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Correlations for the Thermal Conductivity of Metals as a Function of Temperature

S. I. Abu-Eishah[1]

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The objective of this work was to find a suitable correlation that best fits the thermal conductivity of metals as a function of temperature. It was found that a multiple linear regression model of the form $k = aT^b e^{cT} e^{d/T}$ gives the smallest deviations from experimental data among various models. The coefficient of determination, R^2, lies between 0.97 and unity, except for thorium ($R^2 = 0.86$). The average of the absolute relative error, AARE, in the predicted data is less than 4.75%, except for iron (about 11.7%), and the overall AARE for all data points is about 1.4%.

KEY WORDS: correlation; metals; thermal conductivity.

1. INTRODUCTION

Thermal properties represent, in one way or another, the response of a material to the application of heat. As a solid absorbs energy in the form of heat, its temperature rises and its dimensions increase. The energy may be transported to cooler regions of the specimen if temperature gradients exist and thermal conduction is the phenomenon by which heat is transported from regions of high to low temperature in a substance.

Many applications of metals, ceramics, polymers, and composites are based upon their unique thermal properties. Some chemical reactors require a high thermal resistance, high resistance to thermal shock, and low conduction of heat. Thus, heat capacity, thermal conductivity, and thermal diffusivity are properties that are often critical in practical utilization of solids as materials of construction.

[1] Department of Chemical Engineering, University of Bahrain, P.O. Box 32038, Isa Town, Bahrain. E-mail: siam@just.edu.jo

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Thermal conductivity is the property that characterizes the ability of a material to transfer heat, and it is defined as the rate of heat transfer per unit area and per unit temperature gradient imposed normal to the unit area. Thermal conductivity is a nonequilibrium property usually determined in a steady-state experiment utilizing the Fourier law for unidirectional heat transfer in a homogeneous, isotropic substance:

$$Q = -kA\,\mathrm{d}T/\mathrm{d}x \tag{1}$$

where Q is the rate of transfer of thermal energy (W), k is the thermal conductivity ($\mathrm{W \cdot m^{-1} \cdot K^{-1}}$), A is the cross-sectional area ($\mathrm{m^2}$) perpendicular to the direction of heat flow, and $\mathrm{d}T/\mathrm{d}x$ is the temperature gradient ($\mathrm{K \cdot m^{-1}}$). As the thermal conductivity increases, the possibility of thermal shock decreases [1].

It is usually assumed that the thermal conductivity is not a function of the temperature gradient but is a function of the state, composition, purity, perfection, physical structure, and other similar intensive parameters of the material. Thermal conductivity depends strongly on the temperature and, to a lesser extent, on the pressure to which the material is subjected. In nonisotropic materials the thermal conductivity varies with the direction of heat flow across the material. It is also assumed that the conductivity is independent of size or shape, although this is not always true. Effects of size and/or shape become significant whenever the size of the conductor is comparable to the mean free path for motion of the particles (or quasiparticles) that transport the thermal energy.

In the modern view of materials, a solid may be comprised of free electrons and of atoms bound in a periodic arrangement called the lattice. Since heat is conducted in solid materials by migration of free electrons and by lattice vibrational waves (phonons), a thermal conductivity term is associated with each of these mechanisms, and the total thermal conductivity of solids is assumed to be the sum of the two contributions [2]; ignoring effects of interactions (scattering) between the electrons and the phonons,

$$k = k_\ell + k_\mathrm{e} \tag{2}$$

where k_ℓ is the thermal conductivity term due to the lattice vibrational waves (phonons) and k_e is that due to the migration of free electrons, and usually one or the other predominates. The thermal energy associated with lattice vibrational waves (phonons) is transported in the direction of their motion. The k_ℓ contribution results from the net movement of the phonons from high-temperature regions of a body to low-temperature regions across which a temperature gradient exists [3].

The free electrons in a hot region of a solid specimen are imparted a gain in their kinetic energy, where some of this energy is transferred to the atoms themselves as vibrational energy as a consequence of collisions with phonons or other imperfections in the crystal. The relative contribution of k_e to the total thermal conductivity increases with the increase in the concentration of free electrons, since more free electrons are available to participate in this heat transfer process [3].

In high-purity metals, the mechanism of heat transport by electrons is more efficient than the phonon contribution because electrons are not easily scattered as phonons and have higher velocities [3]. Because of the nature of the metallic bond, these electrons are relatively free to move throughout the structure. This large number of carriers plus the large mean free path results in the high thermal conductivity of pure metals.

Alloying metals with impurities results in a reduction in thermal conductivity for the same reason that the electrical conductivity is diminished. Alloying reduces the mean free path and thus results in a decrease in the thermal conductivity. This is because the impurity atoms, especially if in solid solution, act as scattering centers that lower the efficiency of the electrons' motion [3].

Since free electrons are responsible for both electrical and thermal conduction in pure metals, theoretical treatments suggest that the electrical and thermal conductivities of pure metals should be related according to the Wiedemann–Franz–Lorenz law, and the electrical conductivity of a metal or alloy can by estimated by

$$\sigma = L_0 T / k \tag{3}$$

where σ is the electrical conductivity $(\Omega \cdot \mathrm{m})^{-1}$, T is the absolute temperature (K), and L_0 (the Lorenz number) is a constant that has a theoretical value of $2.443 \times 10^{-8}\ \Omega \cdot \mathrm{W} \cdot \mathrm{K}^{-2}$. L_0 should be independent of temperature, and the same for all metals, if the heat energy is transported entirely by free electrons [3]. The electrical conductivity of electrolytes directly influences the energy consumption of the melting process [4]. Thus, knowledge of accurate thermal conductivity data is essential in prediction of the electrical conductivity and estimation of the energy required for the melting process.

