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Polynomial Expression of the Bloch-Grüneisen Integral - Application to an Analysis of the Resistivity-Temperature Variation of Metals

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In many metals, the electrical resistivity (ρ_i) caused by electron-phonon interaction is represented by the following semi-empirical expression, known as the Bloch-Grüneisen relation /1/:

$$\rho_i = (C/\Theta)(T/\Theta)^5 \int_0^{\Theta/T} x^5\{(e^x - 1)(1 - e^{-x})\}^{-1} dx\,, \tag{1}$$

where T, C, and Θ are the absolute temperature, a normalization constant, and a characteristic temperature of the lattice resistivity of the metal, respectively.

Equation (1) has an undetermined constant C and a characteristic temperature Θ. Once the parameters C and Θ are suitably chosen, (1) can represent the experimental data on the temperature variation of the resistivity for a variety of metals, such as not only simpler monovalent metals but also many polyvalent and transition metals as well. It is a difficult, however, laborious and time-consuming task to analyse experimental data by using (1) to estimate two unknown parameters C and Θ simultaneously, because (1) involves the integration procedure. In fact, the analysis of data has been limited in the special cases /2, 3/ that one or both of them were known. Therefore, it may be highly desired to devise a certain simpler method that will allow us to estimate the two parameters.

In Fig. 1, log $F(\Theta/T)$ is plotted as a function of log (Θ/T). Here, $F(\Theta/T)$ is the integral term in (1). The values of F were computed to five significant digits by using Simmpson's rule. In a range of smaller log (Θ/T), log F increases nearly as a linear function of log (Θ/T) and as the log (Θ/T) value increases, the slope of the tangent decreases to zero near log $(\Theta/T) = 1$. Therefore, it can be reasonably expected that log F may be represented by a poly-

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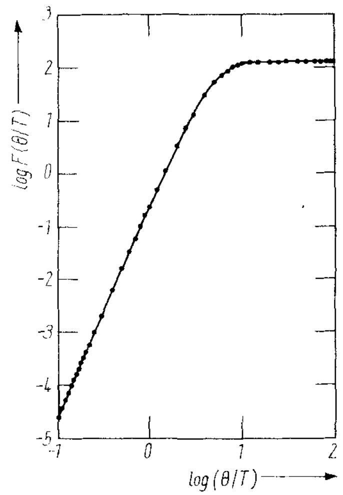

Fig. 1. log F(Θ/T) versus log (Θ/T) plot: F(Θ/T) is the integral term in (1). The solid line is log F(Θ/T) represented by (2); here, Θ is the characteristic temperature of the lattice resistivity in metals

nomial of log (Θ/T).

The polynomial function is designated as log $\bar{F}$(ΘT). When log $\bar{F}$ is represented by a polynomial to ninth order of log (Θ/T), the function was obtained as follows;

$$\log \bar{F}(\Theta/T) = \sum_{i=0}^{9} A_i (\log (\Theta/T))^i , \tag{2}$$

where $A_0 = -0.63212$, $A_1 = 3.8883$, $A_2 = -0.039627$, $A_3 = -0.29215$, $A_4 = -1.2893$, $A_5 = -0.51468$, $A_6 = 1.1127$, $A_7 = 0.15772$, $A_8 = -0.44200$, $A_9 = 0.099955$. The constans A_i in (2) were determined by using the Gauss-Newton method. The maximum value of $|(F - \bar{F})/F|$ was 3.12 % and the average value was 1.09 %. Thus it is concluded that $\bar{F}$ is a good approximate function of F. In Fig. 1, log $\bar{F}$ is also shown by the solid curve.

In general, the resistivity of metals can be divided up into the resistivity caused by electron-phonon interaction, represented by (1), and the resistivity independent of temperature, known as the residual resistivity. Thus, the resistivity is represented as follows;

$$\varrho = \varrho_0 + (C/\Theta)(T/\Theta)^5 \bar{F}(\Theta/T) , \tag{3}$$

where ϱ_0 is the residual resistivity that is approximated by the resistivity measured at 4.2 K. Now, we define a function f(C,Θ) as follows;

$$f(C,\Theta) = \sum_j \left\{ \varrho_c^j(C,\Theta) - \varrho_{exp}^j \right\}^2 , \tag{4}$$

where ϱ_c^j and ϱ_{exp}^j are resistivities calculated and measured at temperature T_j, respectively, and j represents a series of data measured at T_j and equals the number of data of a given sample. Therefore, we can find an equation which represents the resistivity-temperature variation of a given metal by estimating C and Θ so as to minimize f(C,Θ). In the present study, Powell's function minimization method /4/ was used in order to analyse the data and find the unknown

