InSb and InAs-InP from thermal diffusivity measurements. Data for the system GaSb-InAs published by Abrahams et al. have also been included in the test of the model. Experimental data for the system Si-Ge have been obtained by Abeles⁹ and Kudman and Steigmeier.⁵⁰ All of the preceding data sets are at 300 K.

The failure of the LS equation to give accurate values for W_{pp}^* has been partly compensated by inserting an adjustable parameter in the equation to normalize calculated and measured W_{pp}^* values at 300 K. The LS factors used in the calculations are listed in Table 3 with the other pertinent physical property data.

Consideration has been given to an appropriate averaging scheme for the properties of the virtual crystal. The result is that composition weighted averages have been used for θ_D , γ , M and δ . Abeles et al.⁵¹ have used a modified Lindemann rule combined with melting point data to compute alloy Debye temperatures. Calculations completed as part of this work show that replacing composition averages with the modified Lindemann rule for computing θ_D for the Si-Ge system instead of composition averaging reduces the average difference, based on 10 points, between calculated and experimental values from 19 to 13%. The θ_D based on the modified Lindemann rule clearly improves the agreement between

Table 3. Values Used for Lattice Thermal Conductivity Calculations

Compound (Element)	Molecular (Atomic) Weight	Molecular Atomic Volume (m ³ /G.Mol)	Debye Temperature (K)	Gruneisen Constant	LS Factor (see text)
GaAs	144.64	12.376 E-6	344	.685	3.72
GaSb	191.47	14.780 E-6	265.5	.685	3.00
InAs	189.74	14.301 E-6	249	.685	3.03
InSb	236.57	16.941 E-6	202.5	.685	3.45
InP	145.79	14.827 E-6	321	.685	2.14
Si	28.09	13.64 E-6	692	.57	4.70
Ge	72.59	12.07 E-6	403	.80	4.90
KCl	74.56	18.82 E-6	220	1.46	.98
KBr	119.02	21.64 E-6	160	1.33	2.06
RbCl	120.92	21.90 E-6	190	1.45	2.64
Fe	55.85	7.094 E-6	373	1.81	1.00
Cr	52.01	7.231 E-6	424	1.53	1.00
Ni	58.71	6.593 E-6	345	2.00	1.00
W	183.86	9.551 E-6	312	1.78	1.00
Re	186.22	8.860 E-6	275	2.66	1.00
Ta	180.95	10.80 E-6	225	1.82	1.00

calculated and measured W_{pp} and should be used when the required melting point data are available. Experimental θ_D values derived from specific heat data for the alloy are also preferred, if available.

Calculations of W_{pp} as a function of composition at 300 K have been completed for the six semiconducting systems for a range of ϵ values from 39 to 15 and an α of 1.8. Inspection of the calculated W_{pp} curves indicates that an $\epsilon = 75$ is a reasonable compromise value which results in agreement between calculated and experimental results to within approximately $\pm 25\%$ if two points on the Si-Ge curve given by Kudman and Steigmeier are discounted in favor of the later Si-Ge data obtained by Abeles.

Figure 3 is a plot of the difference between calculated and experimental W_{pp} for the seven sets of data that were considered. There is

Fig. 3. Comparison of Calculated and Measured Lattice Thermal Resistivities for Binary Alloys of Semiconductors at 300 K (●Data of Abrahams et al.,⁴⁹ ▼Data of kudman and Steigmeier⁵⁰).

a noticeable upward trend in the collection of points shown in Fig. 3. The model tends to overestimate the W_{pp} for alloys concentrated in the heavy component and underestimates W_{pp} for the alloys concentrated in the light component. The appearance of the upward trend in the results in Fig. 3 is due in large part to the presence of data for the Si-Ge system. Figure 4 is a plot of percent differences between calculated and observed W_{pp} values. It has been observed that the incorrect skewness in the calculated curve for W_{pp} for the Si-Ge system is not due entirely to the way in which Γ is defined.

Ackerman's definition for Γ has also been used to calculate W_{pp} values for the semiconductor alloys.¹¹ The lines shown in Fig. 5 are the least square representations of results obtained using Ackerman's expression for Γ or the Abeles formulation. Both lines exhibit the skew of the calculated results that was mentioned above although the Ackerman treatment reduces the effect slightly. The W_{pp} values calculated with

Fig. 4. Differences Between Experimental and Measured W_{pp} for Binary Alloys of Semiconductors at 300 K Expressed as Percentage of Measured Value.

Fig. 5. Comparison of Lattice Thermal Resistivities for Semiconducting Alloys Calculated Using Alternative Γ Formulations.

the Abeles Γ and the adjusted value for ϵ compare more closely with the measured values than those calculated using Ackerman's Γ . The line in Fig. 5 representing calculations with Ackerman's Γ was obtained using $\alpha = 1.8$ and no adjustable parameters other than the LS factors for the pure components. Ackerman's formulation with α treated as an adjustable parameter could be used to describe the data under discussion. For example, the 300 K Si-Ge data⁹ can be described using Ackerman's Γ and an α value of approximately three.

LATTICE THERMAL CONDUCTIVITY OF ALKALI HALIDE ALLOYS

The model for calculating W_{pp} has also been tested by comparing calculated and measured results for a limited amount of alkali halide data. Anthony and Wurst⁵² have measured lattice thermal conductivities for KCl and the binary alloys KCl-5% KBr and KCl-5% RbCl as a function of temperature. The data required for determination of LS factors were

obtained from Moore et al.¹⁵ for RbCl, Anthony and Wurst⁵² for KCl and McCarthy and Ballard⁵³ for KBr. Table 3 contains the numerical data that were used in the alkali halide calculations.