To a first approximation, k_e is proportional to the electrical conductivity, σ. For pure metals, which are of a high σ, k_e is much larger than k_ℓ. In contrast, for alloys, which have a substantially lower σ, the contribution of k_e to k is no longer negligible. For nonmetallic solids, k is determined primarily by k_ℓ, which depends on the frequency of interactions between the atoms of the lattice. The regularity of the lattice arrangement has an important effect on k_ℓ, with crystalline (well-ordered) materials like quartz

having a higher thermal conductivity than amorphous materials like glass. In fact, for crystalline, nonmetallic solids such as diamond and beryllium oxide, k_ℓ can be quite large, exceeding the values of k associated with good conductors [2].

The theory of thermal conductivity of metallic materials is covered in detail by Touloukian et al. [5]. They presented a correlation for calculating the "recommended" thermal conductivity at temperatures below about $1.5T_m$ (the temperature at maximum thermal conductivity on the k–T curve). This correlation has the following form:

$$k_e = 1/((\alpha' T^n + \beta)/T) \tag{4}$$

where

$$\alpha' = \alpha''(\beta/(n\alpha''))^{(m-n)/(m+1)} \tag{5}$$

and α'', m, and n are constants for a metal. The value of n lies between 2.0 and 3.0 for most metals. The parameter β is defined as the ratio between the residual electrical resistivity and the Lorenz number, i.e., $\beta = \rho_0/L_0$. The purity of the studied metals, values of available residual electrical resistivity ρ_0, and accuracy of the "recommended" data used in this work are presented in Ref. 5 and summarized in Table I. The available values of the above parameters (m, n, β, α'', and α') are listed in Table II for reference.

Touloukian et al. [5] also presented the lattice part of the thermal conductivity k_ℓ as

$$k_\ell = \gamma/T^\delta \tag{6}$$

where γ is some function of the atomic concentration of point defects, and the exponent parameter δ has values between 0.50 (at high temperatures) and 2.0 (at low temperatures).

The accuracy of engineering calculations depends on the accuracy with which the thermophysical properties are known. Selection of reliable property data is an integral part of any careful engineering analysis [3]. The casual use of data from the literature or handbooks, which have not been well characterized or evaluated, is to be avoided. Recommended data values for many thermophysical properties can be obtained from Ref. 5. The objective of this work was to find a suitable correlation that best fits the thermal conductivity of pure metals as a function of temperature.

2. RESULTS AND DISCUSSION

The "recommended" data of the thermal conductivity of metals compiled by Touloukian et al. [5] cover a wide range of temperatures

Table I. Some Characteristics of the "Recommended Data" Used in this Study [5][a]

Metal	Purity	Residual electrical resistivity, ρ_0 ($\mu\Omega \cdot$ cm)	Accuracy near room temperature	Accuracy at other temperatures
Aluminum	Well annealed, 99.9999% pure	0.000593	2–3%	3–5%
Antimony, PC	Well annealed, high purity	0.054	Up to 5%	5–10%
Beryllium, PC	Well annealed, high purity	0.0135	Up to 5%	5–15%
Bismuth, P	99.997$^+$% pure	—	Up to 4%	4–10%
Bismuth, /c/	99.997$^+$% pure	—	Up to 4%	4–10%
Bismuth, PC	99.997$^+$% pure	—	Up to 4%	4–10%
Boron, PC	High purity	—	Up to 5%	5–10%
Cadmium, P	Well annealed, 99.999% pure	0.000463	Up to 4%	4–10%
Cadmium, /c/	Well annealed, 99.999% pure	0.000606	Up to 4%	4–10%
Cadmium, PC	Well annealed, 99.999% pure	0.000502	Up to 4%	4–10%
Cesium	High purity	0.0465	Up to 5%	5–10%
Chromium	99.998$^+$% pure	0.0609	Up to 3%	3–10%
Cobalt, PC	Above 99.999$^+$% pure	0.0905	Up to 4%	4–10%
Copper	Above 99.999$^+$% pure	0.000851	Up to 3%	3–5%
Gallium, /a/[b]	99.9999% pure	0.000100	Up to 4%	4–15%
Gallium, /b/	99.9999% pure	0.000341	Up to 4%	4–15%
Gallium, /c/	99.9999% pure	0.000424	Up to 4%	4–15%
Germanium	High purity	—	Up to 4%	4–10%
Gold	Well annealed, 99.999$^+$% pure	0.0055	Up to 3%	3–6%
Iridium	Well annealed, 99.995$^+$% pure	0.0188	Up to 4%	4–10%
Iron	Well annealed, 99.998$^+$% pure	0.0327	Up to 3%	3–8%
Lead	Well annealed, 99.99$^+$% pure	0.00088	Up to 3%	3–10%
Lithium	High purity	0.0371	Up to 5%	5–10%
Magnesium, PC	Well annealed, 99.98$^+$% pure	0.0189	Up to 3%	3–10%
Manganese	Well annealed, 99.99$^+$% pure	11.3	Up to 5%	5–15%
Molybdenum	Well annealed, 99.95$^+$% pure	0.167	Up to 4%	4–10%
Nickel	Well annealed, 99.99$^+$% pure	0.0384	Up to 5%	5–10%
Niobium	Well annealed, 99.9$^+$% pure	0.0975	Up to 5%	5–10%
Palladium	Well annealed, 99.995$^+$% pure	0.0123	Up to 4%	4–10%
Platinum	Well annealed, 99.999$^+$% pure	0.0106	Up to 5%	5–10%
Plutonium, PC	Well annealed, 99.98$^+$% pure	—	Up to 10%	10–20%
Potassium	99.97$^+$% pure	0.00237	Up to 5%	5–10%
Rhenium, PC	Well annealed, 99.99$^+$% pure	0.0140	Up to 4%	4–10%
Rhodium	Well annealed, 99.997$^+$% pure	0.0084	Up to 4%	4–10%
Silicon	High purity	—	Up to 4%	4–10%
Silver	Well annealed, 99.999$^+$% pure	0.00062	Up to 2%	2–5%
Sodium	High purity	0.00147	Up to 5%	5–10%
Tantalum	Well annealed, 99.9$^+$% pure	0.212	Up to 5%	5–10%
Thorium	Well annealed, high pure	0.72	10–15%	10–15%
Tin, P	Well annealed, 99.999$^+$% pure	0.00012	Up to 3%	3–15%
Tin, /c/	Well annealed, 99.999$^+$% pure white	0.000172	Up to 3%	3–15%
Tin, PC	Well annealed, 99.999$^+$% pure	0.000133	Up to 3%	3–15%
Titanium, PC	Well annealed, 99.99$^+$% pure	1.7	Up to 5%	5–15%
Tungsten	Well annealed, 99.99$^+$% pure	0.0017	Up to 3%	3–5%
Uranium, PC	Well annealed, high purity	2.2	Up to 5%	5–10%
Vanadium	Well annealed, high purity	1.72	Up to 5%	5–15%
Zinc, PC	Well annealed, 99.999$^+$% pure	0.00128	Up to 3%	3–10%
Zirconium, PC	Well annealed, 99.95$^+$% pure	0.219	Up to 5%	5–15%

