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LETTER TO THE EDITOR

An accurate analytic representation for the Bloch–Gruneisen integral

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Abstract. An analytic representation for the Bloch-Gruneisen integral, describing the electron-photon interaction contribution to the electrical resistivity of metals, is presented. The representation takes the form of an originally infinite series, truncated to K terms. The approximation is highly accurate yielding relative errors less than 1% for even a single term ($K=1$) for $T \leqslant \theta/4$ and less than 0.1% with $K=20$ for all $T \leqslant 10\theta$, where θ is the Debye temperature. The series approximation is shown to be superior to the previously suggested ninth-order polynomial in $\log(\theta/T)$. Two other infinite series approximations are also discussed.

The contribution of the electron-photon interaction to the electrical resistivity of many metals is given by the Bloch-Gruneisen law (Gruneisen 1933):

$$\rho_i = (c/\theta)(T/\theta)^5 \int_0^{\theta/T} z^5[(e^z-1)(1-e^{-z})]^{-1}\,dz \tag{1}$$

where c is a constant, θ is the Debye temperature of the metal and T is the absolute temperature. The temperature dependence of the resistivity of simple monovalent metals, as well as polyvalent and even some transition metals, obeys this law closely so that c and θ determine the resistivity of the metal over a wide temperature range (White and Woods 1959, Karamargin *et al* 1972, Kong *et al* 1977, Igasaki and Mitsuhashi 1980, 1983). The determination of θ and c from measured data using (1) is, however, a rather delicate and time-consuming job as the non-linear least-squares fit requires a rather accurate numerical integration at each temperature. Very few such determinations have therefore been done. An appropriate analytic approximation to the integral would greatly facilitate the task of determining c and θ from resistivity data.

Such an approximation in the form of a ninth-order polynomial in $\log(\theta/T)$ was recently proposed by Igasaki and Mitsuhashi (1987). This polynomial, however, deviates at points from the exact value by up to a few per cent and the range of θ/T over which it applies is necessarily restricted. In this letter we present an analytic representation of the integral in (1) in terms of an infinite series, which is valid for all temperatures and yields high accuracy results for a small number of terms. The number of terms required for a given level of accuracy at a given temperature is also discussed.

Note first, that

$$[(e^z-1)(1-e^{-z})]^{-1} = e^{-z}[1-e^{-z}]^{-2} = X(1-X)^{-2}$$

where $X = e^{-z} < 1$ for all finite temperatures. Under this condition we substitute in (1) the series expansion (Gradshteyn and Ryzhik 1980, equation (1.113)):

$$X(1-X)^{-2} = \sum_{k=1}^{\infty} kX^k$$

and obtain

$$I(\theta/T) = \int_0^{\theta/T} z^5[(e^z-1)(1-e^{-z})]^{-1}\,dz = \sum_{k=1}^{\infty} k \int_0^{\theta/T} z^5\,e^{-kz}\,dz.$$

The last integral is readily calculated to yield

$$I(\theta/T) = 120\zeta(5) - \sum_{k=1}^{\infty} \exp(-ky) \times [y^5 + (5/k)y^4 + (20/k^2)y^3 + (60/k^3)y^2 + (120/k^4)y + 120/k^5] \qquad (2)$$

where $\zeta(p) = \Sigma_{k=1}^{\infty} k^{-p}$ is the Riemann zeta function and $y = \theta/T$.

A computer program was written to integrate $I(\theta/T)$ numerically (I_0) to an accuracy of 10^{-8} and to calculate corresponding approximate values using (2) for a given number K of terms in the infinite series (I_k). It also calculates approximate values (I_{IM}) using the ninth-order polynomial of Igasaki and Mitsuhashi (1987). The relative errors $|I_0 - I_k|/I_0$ and $|I_0 - I_{IM}|/I_0$ so obtained are given in figure 1, for $\theta/100 \leqslant T \leqslant \theta$. The constant level of relative error at $\sim 10^{-8}\%$ for large θ/T reflects the accuracy of the numerical integration of I_0. Note that even when truncating the series in (2) after the first term, the accuracy is better than 1% up to $T \sim \theta/4$, e.g., $T \approx 100$ K for Ti having $\theta \approx 400$ K (Igasaki and Mitsuhashi 1987). With five terms in the series, a $\leqslant 1\%$ accuracy persists up to $T \approx 0.9\theta$, i.e. over two decades in θ/T. For 50 terms a relative error