Results for the calculation of W_{pp} for the alkali halide alloys for which data are available are summarized in Fig. 6 in terms of percentage deviation of calculated from measured values. The points shown for alloys were obtained using $\alpha = 1.8$ and $\epsilon = 40$. As indicated in the figure, the complete set of alloy data are described to within $\pm 20\%$ using the above parameters. The average deviation for the two sets of alloy data is 11%.

A series of points are also shown in Fig. 6 for KCl. The KCl data were included to provide an additional measure of the adequacy of the model to predict the variation of W_{pp} with temperature. It can also be

Fig. 6. Comparison of Calculated and Measured Lattice Thermal Resistivities of KCl and the Binary Alloys KCl-5% KBr and KCl-5% RbCl.

seen that the model correctly predicts the magnitude of the thermal conductivity for this nearly unit mass ratio, FCC alkali halide.

In summary, Eq. (16) gives results for the alloys KCl-5% and KCl-5% RbCl using $\sigma = 1.8$ and $\epsilon = 40$ that are comparable in accuracy with results obtained for the semiconductor alloys. Additional alkali halide data are needed to provide for a thorough test of the W_{pp} model and refinement of the value for ϵ for alkali halide solid solutions.

LATTICE THERMAL CONDUCTIVITY OF METALLIC ALLOYS

The final test of the model for the lattice thermal conductivity is a comparison of predicted with measured λ_l for alloys having a non-negligible W_{ep} . Unfortunately, the collection of binary alloy data available for comparison is somewhat limited. The determination of the lattice component of the thermal conductivity is complicated by the fact that there is no universally accepted procedure for making the determination. The experimental data used in this section were obtained from thermal conductivity measurements using the two alloy separation technique described by Williams and Fulkerson.²³ Values obtained for the lattice thermal conductivity using the two alloy separation were extrapolated to zero alloying element content to provide best estimates for λ_l and the Lorenz function, $L(T)$, for the pure metal.³² Values for W_l (or λ_l) were then obtained using the electrical resistivity and Lorenz function of the pure metal and the electrical resistivity of the element to calculate λ_e (ref. 23). LS factors used in the calculations for the metal alloys were one in all cases. Epsilon values from 25 to 75 were used to generate lattice thermal resistivities for the tungsten base and iron base alloys discussed in the following two sections. A value $\epsilon = 40$ was chosen after an examination of the differences between experimental and calculated λ_l values. The remaining input information required to complete the calculation is given in Table 3.

Tungsten Base Alloys

Thermal conductivity and electrical resistivity data for tungsten and two alloys of tungsten and rhenium have been analyzed by Williams and Fulkerson²³ to provide λ_L and $L(T)$ as a function of temperature for tungsten. The results obtained for the lattice thermal conductivity of tungsten were extrapolated to zero rhenium content and used to calculate λ_L for the W-Re alloys.⁵⁴ Thermal conductivity and electrical resistivity measurements for a single W-Ta alloy⁵⁴ were combined with the pure tungsten λ_L to provide an additional set of points for the correlation shown in Fig. 7. A series of points for unalloyed W are also shown in the figure. Table 4 contains a listing of the values obtained for W_{pp} and W_{ep} for the three tungsten alloys that were considered.

Fig. 7. Comparison of Calculated and Measured Lattice Thermal Resistivities of Several Binary Metal Alloys.

Table 4. Calculated Values for W_{ep} and W_{pp} for
Binary Alloys of Fe-Cr, Fe-Ni, W-Re and W-Ta^a

T(K)	Fe + 1.14% Cr		Fe + 2.96% Cr		Fe + 3.15% Ni		W + 2.8% Re		W + 5.4% Re		W + 1.5% Ta	
	W_{pp}	W_{ep}	W_{pp}	W_{ep}	W_{pp}	W_{ep}	W_{pp}	W_{ep}	W_{pp}	W_{ep}	W_{pp}	W_{ep}
100	.0264 ^b	.0726	.0266	.0722	.0313	.0732	.0158	.0072	.0192	.0073	.0174	.0077
140	.0309	.0570	.0310	.0566	.0357	.0576	.0183	.0060	.0220	.0061	.0200	.0064
180	.0365	.0511	.0365	.0507	.0414	.0516	.0212	.0056	.0252	.0056	.0229	.0059
220	.0426	.0482	.0426	.0478	.0476	.0487	.0242	.0053	.0285	.0054	.0260	.0057
260	.0490	.0466	.0489	.0462	.0541	.0471	.0274	.0052	.0318	.0053	.0291	.0056
300	.0556	.0456	.0554	.0452	.0607	.0461	.0306	.0051	.0352	.0052	.0323	.0055
340	.0623	.0449	.0619	.0446	.0676	.0454	.0338	.0051	.0386	.0051	.0355	.0054
380	.0690	.0444	.0686	.0441	.0744	.0449	.0371	.0050	.0421	.0051	.0387	.0054

^a The entries in this table were computed using $\alpha = 1.8$ and $\epsilon = 40$.

^b $\text{watt}^{-1} \text{ m K}$.

Iron Base Alloys

Thermal conductivity and electrical resistivity data for two Fe-Cr alloys and a single Fe-Ni alloy have been collected and analyzed by Holder.³² Holder's alloy data and values for λ_l of Fe provide the basis for comparing predicted and measured W_l values shown in Fig. 7. The lattice conductivity of iron was obtained using the two alloy separation calculation applied to the Fe-Cr data. Lattice thermal resistivities for the Fe-Ni alloy were computed using λ_l for Fe deduced from the Fe-Cr measurements. The W_{ep} and W_{pp} values obtained for the three iron-base alloys considered are shown in Table 4.