[a] PC, polycrystalline; P, perpendicular to *c*-axis; /a/, parallel to *a*-axis; /b/, parallel to *b*-axis, /c/, parallel to *c*-axis.

[b] Values are also good for polycrystalline gallium.

Table II. Values of the Parameters of the Proposed Fitting Eqs. (4) and (5) for the Thermal Conductivity of Metals ($W \cdot m^{-1} \cdot K^{-1}$), up to $T = 1.5T_m$ (from Touloukian et al. [5])[a]

Metal	T_m (K)	n	m	β	α''	α'
Aluminum	10	2.0	2.61	0.0245	4.87×10^{-6}	1.829×10^{-4}
Beryllium, PC	14	2.8	—	0.553	—	2.56×10^{-7}
Cadmium, P	3	2.5	—	0.0188	—	1.77×10^{-4}
Cadmium, /c/	3	2.5	—	0.0246	—	1.90×10^{-4}
Cadmium, PC	3	2.5	—	0.0204	—	1.80×10^{-4}
Chromium	25	2.0	—	2.49	—	1.04×10^{-4}
Cobalt, PC	25	2.1	—	3.71	—	0.747
Copper	10	2.4	2.0	0.0348	4.16×10^{-6}	6.973×10^{-6}
Gallium, /a/[b]	2	2.0	—	0.00409	—	3.28×10^{-4}
Gallium, /b/	2	2.0	—	0.0014	—	1.26×10^{-4}
Gallium, /c/	2	2.0	—	0.0174	—	11.2×10^{-4}
Gold	10	2.0	2.46	0.225	4.6×10^{-5}	1.298×10^{-4}
Iridium	20	3.0	—	0.770	—	1.75×10^{-6}
Iron	20	2.1	2.47	1.34	2.05×10^{-5}	6.178×10^{-5}
Lead	2	3.0	—	0.0353	—	7.40×10^{-4}
Lithium	16	2.0	—	1.52	—	1.57×10^{-4}
Magnesium, PC	15	2.0	—	0.772	—	0.83×10^{-4}
Molybdenum	35	2.6	—	6.85	—	7.76×10^{-6}
Nickel	20	2.0	—	1.57	—	9.57×10^{-5}
Niobium	15	2.0	—	3.99	—	5.92×10^{-4}
Palladium	9	2.0	2.4	0.502	1.54×10^{-4}	3.676×10^{-4}
Platinum	8	2.1	—	0.433	—	3.01×10^{-4}
Potassium	3	2.0	—	0.0973	—	2.06×10^{-3}
Rhenium, PC	12	2.5	—	0.57	—	4.56×10^{-5}
Rhodium	18	2.7	—	0.344	—	3.16×10^{-6}
Silver	7	2.2	2.75	0.0254	7.3×10^{-6}	2.150×10^{-5}
Sodium	5	2.0	—	0.060	—	3.5×10^{-4}
Tantalum	20	2.1	—	8.69	—	4.52×10^{-4}
Titanium, PC	40	2.6	—	69.5	—	4.32×10^{-5}
Tungsten	9	2.4	—	0.0696	—	2.06×10^{-5}
Zinc, PC	5	3.0	—	0.0525	—	1.88×10^{-5}
Zirconium, PC	15	2.2	—	8.98	—	7.45×10^{-4}

[a] PC, polycrystalline; P, perpendicular to *c*-axis; /a/, parallel to *a*-axis; /b/, parallel to *b*-axis; /c/, parallel to *c*-axis.
[b] Values are also good for polycrystalline gallium.

(from as low as 0 K up to the melting point of the solid phase of the metal and above that for the melt phase.). Practical application of these data might not extend to very low temperatures. Some values of the "recommended" thermal conductivity data have been estimated by Touloukian et al. [5], especially at the low and/or the high end of the temperature range. Anyway, since Touloukian et al. [5] already correlated the low-temperature side

of these data (up to $1.5T_m$), with T_m the temperature corresponding to the maximum thermal conductivity of the curve, this work is concerned only with fitting the k–T data from above $1.5T_m$ up to the melting point, where available.