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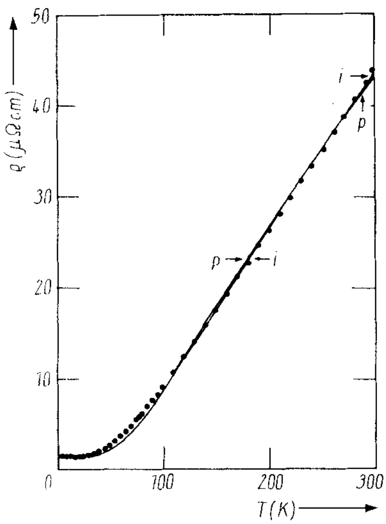
Values of C and Θ for the four samples obtained by a computer analysis by using Powell's function minimization method

material	thickness (nm)	ρ_0 ($\mu\Omega$cm)	C ($\mu\Omega$cmK))	Θ (K)	remarks
Ti		0.0[1]	91000	380.0	bulk /6/
Ti	1060	1.358	97720	396.6	single crystal film
Ti_2N	580	21.41	108300	410.8	reactively sputtered film
TiN	260	11.94	39090	451.5	reactively sputtered film /7/

1) The resistivities given in the reference were ideal resistivities (ρ - ρ_0).



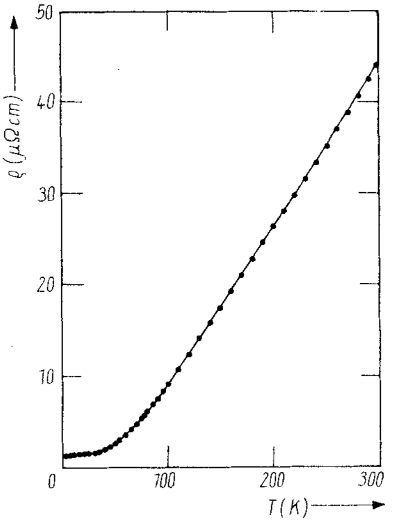


Fig. 2. Temperature-resistivity variation of a Ti single crystal film with (0001) orientation: solid curves are the calculated values using $F(\Theta/T)$ or $\bar{F}(\Theta/T)$ with $C = 97720$ and $\Theta = 396.6$, respectively: i and p beside the curve indicate $F(\Theta/T)$ and $\bar{F}(\Theta/T)$, respectively

Fig. 3. Temperature-resistivity variation of a Ti film calculated by using the temperature-dependent $\Theta(T)$ function presented in the text

parameters.

In Table 1, the values of C and Θ obtained by analysing the experimental resistivity-temperature data of a titanium epitaxial film (1060 nm thick) deposited on a sapphire substrate are indicated with those of other three samples. In the case of titanium, the estimated value of Θ is considered to be reasonable since the values reported by other investigators also cover from $\approx$ 280 to $\approx$420 K /5/. The validity of the C value for the present example, however, cannot be discussed because no information on that is available at all.

Fig. 2 shows the resistivity-temperature variation of a Ti film. Solid circles represent the experimental values and the two solid curves show the resistivities of the sample calculated by using (3) with the values of C and Θ ; one curve, the tangential slope of which is larger in the lower temperature range and smaller in the higher temperature range than that of the other, represents the result calculated by using $\bar{F}(\Theta/T)$, and the other by using $F(\Theta/T)$. These two calculated results agree considerably well with each other. Thus, it may be concluded that the polynomial formula presented here is very useful in the computer analysis of resistivity-temperature variations of metals, especially in which a resistivity minimum is observed at a certain temperature /6/.

In the above discussion, the value of Θ is considered to be constant independent of temperature, however, a closer agreement between the experimental and the calculated values of resistivity may be obtained by taking account of the temperature dependence of Θ. Fig. 3 shows the temperature-resistivity variation of a Ti film using a temperature dependent Θ formulated as follows;

$$\Theta(T) = \sum_{i=0}^{4} B_i T^i , \tag{5}$$

where $B_0 = 284.78$, $B_1 = 2.1147$, $B_2 = -1.4310\times10^{-2}$, $B_3 = 4.1122\times10^{-5}$, and $B_4 = -4.3658\times10^{-8}$. But the discussion about the temperature dependence of Θ obtained is outside the scope of the present study.

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