The differences between measured and calculated lattice thermal resistivities shown in Fig. 7 are larger than the corresponding differences shown for the semiconductor alloys or the alkali halide data. This last set of comparisons, however, involves the estimation of W_{ep} as well as the calculation of W_{pp} . Lattice conductivity values for the metals are also burdened by the fact that they are not measured directly but rather must be deduced from thermal conductivity and electrical resistivity measurements with the aid of a mathematical model. Indications are, however, that the procedure described in this report can conservatively provide W_l (or λ_l) estimates to within a factor of 2.

Copper-Nickel and Silver-Palladium Alloys

Figures 8 and 9 compare lattice thermal conductivity values given by Ackerman et al.¹¹ with values obtained in this study. The curves shown for the Cu-Ni alloy and the Ag-Pd alloy illustrate the magnitude of the difference between the two sets of calculations. The present calculations for the Cu-Ni and Ag-Pd alloys followed the pattern for the other sets of calculations that have been discussed except that electronic specific heat coefficients for the alloys^{55,56} were used rather than composition averages of the coefficients for the constituent elements.

The curves obtained in this work differ significantly from Ackerman's values because of the inclusion of an estimate for W_{ep} in the present calculation and because of differences in the strain factor.

Fig. 8. Lattice Thermal Conductivity for a 50% Cu and 50% Ni Alloy.

Fig. 9. Lattice Thermal Conductivity for a 50% Ag and 50% Pd Alloy.

Results obtained for W_{ep} and W_{pp} that are shown in Table 5 show that there is a decrease of approximately 18% in the predicted lattice conductivity for the Cu-Ni alloy at 300 K resulting from the W_{ep} term. The corresponding reduction for the Ag-Pd alloy is 2.4%. A significant fraction, therefore, of the differences between the two curves shown for Cu-Ni or Ag-Pd are due to differences in the magnitude of the strain factor. Curves which approach Ackerman's values can be generated using Eqs. (15) and (16) with epsilon values in the range 10 to 25. In view of the observation that the several data sets discussed earlier in the report were best described using ϵ values of 40 or 75 there is no justification available for reducing ϵ to well below 40 for the Cu-Ni or Ag-Pd systems.

Table 5. Calculated Values for W_{ep} and W_{pp} for 50-50 Alloys of Cu-Ni and Ag-Pd^a

Temperature (K)	Cu-Ni		Ag-Pd	
	W_{pp}	W_{ep}	W_{pp}	W_{ep}
100	.0759 ^b	.0416	.1728	.0093
200	.1034	.0306	.2461	.0077
300	.1329	.0287	.3129	.0074
400	.1625	.0281	.3755	.0073
500	.1919	.0278	.4355	.0073
600	.2212	.0276	.4937	.0073

^aEntries in this table were computed using $\alpha = 1.8$, $\epsilon = 40$, $\gamma_e = 1.6$ j/kg at. wt. deg² for the Ag-Pd alloy, and $\gamma_e = 7$ j/kg at. wt. deg² for the Cu-Ni alloy.

^b W_{watt}^{-1} m K.

DISCUSSION AND CONCLUSIONS

The method for calculating the lattice thermal conductivity of alloys that has been detailed in the opening sections of this report has been compared with experimental data for 13 binary alloys. Systems for which calculations were completed include alkali halide alloys, alloys of semiconductor materials and binary metallic alloys. For each binary alloy studied, results for the lattice thermal resistivity were computed for a fixed α of 1.8 and a range of ϵ values. Recommended values for ϵ were chosen after a study of the comparisons of calculated with experimental W_ℓ values. In the case of the semiconductor alloys a value $\epsilon = 75$ was chosen as representative. An $\epsilon = 40$ was chosen as the recommended value for the alkali halide and metallic alloy data. The separation of the points shown in Fig. 7 into a magnetic (Fe) group and a non-magnetic (W) group suggests a refinement of the model which would distinguish between magnetic and non-magnetic materials.

Epsilon was chosen to be adjustable rather than the ratio α since a plausible value for α has been established in the literature. The choice of ϵ as an adjustable parameter in the model is also tied in part to the use of the Abeles formulation for Γ rather than the Ackerman formulation. The Abeles Γ was chosen since the expression is readily extended to multicomponent alloys and at least for $\alpha = 1.8$ the calculated results for W_ℓ agree more closely with the measured values than those obtained using Ackerman's Γ .

Comparisons between calculated and measured λ values for the semiconductor alloys and the alkali halide alloys establish an error bound on the calculation of $\pm 30\%$. The quality of the numerical calculation can be improved if data for the system in question or for similar systems are available to establish an epsilon value.

Further testing of this and other theoretical models for the lattice thermal conductivity is dependent on continued expansion of the alloy data collection which can be used to determine lattice conductivity. At present the alloy separation technique appears to be the most promising approach for obtaining λ_ℓ but requires highly accurate thermal conductivity measurements. Data for binary systems such as Fe-Ti or Fe-V where the

effect of alloying on the lattice thermal conductivity is anticipated to be large would represent a meaningful test of the calculational procedure outlined in this report. The collection of experimental data available for alkali halide solid solutions is small and should be expanded to provide for a better understanding of that type of system.

The extension of the present calculation for the lattice thermal conductivity of alloys has not been tested against data for ternary or higher alloys. Calculation of λ_l for multicomponent alloys can be accomplished within the framework of the present model but a method for the analysis of experimental data to obtain λ_l values for a multicomponent alloy has not been embraced by researchers in the field. Obvious numerical refinements of the model such as optimization of the data fit by parameter adjustment or modification of Γ are being pursued as part of the present project.