Throughout the analysis of results, the following basic definitions have been used.

Absolute error, $\mathrm{AE} = |k_{\mathrm{exp}} - k_{\mathrm{cal}}|$.
Absolute relative error, $\mathrm{ARE} = |k_{\mathrm{exp}} - k_{\mathrm{cal}}| / k_{\mathrm{exp}}$.
Average of absolute errors, $\mathrm{AAE} = \sum$ (absolute errors)$/M$.
Average of absolute relative errors, $\mathrm{AARE} = \sum$ (absolute relative errors)$/M$.

M is the number of data points in the set of data used to compute the averages.

The coefficient of determination, R^2, defined by Eq. (7) can be used as one measure to test the accuracy of fitting. The best fit is obtained when R^2 approaches unity.

$$R^2 = \sum (k_{i,\,\mathrm{exp}} - k_{\mathrm{avg}})^2 / \sum (k_{i,\,\mathrm{cal}} - k_{\mathrm{avg}})^2 \tag{7}$$

where $k_{i,\,\mathrm{exp}}$ and $k_{i,\,\mathrm{cal}}$ are, respectively, the ith experimental and calculated values of k, and k_{avg} is the average value of experimental k.

Two fitting equations have been used in this study.

(1) nth-order polynomial regression of the form

$$k = B_0 + B_1 T + B_2 T^2 + B_3 T^3 + \cdots + B_n T^n \tag{8}$$

where B_0, B_1, ..., B_n are the polynomial fitting parameters and T is the temperature in K.

(2) Multilinear regression of the form

$$k = aT^b e^{cT} e^{d/T} \tag{9}$$

where a, b, c, and d are fitting constants. If the exponential terms in Eq. (9) are expanded by a Taylor's series, then

$$k = aT^b(1 + cT + (cT)^2/2! + (cT)^3/3! + \cdots)$$
$$\times (1 + (d/T) + (d/T)^2/2! + (d/T)^3/3! + \cdots)$$
$$k = aT^b\{1 + cd + (cd)^2/4 + \cdots + c(1 + (cd/2))\,T$$
$$+ (c^2/2)\,T^2 + \cdots + d(1 + (c^2/2))/T + (d^2/2)/T^2 + \cdots\}$$

or

$$k = aT^b\{A + BT + CT^2 + \cdots + D/T + E/T^2 + \cdots\} \qquad (10)$$

Thus, Eq. (9) is general in its nature; it is more than just a polynomial, a power series, or an exponential function; it is a combination of all of these functions. It can have positive and negative exponents, with integer and noninteger values. Also, the parameter a will always be a nonnegative value, which is needed for representing thermophysical data, in general. Taking the logarithm of both sides of Eq. (9) gives

$$\ln k = \ln a + b \ln T + cT + (d/T) \qquad (11)$$

That is, all the right hand-side terms are linear, from which the multilinear name of the proposed function is derived.

Although the polynomial regression method is well known and easy to implement on digital computers, its main disadvantages are that more fitting parameters are needed to get a higher accuracy, and it might give impractical (or unrealistic negative) values for the predicted property. Polynomials are based on power laws and diverge greatly at or near the end points of the data region. They are thus poor candidates for fitting "smooth" curves.

The method of multilinear regression, which is a combination of power and exponential series, is characterized by (a) a smaller number of fitting parameters and (b) a more realistic representation of the experimental data. The main disadvantage of this method is that it does not predict sharp drops or increases in the physical properties, as is the case for thorium, for example.

All the metals studied here, except manganese, plutonium, and uranium, have a maximum in their k–T curve. Palladium has a constant thermal conductivity of about 75.5 $W \cdot m^{-1} \cdot K^{-1}$ for $T \geqslant 150$ K.

As shown in Table III, the coefficient of determination, R^2, lies for all systems between 0.97 and unity, except for thorium ($R^2 = 0.86$). The average of the absolute relative error, AARE, in the predicted data is less than 4.75%, except for iron (about 11.7%), and the overall AARE for all data points is about 1.4%.

The effect of using more data points in the lower side of the temperature range on the accuracy of fitting is demonstrated by comparing the results presented in Tables III and IV. The overall AARE in Table III is about 1.41%, with a maximum of about 4.75%, except for iron (AARE = 11.73%). On the other hand, the overall AARE in Table IV is about 4.22% and the same is still true for iron (AARE = 11.62%). For the

Table III. Multilinear Fitting Parameters of Eq. (9) for the Thermal Conductivity of Metals ($W \cdot m^{-1} \cdot K^{-1}$) Starting from $T > 1.5T_m$ [a]