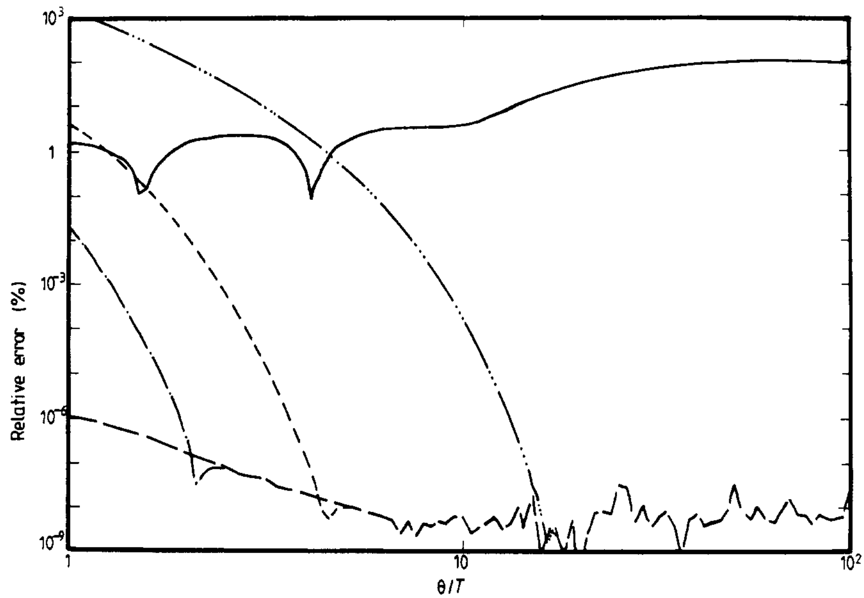

Figure 1. Relative deviation from the Bloch-Gruneisen integral of the ninth-order polynomial approximation of Igasaki and Mitsuhashi (1987) (——) and of the infinite series in equation (2) truncated to 1(— · · · —), 5(- - -), 10(— · —) and 20(— —) terms.

below 0.1% persists to well above $T = 10\theta$. By comparison, the ninth-order polynomial approximation is seen to yield inferior accuracies to even a single term series below $T \approx \theta/6$, with deviations of the order of 1.5% over several subintervals in the range $\theta/6 < T < 10\theta$. The deviations near $T \approx 10\theta$ are ~5%.

Finally, using

$$[(e^z+1)(1-e^{-z})] = 4\sinh^2(z/2)$$

we obtain

$$I(\theta/T) = \int_0^{\theta/2} z^5[(e^z+1)(1-e^{-z})]\,dz = 16\int_0^{\theta/2T} z^5 \sinh^{-2} z\,dz$$

and after a single integration by parts

$$I(\theta/T) = -0.5y^5\coth(y/2) + 80\int_0^{\theta/2T} z^4 \coth z\,dz \qquad (3)$$

where $y = \theta/T$. Expansion of coth z in powers of z yields a very slowly converging power series representation for the integral in (3), valid only for $T > \theta/2\pi$. Another expansion (Gradshteyn and Ryzhik 1980, equation (2.321.2)):

$$\coth z = z^{-1} + 2\sum_{k=1}^{\infty} z[z^2 + (\pi k)^2]^{-1}$$

yields a divergent representation for $I(\theta/T)$. Neither of these two series is useful as a representation of the integral.

We conclude therefore that the series in (2) accurately approximates the integral in (1) for a small number of terms. The exact number of terms required to obtain a given accuracy depends upon the minimal (θ/T). For temperatures up to $T \sim \theta$ however, less than 15 terms suffice to approximate even the most accurate experimental data.

References

Gradshteyn I S and Ryzhik I M 1980 *Tables of Integrals, Series and Products* (New York: Academic)
Gruneisen E 1933 *Ann. Phys., Lpz* **16** 530
Igasaki Y and Mitsuhashi H 1980 *Thin Solid Films* **70** 17
—— 1983 *J. Appl. Phys.* **54** 836
—— 1987 *Phys. Status Solidi* a **99** K111
Karamargin M C, Reynolds C A, Lipschultz F P and Klemens P G 1972 *Phys. Rev.* B **5** 2856
Kong W M T, Polan J S and Rose K 1977 *J. Appl. Phys.* **48** 5170
White G K and Woods S B 1959 *Phil. Trans. R. Soc.* A **251** 273