REFERENCES

1. J. Callaway, *Phys. Rev.* 113: 1046 (1959).
2. J. Callaway and H. C. von Baeyer, *Phys. Rev.* 120: 1149 (1960).
3. J. Callaway, *Phys. Rev.* 122: 787 (1961).
4. J. E. Parrott, *Proc. Phys. Soc.* 81: 726 (1963).
5. P. G. Klemens, *Proc. Roy. Soc.* 68(A): 1113 (1955).
6. P. G. Klemens, *Solid State Physics*, Vol. 7 Ed., F. Seitz and D. Turnbull, Academic Press (1958).
7. M. G. Holland, *Phys. Rev.* 132: 2461 (1963).
8. P. C. Sharma, K. S. Dubey and G. S. Verma, *Phys. Rev. (B)* 4: 1306 (1971).
9. B. Abeles, *Phys. Rev.* 131: 1906 (1963).
10. I. Kudman, *Proc. of the Seventh International Conference on Thermal Conductivity*, pp. 97-102, 1967.
11. M. W. Ackerman, K. Y. Wu and C. Y. Ho, *Proc. of the Fourteenth International Conf. on Thermal Conductivity*, p. 245, 1975.
12. A. H. Wilson, "The Theory of Metals," Cambridge University Press, pp. 294-295, 1953.
13. C. L. Julian, *Phys. Rev.* 137(1A): 128 (1965).
14. G. K. White and S. B. Woods, *Phil. Mag.* 3H: 785 (1958).
15. J. P. Moore, R. K. Williams and R. S. Graves, *Phys. Rev. B* 11: 3107 (1975).
16. P. G. Klemens, "Thermal Conductivity of Solids at Low Temperatures," *Handbuch Der Physik*, pp. 253-255, 259-266, 1965.
17. G. K. White, S. B. Woods and M. T. Eiford, *Phil. Mag.* 4: 688 (1959).
18. W.R.G. Kemp and P. G. Klemens, *J. Phys.* 13: 247 (1960).
19. A. J. Buhl and W. F. Giauque, *Rev. Sci. Instr.* 36: 703 (1965).
20. K. A. Gschneidner, Jr., "Physical Properties and Interrelationships of Metallic and Semimetallic Elements," *Solid State Physics*, Vol. 10, Ed. C. Y. Ho and R. E. Taylor, Plenum Press, pp. 389-456 (1969).
21. W. van Witzenburg and M. J. Laubitz, *Can. J. Phys.* 46: 1887 (1968).
22. J. P. Moore, R. K. Williams and R. S. Graves, *Phys. Rev. (B)* 11: 3107 (1975).

23. R. K. Williams and W. Fulkerson, "Separation of the Electronic and Lattice Contributions to the Thermal Conductivity of Metals and Alloys," *Thermal Conductivity*, Proc. of the 8th Conf. Ed. C. Y. Ho and R. E. Taylor, Plenum Press, pp. 389-456 (1969).
24. S. H. Chen and B. N. Brockhouse, *Solid State Comm.* 2: 73 (1964).
25. R. K. Williams, *J. Appl. Phys.* 46: 475 (1975).
26. D. K. Wagner, *Phys. Rev. (B)* 5: 336 (1972).
27. R. Fletcher and D. Greig, *Phil. Mag.* 16: 303 (1907).
28. W.R.G. Kemp, P. G. Klemens, A. K. Sreedhar and G. K. White, *Proc. Roy. Soc. (London)* A233: 480 (1956).
29. R. K. Williams, J. P. Moore and R. S. Graves, ORNL-5089, pp. 29-30 (October 1975).
30. R. K. Williams, J. P. Moore and D. L. McElroy, *Thermal Conductivity*, Proc. of the 10th Conf. Ed. pp. VII 9-VII 10 (1970).
31. J. W. Masey, M.S. Thesis, Tennessee Technological University, Cookeville, Tennessee (1977).
32. T. K. Holder, ORNL/TM-5539 (June 1977).
33. G. K. White and S. B. Woods, *Can. J. Phys.* 33: 58 (1955).
34. J. K. Hulm, NBS Circular 519 pp. 37-41 (1952).
35. H. M. Rosenberg, *Phil. Trans. Roy. Soc. (London) Ser. A* 247: 441 (1955).
36. R. W. Klaffky, N. S. Mohan and D. H. Damon, *Phys. Rev. (B)* 11: 1297 (1975).
37. F. W. Gorter and L. J. Noordermeer, *Physica* 46: 507 (1970).
38. J. R. Pernicone and P. A. Schroder, *Phys. Rev. (B)* 11: 588 (1975).
39. M. C. Karamargin, C. A. Reynolds, F. P. Eifschultz and P. G. Klemens, *Phys. Rev. (B)* 6: 3624 (1972).
40. N. S. Natarajan and M.S.R. Chari, *Indian J. Pure and Appl. Phys.* 9: 439 (1971).
41. G. T. Meaden, "Electrical Resistance of Metals," Plenum Press, New York, pp. 15-18 (1965).
42. C. Y. Ho, R. W. Powell and P. E. Liley, *J. Phys. Chem. Ref. Data* 1: 279 (1972).
43. J. M. Ziman, *Electrons and Phonons*, Oxford at the Clarendon Press, pp. 320-322 (1960).

44. R. Hultgren, P. D. Desai, D. T. Hawkins, M. Glaisien and K. Kelley, "Selected Values of the Thermodynamic Properties of the Elements," American Society for Metals (1973).
45. W. L. McMillan, *Phys. Rev.* 167: 331 (1968).
46. W. Fulkerson, J. P. Moore and D. L. McElroy, *J. Appl. Phys.* 37: 2639 (1966).
47. W. M. Rogers and R. C. Powell, "Tables of Transport Integrals," NBS Circular 595 (1958).
48. M. Abramowitz and I. A. Stegun, *Handbook of Mathematical Functions*, NBS Applied Math Series 55, U.S. Government Printing Office (1964).
49. M. S. Abrahams, R. Braunstein and F. D. Rosi, *J. Phys. Chem. Solids* 10: 204 (1959).
50. I. Kudman and E. F. Steigmeier, Proc. of the Fourth Conference on Thermal Conductivity, pp. IV-D 1-9 (1964).
51. B. Abeles, D. S. Beers, G. D. Cody and J. P. Dismukes, *Phys. Rev.* 125: 44 (1962).
52. P. J. Anthony and J. C. Wurst, *J. Am. Ceram. Soc.* 57: 504 (1974).
53. Kathryn A. McCarthy and Stanley S. Ballard, *J. Appl. Phys.* 31: 1410 (1960).
54. J. P. Moore, unpublished data for the thermal conductivity and electrical resistivity of W-Re alloys and a W-Ta alloy.
55. G. M. Stocks, R. W. Williams and J. S. Faulkner, *Phys. Rev. (B)* 4: 4390 (1971).
56. F. E. Hoare and B. Yates, *Proc. of the Royal Soc. (London)* 240: 42 (1957).