Metal	M	Temperature range (K)	a	b	$c \times 10^4$	d	R^2	AARE (%)
Aluminum	15	100–933.2	1.610073	0.857540	−12.3355	140.2813	0.9872	0.7753
Antimony, PC	14	100–903.7	906.3572	−0.669837	6.15011	4.880814	1.0000	0.2429
Beryllium, PC	18	100–1400	7.009381	0.475543	−10.45180	287.6711	0.9997	1.0043
Bismuth, P	9	100–544.5	142.242	−0.548250	7.91260	42.13569	0.9995	0.4642
Bismuth, /c/	9	100–544.5	257.6239	−0.764014	11.81820	32.33529	0.9991	0.7150
Bismuth, PC	9	100–544.5	108.1828	−0.531360	8.19123	48.44849	1.0000	0.1510
Boron, PC	18	100–1400	1073.03	−1.114956	1.44057	110.8195	0.9998	1.1067
Cadmium, P	10	100–594.2	38.41291	0.196614	−6.57815	21.36565	0.9951	0.3041
Cadmium, /c/	10	100–594.2	30.55295	0.197260	−6.55921	21.95176	0.9972	0.2253
Cadmium, PC	10	100–594.2	37.66306	0.187388	−6.38126	20.83231	0.9943	0.2574
Cesium	7	100–301.9	50.70952	−0.075761	1.97161	8.43343	1.0010	0.0445
Chromium	21	100–2000	60.63089	0.044844	−2.90323	79.82282	0.9919	2.0951
Cobalt, PC	14	50–1500	4032.682	−0.643275	1.21289	−23.04691	0.9993	0.7387
Copper	18	100–1356	82.56648	0.262301	−4.06701	59.72934	0.9997	0.1332
Gallium, /a/ [b]	8	90–302.9	98.35468	−0.174878	3.30884	4.185883	0.9996	0.0764
Gallium, /b/	8	90–302.9	394.9374	−0.300026	8.50985	−12.68498	0.9997	0.0509
Gallium, /c/	8	90–302.9	2.934731	0.295647	−5.58252	51.40721	0.9991	0.1259
Germanium	16	100–1200	1341501.0	−1.784770	11.59350	−59.03847	0.9983	2.7459
Gold	18	100–1336.2	91.34061	0.221831	−4.62083	36.2277	0.9943	0.6415
Iridium	19	100–1500	63.35366	0.144685	−3.48051	36.77638	0.9999	0.1190
Iron	32	50–1810	2227.664	−0.627271	2.09554	22.35452	0.9681	11.7289
Lead	11	100–600.5	14.92863	0.169272	−6.49013	26.11494	0.9985	0.1707
Lithium	9	100–453.7	7350.188	−0.857875	15.22240	−36.90931	1.0000	0.2293
Magnesium, PC	14	100–923	141.7137	0.015169	−1.04937	11.34289	0.9910	0.3082
Manganese	11	20–300	0.472542	0.585013	−17.8544	−1.832767	0.9992	0.8834
Molybdenum	25	100–2800	185.5698	−0.055329	−1.54776	19.51821	0.9875	2.0265
Nickel	20	100–1500	13802.17	−0.927164	11.45850	−33.13548	0.9804	2.6502
Niobium	20	100–2200	20.07295	0.147295	1.17388	32.17986	0.9999	0.1549
Palladium	16	20–1000	6.011879	0.421147	−4.47875	68.80641	0.9888	4.7515
Platinum	22	100–2000	97.64839	−0.076700	3.08766	9.166382	0.9964	0.3984
Plutonium, PC	7	100–350	0.4197818	0.346780	23.99130	22.84283	1.0000	0.1675
Potassium	10	20–336.8	17.36068	0.376505	−15.4475	23.26408	0.9952	0.8864
Rhenium, PC	21	100–2600	161.7389	−0.231703	3.12640	2.488815	0.9986	0.3291
Rhodium	13	100–1400	58.26164	0.157359	−3.87659	45.66854	0.9859	1.3545
Silicon	19	100–1685	335769.8	−1.405104	4.30785	46.06461	0.9990	2.6110
Silver	16	100–1234	230.9532	0.113561	−3.19146	17.17667	0.9976	0.2798
Sodium	12	20–371	0.5138235	1.123792	−37.4489	75.81478	0.9993	1.0557
Tantalum	23	100–3200	38.88549	0.058179	0.227751	15.27868	0.9985	0.2559
Thorium	23	20–1000	63.40096	−0.056958	1.96976	0.687997	0.8558	1.2696
Tin, P	15	20–505.1	32.62162	0.165472	−8.05469	38.33054	0.9997	0.6689
Tin, /c/	11	20–505.1	20.32804	0.188061	−8.69687	39.0890	0.9996	0.8637
Tin, PC	11	20–505.1	28.16529	0.172732	−8.12943	38.50249	0.9997	0.7591
Titanium, PC	15	100–1900	189.327	−0.416822	6.56393	5.564995	0.9963	0.7608
Tungsten	22	100–3653	1675.621	−0.388818	0.717926	−18.4985	0.9983	0.8949
Uranium, PC	16	100–1200	18.94832	0.043816	5.44897	−12.05495	0.9998	0.2726
Vanadium	15	100–2000	7.947953	0.195897	1.70438	58.72758	0.9981	0.5473
Zinc, PC	10	100–692.6	29.54797	0.285617	−9.86623	21.50571	0.9964	0.4012
Zirconium, PC	17	100–2000	39.4099	−0.152855	4.77081	49.96284	0.9689	2.2077

[a] PC, polycrystalline; P, perpendicular to c-axis; /a/, parallel to a-axis; /b/, parallel to b-axis; /c/, parallel to c-axis.

[b] Values are also good for polycrystalline gallium.

Table IV. Multilinear Fitting Parameters of Eq. (9) for the Thermal Conductivity of Metals ($W \cdot m^{-1} \cdot K^{-1}$) Starting from $T \sim 1.5T_m$ [a]

Metal	M	Temperature range (K)	a	b	$c \times 10^4$	d	R^2	AARE (%)
Aluminum	24	30–933.2	1.724468	0.815012	−9.953	164.93990	0.9924	6.0021
Antimony, PC	23	15–903.7	1072.298	−0.714528	7.736	11.79019	0.9985	2.6479
Beryllium	21	70–1400	58.63311	0.125506	−7.020	224.96950	0.9989	2.8208
Bismuth, P	24	6–544.5	1036.199	−0.920326	15.907	8.27410	0.9998	1.4461
Bismuth, /c/	17	20–544.5	1247.266	−1.059973	18.242	5.39253	0.9998	1.0200
Bismuth, PC	17	20–544.5	1232.348	−0.986320	17.905	6.30495	0.9998	1.0484
Boron, PC	20	80–1400	48225.34	−1.359888	3.73143	62.86083	0.9994	2.3538
Cadmium, P	20	10–594.2	22.52796	0.296909	−8.752	30.56886	0.9998	0.5560
Cadmium, /c/	22	8–594.2	17.45152	0.304484	−9.069	30.78216	0.9999	0.6647
Cadmium, PC	23	6–594.2	29.78960	0.220767	−6.006	28.26045	0.9987	2.1301
Cesium	22	5–301.9	70.96258	−0.138910	3.32367	3.01810	0.9994	0.6240
Chromium	29	35–2000	106.5083	−0.046444	−2.12815	62.37709	0.9982	2.2474
Cobalt, PC	22	35–1500	485.1704	−0.288266	−2.44991	31.85364	0.9986	2.3866
Copper	27	30–1356	6.327957	0.691340	−8.530	128.08440	0.9972	3.2272
Gallium, /a/ [b]	21	8–302.9	750.972	−0.775465	51.077	21.54189	0.9948	8.1675
Gallium, /b/	21	8–302.9	10093.96	−1.241021	8.0647	16.13929	0.9949	8.6073
Gallium, /c/	21	8–302.9	194.8016	−0.650103	39.749	20.08618	0.9988	3.3824
Germanium	26	25–1200	324619.10	−1.553354	9.371	−13.44210	0.9995	2.8519
Gold	31	16–1336.2	49.21633	0.328633	−5.871	47.35758	0.9953	2.5634
Iridium	27	35–1500	2.229822	0.697966	−8.866	130.19120	0.9942	3.9701
Iron	34	35–1810	460.7027	−0.360733	−0.7061	57.67840	0.9813	11.6225
Lead	32	5–600.5	7.299241	0.337133	−13.225	24.20599	0.9971	4.3464
Lithium	18	30–453.7	40.86097	0.078706	−1.76773	71.00054	0.9964	3.1190
Magnesium, PC	22	35–923	1.228	0.838051	−12.107	122.90840	0.9945	3.2238
Manganese	20	2–300	0.3749391	0.634457	−19.791	0.22496	0.9998	0.8749
Molybdenum	30	50–2800	84.13335	0.065655	−2.24456	50.99060	0.9933	2.3505
Nickel	29	30–1500	1001.544	−0.493261	7.220	39.46008	0.9970	3.2678
Niobium	30	25–2200	8.433121	0.288897	0.01541	54.67941	0.9957	1.7421
Palladium	21	18–1000	11.91315	0.289615	−1.93013	61.50173	0.9873	6.5699
Platinum	35	16–2000	19.24495	0.188281	0.841185	52.08891	0.9959	3.1835
Plutonium, PC	9	80–350	0.7956418	0.226190	26.866	11.34326	1.0000	0.1605
Potassium	25	7–336.8	31.77876	0.225461	−6.222	20.73039	0.9925	4.3803
Rhenium	32	20–2600	9.419294	0.229360	−0.33746	76.11647	0.9919	5.6055
Rhodium	20	40–1400	0.7590507	0.887924	−11.667	158.93790	0.9952	3.6527
Silicon	25	45–1685	2074310	−1.708188	7.201	1.14520	0.9992	4.0221
Silver	27	20–1234	13.3066	0.596469	−8.590	85.97233	0.9934	4.4148
Sodium	23	10–371	156.7575	−0.153778	18.785	32.35447	0.9829	10.6193
Tantalum	33	30–3200	17.67491	0.182707	−0.54682	36.60055	0.9758	2.0385
Thorium	23	20–1000	63.40096	−0.056958	1.9698	0.687997	0.8558	1.2696
Tin, P	29	6–505.1	264.1387	−0.312668	12.527	26.17066	0.9939	9.5058
Tin, /c/	25	6–505.1	230.1577	−0.374470	15.337	25.35363	0.9934	10.2018
Tin, PC	27	6–505.1	268.8969	−0.348999	14.609	25.74366	0.9936	9.9114
Titanium, PC	20	50–1900	243.7518	−0.457710	6.899	−2.07962	0.9986	0.6529
Tungsten	32	20–3653	102.6421	0.042155	−1.6266	68.29091	0.9912	7.4943
Uranium, PC	34	3–1200	11.77491	0.135091	3.74171	−4.618909	0.9948	3.4893
Vanadium	31	10–1200	213.8358	−0.349107	6.529	−20.38209	0.9600	5.3778
Zinc	24	14–692.6	62.51884	0.062945	1.20435	50.65238	0.9881	9.2104
Zirconium, PC	28	25–2000	121.0481	−0.334302	6.197	18.61243	0.9955	2.1326

[a] PC, polycrystalline; P, perpendicular to c-axis; /a/, parallel to a-axis; /b/, parallel to b-axis; /c/, parallel to c-axis.

[b] Values are also good for polycrystalline gallium.

temperature range used in Table III, the maximum point-by-point relative error very rarely goes beyond 5% and reaches a maximum of about 13.6% for palladium at 30 K. For the temperature range used in Table IV, the maximum point-by-point relative error occurs, in most cases, at the low-temperature side (mostly around $1.5T_m$) and reaches a maximum of 26% for aluminum at 30 K.