APPENDIX A

Table A-1. Values for $J_2 + 1.8 J_4^2/J_6$ Computed Using 40 Point Gauss-Legendre Quadrature

θ_D/T	0.0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9
0.0	—	0.19993	0.39945	0.59816	0.79565	0.99154	1.18542	1.37695	1.56575	1.75150
1.0	1.93386	2.11255	2.28726	2.45776	2.62380	2.78518	2.94171	3.09322	3.23959	3.38069
2.0	3.51644	3.64679	3.77167	3.89109	4.00503	4.11351	4.21659	4.31431	4.40675	4.49399
3.0	4.57614	4.65331	4.72562	4.79320	4.85620	4.91477	4.96905	5.01921	5.06540	5.10778
4.0	5.14653	4.18180	5.21377	5.24258	5.26841	5.29141	5.31174	5.32956	5.34500	5.35822
5.0	5.36936	5.37855	—	—	—	—	—	—	—	—

Table A-2. Values for $I_2 + \alpha I_4^2 / (I_6 + T_8/x_0^2)$ Computed Using
40 Point Gauss-Legendre Quadrature

x_0	$\theta_D/T:0.1$	0.2	0.3
0.1	0.179861	0.383344	0.718571
0.2	0.191376	0.359354	0.536108
0.3	0.195674	0.373276	0.538114
0.4	0.197436	0.382363	0.552647
0.5	0.198303	0.387693	0.564334
0.6	0.198789	0.390949	0.572575
0.7	0.199087	0.393048	0.578336
0.8	0.199282	0.394469	0.582437
0.9	0.199417	0.395471	0.585429
1.0	0.199514	0.396201	0.587663
1.1	0.199586	0.396750	0.589370
1.2	0.199641	0.397171	0.590699
1.3	0.199683	0.397502	0.591752
1.4	0.199718	0.397766	0.592600
1.5	0.199745	0.397980	0.593292
1.6	0.199768	0.398156	0.593864
1.7	0.199786	0.398303	0.594341
1.8	0.199802	0.398426	0.594744
1.9	0.199815	0.398530	0.595087
2.0	0.199827	0.398620	0.595381
2.1	0.199836	0.398697	0.595635
2.2	0.199845	0.398763	0.595856
2.3	0.199852	0.398822	0.596049
2.4	0.199859	0.398873	0.596219
2.5	0.199864	0.398919	0.596369
2.6	0.199869	0.398959	0.596503
2.7	0.199874	0.398995	0.596622
2.8	0.199878	0.399027	0.596729
2.9	0.199882	0.399056	0.596826
3.0	0.199885	0.399082	0.596912
3.1	0.199888	0.399105	0.596991
3.2	0.199891	0.399127	0.597063
3.3	0.199893	0.399146	0.597128
3.4	0.199895	0.399164	0.597187
3.5	0.199897	0.399180	0.597242
3.6	0.199899	0.399195	0.597292
3.7	0.199901	0.399209	0.597338
3.8	0.199902	0.399222	0.597381
3.9	0.199904	0.399234	0.597420
4.0	0.199905	0.399244	0.597456
4.1	0.199907	0.399254	0.597490
4.2	0.199908	0.399264	0.597522
4.3	0.199909	0.399273	0.597551
4.4	0.199910	0.399281	0.597578
4.5	0.199911	0.399288	0.597604
4.6	0.199912	0.399296	0.597628
4.7	0.199913	0.399302	0.597650
4.8	0.199913	0.399308	0.597671
4.9	0.199914	0.399314	0.597691
5.0	0.199915	0.399320	0.597710