If the temperature range for iron is taken from 100 K up to the triple point (1183 K) instead of the melting point (1810 K), the results for a total of 23 data points are better than those shown in Table III: $R^2=0.9981$, AARE$=2.5888$, $a=2.899333$, $b=0.5955211$, $c=-0.001783$, and $d=129.5933$. The same is true when the lower temperature starts from 35 K up to the triple point (1183 K) instead of the melting point (1810 K) for a total of 26 data points, instead of those used in Table IV. The results in this case become $R^2=0.9978$, AARE$=3.3049$, and $a=9.273859$, $b=0.3913118$, $c=-0.0015148$, and $d=107.3843$. This might be attributed to the presence of some discontinuity in the k–T data, and k is minimum at 1183 K (as indicated by Fig. 24R-1, p. 169 in Ref. 5) after which k increases with temperature up to the melting point. Also, there are several changes in the crystal structure of iron, starting from 1043 K (Curie temperature), to the triple point at 1183 K (b.c.c.–f.c.c.), to the triple point at 1673 K (f.c.c.–b.c.c.), to the melting point at 1810 K.

Finally, the calculated fitting parameters for the multilinear and polynomial regression methods are listed in Tables III–V for the thermal conductivity of the studied metals. Examination of the last column in Tables III and V for AARE shows that the multilinear regression method used is superior to the polynomial regression method. Here, the multilinear regression prediction is better for 28 systems (of 49) and, at the same time, gives a comparatively very close fit for the other 21 systems. Unfortunately, the polynomial fit gives an overall AARE as high as 11–51% for the thermal conductivity of some systems such as beryllium, boron, germanium, iron, palladium, silicon, sodium, and all forms of tin.

3. CONCLUSIONS

In this work, the multilinear regression model of the form $k=aT^be^{cT}e^{d/T}$ has been found to fit better the thermal conductivity of metals as a function of temperature. The coefficient of determination, R^2, is between 0.97 and unity, except for thorium (0.86). The average of the absolute relative error, AARE, in the predicted data is less than 4.75%, except for iron, with an overall AARE of about 1.4% for all data points.

The Toulokian et al. correlation presented above can be used to predict the thermal conductivity of pure metals at $T<1.5T_m$, while the

Table V. Fifth-Order Polynomial Fitting Parameters of Eq. (8) for the Thermal Conductivity of Metals ($W \cdot m^{-1} \cdot K^{-1}$)[a]

Metal	M	Temperature range (K)	B_0	B_1	$B_2 \times 10^3$	$B_3 \times 10^6$	$B_4 \times 10^9$	$B_5 \times 10^{12}$	R^2	AARE (%)
Aluminum	15	100–933.2	508.7	–3.284	14.41	–28.90	26.82	–9.378	0.9768	1.0396
Antimony, PC	14	100–903.7	82.77	–0.5229	1.869	–3.415	3.053	–1.056	0.9987	0.9759
Beryllium, PC	18	100–1400	1984	–14.690	43.38	–59.35	37.79	–9.055	0.9502	22.2328
Bismuth, P	9	100–544.5	47.19	–0.4748	2.493	–6.692	8.876	–4.603	0.9999	0.2417
Bismuth, /c/	9	100–544.5	32.55	–0.3508	1.898	–5.238	7.137	–3.798	0.9999	0.3647
Bismuth, PC	9	100–544.5	44.19	–0.4782	2.684	–7.77	11.21	–6.355	1.0000	0.1631
Boron, PC	18	100–1400	396.4	–2.9720	8.618	–11.65	7.358	–1.754	0.9685	45.6429
Cadmium, P	10	100–594.2	118.6	–0.1261	0.5219	–1.301	1.643	–0.8853	0.9969	0.1954
Cadmium, /c/	10	100–594.2	95.22	–0.1018	0.4204	–1.08	1.438	–0.8175	1.0000	0.0178
Cadmium, PC	10	100–594.2	108.6	–0.0679	0.1313	–0.1136	–0.0109	–0.01935	1.0000	0.0198
Cesium	7	100–301.9	40.91	0.0822	–1.80	11.33	–30.61	30.61	1.0000	0.0045
Chromium	21	100–2000	221.0	–0.8502	1.954	–2.126	1.068	–0.1988	0.9854	3.4234
Cobalt, PC	14	50–1500	236.4	–0.8858	2.037	–2.475	1.478	–0.3395	0.9988	1.0223
Copper	18	100–1356	593.0	–1.6030	4.814	–6.799	4.441	–1.092	0.9860	0.8211
Gallium, /a/[b]	8	90–302.9	62.92	–0.2665	1.609	–6.199	14.03	–13.76	0.9999	0.0565
Gallium, /b/	8	90–302.9	117.4	–0.4863	4.361	–22.64	59.96	–61.71	1.0000	0.0075
Gallium, /c/	8	90–302.9	41.9	–0.5684	5.214	–24.18	55.74	–50.80	0.9998	0.0867
Germanium	16	100–1200	476.4	–3.488	10.92	–16.53	11.89	–3.254	0.9876	11.3636
Gold	18	100–1336.2	383.0	–0.4927	1.38	–1.944	1.267	–0.3151	0.9995	0.1798
Iridium	19	100–1500	198.3	–0.3674	0.9595	–1.240	0.7412	–0.1664	0.9959	0.6081
Iron	32	50–1810	347.4	–2.111	5.508	–6.472	3.442	–0.6748	0.8618	22.9914
Lead	11	100–600.5	48.31	–0.1361	0.6246	–1.497	1.698	–0.7318	0.9991	0.1329
Lithium	9	100–453.7	198.3	–1.435	8.101	–25.74	42.14	–27.33	1.0000	0.0478
Magnesium, PC	14	100–923	194.5	–0.3922	1.609	–3.286	3.150	–1.136	0.9937	0.2746
Manganese	11	20–300	0.924	0.0822	–0.4281	0.9676	–0.2187	–1.477	0.9999	0.2094
Molybdenum	25	100–2800	186.5	–0.2452	0.3679	–0.2839	0.1004	–0.01303	0.9736	2.2160
Nickel	20	100–1500	215.1	–0.7958	1.719	–1.871	1.023	–0.2200	0.9783	2.7865
Niobium	20	100–2200	56.47	–0.0327	0.1039	–0.0988	0.04265	–0.00686	0.9980	0.5578
Palladium	16	20–1000	565.9	–9.595	55.69	–133.0	138.5	–52.08	0.7000	47.0377
Platinum	22	100–2000	83.39	–0.0851	0.2017	–0.2007	0.09768	–0.01805	0.9987	0.3290
Plutonium, PC	7	100–350	1.229	0.0347	–0.2235	1.041	–2.045	1.520	1.0000	0.0112
Potassium	10	20–336.8	235.5	–4.734	62.21	–370.2	1013.0	–1035.0	0.9480	3.1255
Rhenium, PC	21	100–2600	65.42	–0.0923	0.1419	–0.0987	0.03280	–0.00412	0.9877	0.7935
Rhodium	13	100–1400	232.0	–0.7099	2.264	–3.431	2.364	–0.6007	0.9713	1.7442
Silicon	19	100–1685	1587.	–10.43	26.31	–30.61	16.49	–3.330	0.9480	51.3292
Silver	16	100–1234	480.1	–0.4705	1.61	–2.793	2.167	–0.6196	0.9950	0.3744
Sodium	12	20–371	1080.	–32.73	393.3	–2112.0	5201.0	–4791.0	0.9256	17.8295
Tantalum	23	100–3200	59.39	–0.011	0.0232	–0.0155	0.00467	–0.00053	0.9948	0.2929
Thorium	23	20–1000	57.5	–0.1337	0.6649	–1.402	1.332	–0.4668	0.9305	0.9067
Tin, P	15	20–505.1	493.4	–11.3	109.5	–472.3	923.2	–665.7	0.9088	14.0747
Tin, /c/	11	20–505.1	348.1	–8.197	81.21	–354.9	697.6	–503.7	0.9006	16.0982
Tin, PC	11	20–505.1	476.6	–11.08	107.4	–462.4	899.3	–644.5	0.9316	14.1232
Titanium, PC	15	100–1900	39.2	–0.1049	0.2062	–0.1905	0.08575	–0.01483	0.9918	1.0287
Tungsten	22	100–3653	263.4	–0.3905	0.4112	–0.2142	0.05286	–0.00493	0.9974	1.3480
Uranium, PC	16	100–1200	16.42	0.0663	–0.1569	0.2483	–0.1786	0.04835	1.0000	0.0974
Vanadium	15	100–2000	40.58	–0.075	0.1941	–0.1949	0.08974	–0.01541	0.9948	1.1346
Zinc, PC	10	100–692.6	134.6	–0.2187	1.514	–4.781	6.458	–3.182	0.9963	0.3541
Zirconium, PC	17	100–2000	41.1	–0.110	0.2094	–0.1782	0.07351	–0.01179	0.9812	1.6257

[a] PC, polycrystalline; P, perpendicular to *c*-axis; /a/, parallel to *a*-axis; /b/, parallel to *b*-axis; /c/, parallel to *c*-axis.

[b] Values are also good for polycrystalline gallium.

correlation proposed in this work is suitable for $T > T_m$ up to the melting point.

NOMENCLATURE

A	Heat transfer area, m^2
AARE	Average of the absolute relative errors
a, b, c, d	Constants in multilinear fitting equation, Eq. (9)
$B_0, B_1, B_2, \ldots, B_n$	Constants in polynomial fitting equation, Eq. (8)
dT/dx	Temperature gradient in the x direction, $K \cdot m^{-1}$
k	Thermal conductivity, $W \cdot m^{-1} \cdot K^{-1}$
L_0	Lorenz number $= 2.443 \times 10^{-8}$, $\Omega \cdot W \cdot K^{-2}$
M	Number of data points in a given set of data
m, n	Constants in Eqs. (4) and (5)
Q	Heat transfer rate, W
R^2	Coefficient of determination defined by Eq. (7)
T	Temperature, K
T_m	Temperature at which k is maximum on the k–T curve, K

Greek letters

α', α'', β	Constants in Eqs. (4) and (5) as listed in Table II
γ	Some function of the atomic concentration of point defects, Eq. (6)
δ	Exponent parameter in Eq. (6)
ρ_0	Residual electrical resistivity, $\mu\Omega \cdot cm$
σ	Electrical conductivity ($\Omega^{-1} \cdot m^{-1}$)

Subscripts

cal	Calculated
e	Electronic
exp	Experimental
ℓ	Lattice

REFERENCES

1. J. C. Anderson, K. D. Leaver, R. D. Rawlings, and J. M. Alexander, *Materials Science*, 4th ed. (Chapman and Hall, London, 1990).
2. F. P. Incropera and D. P. DeWitt, *Fundamentals of Heat & Mass Transfer*, 4th ed. (John Wiley, New York, 1996).

3. W. D. Callister, Jr., *Materials Science and Engineering: An Introduction*, 5th ed. (John Wiley, New York, 2000).
4. K. Grotheim and H. Kvande (eds.), *Understanding the Hall-Heroult Process for the Production of Aluminium* (Aluminium Verlag, Dusseldorf, Germany, 1986).
5. Y. S. Touloukian, R. W. Powell, C. Y. Ho, and P. Klemens (eds.), *Thermophysical Properties of Matter, Vol. 1. Thermal Conductivity of Metallic Solids* (Plenum Press, New York, 1972).