Table A-2. Continued

X_0	$\theta_0/T_{\infty,4}$	0.5	0.6
0.1	0.126975 E1	0.209998 E1	0.327256 E1
0.2	0.757343	0.104668 E1	0.142173 E1
0.3	0.708389	0.900874	0.112774 E1
0.4	0.715780	0.682424	0.106214 E1
0.5	0.730466	0.891999	0.105572 E1
0.6	0.743530	0.906687	0.106642 E1
0.7	0.753791	0.920502	0.108106 E1
0.8	0.761629	0.932121	0.109529 E1
0.9	0.767618	0.941557	0.110782 E1
1.0	0.772240	0.949151	0.111845 E1
1.1	0.775855	0.955273	0.112735 E1
1.2	0.778722	0.960240	0.113478 E1
1.3	0.781026	0.964303	0.114098 E1
1.4	0.782901	0.967655	0.114618 E1
1.5	0.784445	0.970446	0.115058 E1
1.6	0.785730	0.972789	0.115430 E1
1.7	0.786809	0.974773	0.115749 E1
1.8	0.787724	0.976465	0.116023 E1
1.9	0.788506	0.977910	0.116259 E1
2.0	0.789178	0.979175	0.116465 E1
2.1	0.789761	0.980268	0.116645 E1
2.2	0.790270	0.981225	0.116803 E1
2.3	0.790716	0.982066	0.116942 E1
2.4	0.791109	0.982810	0.117066 E1
2.5	0.791457	0.983470	0.117176 E1
2.6	0.791767	0.984059	0.117274 E1
2.7	0.792045	0.984587	0.117362 E1
2.8	0.792293	0.985061	0.117442 E1
2.9	0.792517	0.985488	0.117514 E1
3.0	0.792720	0.985875	0.117579 E1
3.1	0.792903	0.986226	0.117638 E1
3.2	0.793070	0.986546	0.117692 E1
3.3	0.793222	0.986838	0.117741 E1
3.4	0.793362	0.987105	0.117786 E1
3.5	0.793489	0.987350	0.117828 E1
3.6	0.793606	0.987576	0.117866 E1
3.7	0.793714	0.987783	0.117901 E1
3.8	0.793814	0.987975	0.117934 E1
3.9	0.793906	0.988153	0.117964 E1
4.0	0.793992	0.988318	0.117992 E1
4.1	0.794071	0.988471	0.118018 E1
4.2	0.794145	0.988613	0.118042 E1
4.3	0.794214	0.988746	0.118065 E1
4.4	0.794278	0.988870	0.118086 E1
4.5	0.794338	0.988986	0.118106 E1
4.6	0.794394	0.989094	0.118124 E1
4.7	0.794447	0.989196	0.118142 E1
4.8	0.794497	0.989292	0.118158 E1
4.9	0.794543	0.989381	0.118173 E1
5.0	0.794587	0.989466	0.118188 E1

Table A-2. Continued

X_0	$\theta_0/T=0.7$	0.8	0.9
0.1	0.484779 E1	0.688223 E1	0.942816 E1
0.2	0.189763 E1	0.248838 E1	0.320653 E1
0.3	0.139739 E1	0.171833 E1	0.209499 E1
0.4	0.126230 E1	0.148845 E1	0.174481 E1
0.5	0.122771 E1	0.141283 E1	0.161485 E1
0.6	0.122735 E1	0.139361 E1	0.156859 E1
0.7	0.123872 E1	0.139678 E1	0.155817 E1
0.8	0.125328 E1	0.140858 E1	0.156359 E1
0.9	0.126773 E1	0.142305 E1	0.157568 E1
1.0	0.128088 E1	0.143761 E1	0.159007 E1
1.1	0.129240 E1	0.145116 E1	0.160465 E1
1.2	0.130234 E1	0.146334 E1	0.161848 E1
1.3	0.131086 E1	0.147411 E1	0.163114 E1
1.4	0.131815 E1	0.148353 E1	0.164255 E1
1.5	0.132440 E1	0.149176 E1	0.165272 E1
1.6	0.132978 E1	0.149894 E1	0.166174 E1
1.7	0.133442 E1	0.150522 E1	0.166974 E1
1.8	0.133844 E1	0.151071 E1	0.167682 E1
1.9	0.134194 E1	0.151554 E1	0.168310 E1
2.0	0.134501 E1	0.151979 E1	0.168868 E1
2.1	0.134770 E1	0.152355 E1	0.169365 E1
2.2	0.135008 E1	0.152689 E1	0.169809 E1
2.3	0.135219 E1	0.152967 E1	0.170206 E1
2.4	0.135406 E1	0.153252 E1	0.170563 E1
2.5	0.135574 E1	0.153490 E1	0.170884 E1
2.6	0.135724 E1	0.153705 E1	0.171174 E1
2.7	0.135859 E1	0.153898 E1	0.171436 E1
2.8	0.135981 E1	0.154073 E1	0.171674 E1
2.9	0.136091 E1	0.154231 E1	0.171890 E1
3.0	0.136191 E1	0.154376 E1	0.172088 E1
3.1	0.136283 E1	0.154508 E1	0.172269 E1
3.2	0.136366 E1	0.154628 E1	0.172434 E1
3.3	0.136442 E1	0.154738 E1	0.172586 E1
3.4	0.136512 E1	0.154840 E1	0.172726 E1
3.5	0.136577 E1	0.154933 E1	0.172855 E1
3.6	0.136636 E1	0.155019 E1	0.172974 E1
3.7	0.136691 E1	0.155099 E1	0.173084 E1
3.8	0.136741 E1	0.155173 E1	0.173186 E1
3.9	0.136788 E1	0.155241 E1	0.173281 E1
4.0	0.136832 E1	0.155305 E1	0.173369 E1
4.1	0.136872 E1	0.155364 E1	0.173451 E1
4.2	0.136910 E1	0.155419 E1	0.173528 E1
4.3	0.136945 E1	0.155470 E1	0.173600 E1
4.4	0.136978 E1	0.155519 E1	0.173667 E1
4.5	0.137009 E1	0.155564 E1	0.173730 E1
4.6	0.137038 E1	0.155607 E1	0.173789 E1
4.7	0.137065 E1	0.155646 E1	0.173845 E1
4.8	0.137091 E1	0.155684 E1	0.173897 E1
4.9	0.137115 E1	0.155719 E1	0.173946 E1
5.0	0.137137 E1	0.155752 E1	0.173992 E1

Table A-2. Continued

x_0	$\theta_D/T=1.0$	1.5	2.0
0.1	0.125331 E2	0.377269 E2	0.807972 E2
0.2	0.406368 E1	0.107471 E2	0.218528 E2
0.3	0.253298 E1	0.577715 E1	0.109565 E2
0.4	0.203473 E1	0.406653 E1	0.716464 E1
0.5	0.183663 E1	0.330317 E1	0.543211 E1
0.6	0.175498 E1	0.291474 E1	0.451312 E1
0.7	0.172537 E1	0.270373 E1	0.397996 E1
0.8	0.172050 E1	0.258658 E1	0.365321 E1
0.9	0.172745 E1	0.252276 E1	0.344660 E1
1.0	0.173974 E1	0.249061 E1	0.331421 E1
1.1	0.175404 E1	0.247771 E1	0.322970 E1
1.2	0.176861 E1	0.247662 E1	0.317702 E1
1.3	0.178260 E1	0.248269 E1	0.314594 E1
1.4	0.179563 E1	0.249300 E1	0.312970 E1
1.5	0.180753 E1	0.250567 E1	0.312371 E1
1.6	0.181830 E1	0.251948 E1	0.312479 E1
1.7	0.182799 E1	0.253367 E1	0.313070 E1
1.8	0.183669 E1	0.254775 E1	0.313987 E1
1.9	0.184449 E1	0.256140 E1	0.315115 E1
2.0	0.185148 E1	0.257446 E1	0.316374 E1
2.1	0.185775 E1	0.258682 E1	0.317705 E1
2.2	0.186339 E1	0.259845 E1	0.319066 E1
2.3	0.186847 E1	0.260934 E1	0.320429 E1
2.4	0.187305 E1	0.261950 E1	0.321772 E1
2.5	0.187720 E1	0.262897 E1	0.323082 E1
2.6	0.188095 E1	0.263777 E1	0.324349 E1
2.7	0.188437 E1	0.264595 E1	0.325567 E1
2.8	0.188747 E1	0.265356 E1	0.326733 E1
2.9	0.189031 E1	0.266062 E1	0.327845 E1
3.0	0.189290 E1	0.266719 E1	0.328904 E1
3.1	0.189527 E1	0.267330 E1	0.329909 E1
3.2	0.189745 E1	0.267899 E1	0.330862 E1
3.3	0.189946 E1	0.268429 E1	0.331765 E1
3.4	0.190131 E1	0.268923 E1	0.332620 E1
3.5	0.190301 E1	0.269384 E1	0.333429 E1
3.6	0.190459 E1	0.269815 E1	0.334194 E1
3.7	0.190606 E1	0.270217 E1	0.334918 E1
3.8	0.190742 E1	0.270594 E1	0.335603 E1
3.9	0.190868 E1	0.270947 E1	0.336252 E1
4.0	0.190986 E1	0.271278 E1	0.336866 E1
4.1	0.191097 E1	0.271589 E1	0.337446 E1
4.2	0.191198 E1	0.271881 E1	0.337997 E1
4.3	0.191294 E1	0.272155 E1	0.338518 E1
4.4	0.191384 E1	0.272414 E1	0.339013 E1
4.5	0.191468 E1	0.272658 E1	0.339482 E1
4.6	0.191548 E1	0.272888 E1	0.339927 E1
4.7	0.191622 E1	0.273105 E1	0.340350 E1
4.8	0.191692 E1	0.273310 E1	0.340751 E1
4.9	0.191758 E1	0.273501 E1	0.341133 E1
5.0	0.191820 E1	0.273688 E1	0.341496 E1

Table A-2. Continued

λ_0	$\theta_r/T=2.5$	3.0	3.5
0.1	0.141305 E3	0.215899 E3	0.299499 E3
0.2	0.372619 E2	0.561351 E2	0.772058 E2
0.3	0.180093 E2	0.265605 E2	0.360494 E2
0.4	0.112877 E2	0.162225 E2	0.216552 E2
0.5	0.819436 E1	0.114517 E2	0.150040 E2
0.6	0.653197 E1	0.887455 E1	0.114027 E2
0.7	0.554719 E1	0.733508 E1	0.924304 E1
0.8	0.492469 E1	0.635007 E1	0.785509 E1
0.9	0.451411 E1	0.568843 E1	0.691168 E1
1.0	0.423498 E1	0.522820 E1	0.624948 E1
1.1	0.404192 E1	0.489977 E1	0.577028 E1
1.2	0.390727 E1	0.466180 E1	0.541605 E1
1.3	0.381340 E1	0.448707 E1	0.515007 E1
1.4	0.374863 E1	0.435818 E1	0.494813 E1
1.5	0.370498 E1	0.426311 E1	0.479371 E1
1.6	0.367681 E1	0.419339 E1	0.467524 E1
1.7	0.366008 E1	0.414291 E1	0.458434 E1
1.8	0.365183 E1	0.410717 E1	0.451489 E1
1.9	0.364987 E1	0.408282 E1	0.446227 E1
2.0	0.365256 E1	0.406729 E1	0.442298 E1
2.1	0.365866 E1	0.405861 E1	0.439429 E1
2.2	0.366723 E1	0.405527 E1	0.437408 E1
2.3	0.367755 E1	0.405606 E1	0.436068 E1
2.4	0.368907 E1	0.406005 E1	0.435274 E1
2.5	0.370137 E1	0.406649 E1	0.434920 E1
2.6	0.371413 E1	0.407479 E1	0.434918 E1
2.7	0.372711 E1	0.408449 E1	0.435198 E1
2.8	0.374013 E1	0.409519 E1	0.435702 E1
2.9	0.375303 E1	0.410661 E1	0.436384 E1
3.0	0.376573 E1	0.411851 E1	0.437205 E1
3.1	0.377814 E1	0.413069 E1	0.438134 E1
3.2	0.379022 E1	0.414300 E1	0.439144 E1
3.3	0.380197 E1	0.415534 E1	0.440215 E1
3.4	0.381323 E1	0.416760 E1	0.441328 E1
3.5	0.382413 E1	0.417971 E1	0.442469 E1
3.6	0.383461 E1	0.419161 E1	0.443627 E1
3.7	0.384468 E1	0.420327 E1	0.444792 E1
3.8	0.385433 E1	0.421464 E1	0.445956 E1
3.9	0.386359 E1	0.422572 E1	0.447113 E1
4.0	0.387245 E1	0.423648 E1	0.448257 E1
4.1	0.388093 E1	0.424691 E1	0.449385 E1
4.2	0.388904 E1	0.425701 E1	0.450494 E1
4.3	0.389680 E1	0.426678 E1	0.451581 E1
4.4	0.390422 E1	0.427622 E1	0.452644 E1
4.5	0.391131 E1	0.428533 E1	0.453681 E1
4.6	0.391809 E1	0.429412 E1	0.454693 E1
4.7	0.392458 E1	0.430259 E1	0.455677 E1
4.8	0.393078 E1	0.431076 E1	0.456635 E1
4.9	0.393672 E1	0.431863 E1	0.457565 E1
5.0	0.394239 E1	0.432620 E1	0.458467 E1

Table A-2. Continued

x_0	$\theta_D/T=4.0$	4.5	5.0
0.1	0.386550 E3	0.472027 E3	0.552021 E3
0.2	0.990928 E2	0.120547 E3	0.140601 E3
0.3	0.458671 E2	0.554645 E2	0.644172 E2
0.4	0.272465 E2	0.326923 E2	0.377584 E2
0.5	0.186370 E2	0.221595 E2	0.254253 E2
0.6	0.139697 E2	0.164457 E2	0.187323 E2
0.7	0.111652 E2	0.130085 E2	0.147032 E2
0.8	0.935464 E1	0.107856 E2	0.120949 E2
0.9	0.812298 E1	0.926973 E1	0.103134 E2
1.0	0.725145 E1	0.819337 E1	0.904584 E1
1.1	0.661583 E1	0.740482 E1	0.811462 E1
1.2	0.614130 E1	0.681272 E1	0.741290 E1
1.3	0.578057 E1	0.635935 E1	0.687319 E1
1.4	0.550250 E1	0.600680 E1	0.645120 E1
1.5	0.528592 E1	0.572927 E1	0.611681 E1
1.6	0.511600 E1	0.550373 E1	0.584898 E1
1.7	0.498206 E1	0.533224 E1	0.563264 E1
1.8	0.487626 E1	0.519010 E1	0.545673 E1
1.9	0.479274 E1	0.507582 E1	0.531302 E1
2.0	0.472703 E1	0.498339 E1	0.519523 E1
2.1	0.467566 E1	0.490883 E1	0.509853 E1
2.2	0.463593 E1	0.484889 E1	0.501912 E1
2.3	0.460568 E1	0.480096 E1	0.495402 E1
2.4	0.458320 E1	0.476298 E1	0.490032 E1
2.5	0.456710 E1	0.473324 E1	0.485756 E1
2.6	0.455624 E1	0.471039 E1	0.482267 E1
2.7	0.454969 E1	0.469329 E1	0.479484 E1
2.8	0.454671 E1	0.468102 E1	0.477297 E1
2.9	0.454664 E1	0.467279 E1	0.475617 E1
3.0	0.454898 E1	0.466794 E1	0.474367 E1
3.1	0.455327 E1	0.466594 E1	0.473485 E1
3.2	0.455916 E1	0.466632 E1	0.472910 E1
3.3	0.456633 E1	0.466869 E1	0.472602 E1
3.4	0.457454 E1	0.467271 E1	0.472520 E1
3.5	0.458356 E1	0.467811 E1	0.472629 E1
3.6	0.459321 E1	0.468465 E1	0.472900 E1
3.7	0.460334 E1	0.469212 E1	0.473308 E1
3.8	0.461385 E1	0.470034 E1	0.473832 E1
3.9	0.462456 E1	0.470916 E1	0.474453 E1
4.0	0.463545 E1	0.471847 E1	0.475154 E1
4.1	0.464642 E1	0.472814 E1	0.475922 E1
4.2	0.465740 E1	0.473808 E1	0.476744 E1
4.3	0.466836 E1	0.474823 E1	0.477611 E1
4.4	0.467923 E1	0.475850 E1	0.478512 E1
4.5	0.469000 E1	0.476884 E1	0.479441 E1
4.6	0.470062 E1	0.477920 E1	0.480389 E1
4.7	0.471108 E1	0.478954 E1	0.481353 E1
4.8	0.472135 E1	0.479983 E1	0.482325 E1
4.9	0.473143 E1	0.481005 E1	0.483303 E1
5.0	0.474130 E1	0.482012 E1	0.484282 E1

Table A-3. Values for J_5/J_4^2 Computed Using 40 Point
Gauss-Legendre Quadrature

θ_D/T	J_5/J_4^2	θ_D/T	J_5/J_4^2	θ_D/T	J_5/J_4^2
.40	14.163	.82	3.447	1.24	1.565
.42	12.855	.84	3.290	1.26	1.519
.44	11.722	.86	3.143	1.28	1.475
.46	10.733	.88	3.006	1.30	1.433
.48	9.866	.90	2.879	1.35	1.336
.50	9.100	.92	2.759	1.40	1.250
.52	8.421	.94	2.647	1.45	1.172
.54	7.816	.96	2.542	1.50	1.102
.56	7.275	.98	2.444	1.55	1.039
.58	6.789	1.00	2.351	1.60	.982
.60	6.350	1.02	2.264	1.65	.929
.62	5.954	1.04	2.181	1.70	.881
.64	5.594	1.06	2.104	1.75	.838
.66	5.266	1.08	2.030	1.80	.800
.68	4.966	1.10	1.961	1.90	.727
.70	4.692	1.12	1.895	2.00	.667
.72	4.441	1.14	1.833	2.10	.615
.74	4.209	1.16	1.773	2.20	.570
.76	3.996	1.18	1.717	2.30	.531
.78	3.799	1.20	1.664	2.40	.496
.80	3.616	1.22	1.613	2.50	.466