

## Computation of Mean Debye Temperature of Cubic Crystals from Elastic Constants\*

S. L. QUIMBY AND PAUL M. SUTTON†  
Columbia University, New York, New York  
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An improved method is presented for computing the mean Debye characteristic temperature of cubic crystals from the elastic constants. It is based upon an evaluation of the distribution in solid angle of the roots of the cubic equation which describes the propagation of plane acoustic waves in the crystal, and otherwise employs a device due to Hopf and Lechner. The end result is given in simple closed expressions which present no computational difficulty. The uncertainty in the computed value of the mean Debye temperature due to the approximation made in the method is of the order 0.1 percent when the anisotropy factor of the crystal is as large as 4.

### INTRODUCTION

THE mean Debye temperature,  $\Theta_D$ , of a cubic crystal is given by the expression

$$\Theta_D = (h/k)v_m \{3N/4\pi V\}^{1/3}, \quad (1)$$

where  $N$  is the number of atoms in volume  $V$  of the crystal and  $v_m$  is defined by the formula

$$3/v_m^3 = \sum_i (1/v_{mi}^3), \quad i=1, 2, 3, \quad (2)$$

in which the  $v_{mi}$  are the three velocities of propagation of plane elastic waves in the crystal, averaged over all directions in the crystal. A given direction of propagation in a cubic crystal is conveniently specified by its direction cosines,  $\alpha, \beta, \gamma$ , with respect to the principal crystal axes. The corresponding propagation velocities are then given in terms of the elastic constants,  $c_{jk}$ , of the lattice by the expression

$$z_i = (\rho v_i^2 - c_{44}) / (c_{11} - c_{44}), \quad (3)$$

provided the  $z_i$  are the three real roots of the cubic equation,<sup>1</sup>

$$z^3 - z^2 + (1 - K^2)\Gamma z - (1 - 3K^2 + 2K^3)\chi = 0, \quad (4)$$

where

$$K = (c_{12} + c_{44}) / (c_{11} - c_{44}), \quad \Gamma = \alpha^2\beta^2 + \beta^2\gamma^2 + \gamma^2\alpha^2, \\ \chi = \alpha^2\beta^2\gamma^2.$$

It follows immediately from Eqs. (2) and (3) that

$$\frac{3}{v_m^3} = \left[ \frac{\rho}{c_{11} - c_{44}} \right]^{1/3} \int_0^{4\pi} \left[ \sum_i \frac{1}{(C + z_i)^3} \right] \frac{d\Omega}{4\pi}, \quad (5)$$

where  $C = c_{44} / (c_{11} - c_{44})$ , and  $d\Omega$  is an element of solid angle. The present paper is concerned with the evaluation of the integral in Eq. (5).

Hopf and Lechner<sup>2</sup> devised a method for the approxi-

mate evaluation of the integral which is, briefly, as follows: The function  $f(z) = (C+z)^{-3}$  is replaced in the interval  $0 < z < 1$  by a fifth degree polynomial in  $z$ . The coefficients of  $z$  in this polynomial are obtained by the Lagrange interpolation method. This amounts to forcing the representative function through the points  $f(0), f(1)$  and four equally spaced intermediate points. The sum in the integrand then appears as a series of sums of powers, up to the fifth, of the roots of the cubic Eq. (4), multiplied by numerical coefficients. But such sums of powers are directly expressible in terms of the coefficients of the cubic, which are constants apart from the quantities  $\Gamma$  and  $\chi$ . Accordingly, the approximate evaluation of the integral requires only computation of the average values of various functions of the direction cosines,  $\alpha, \beta$ , and  $\gamma$ . These averages are, of course, the same for all cubic crystals and are given by Hopf and Lechner.

Three defects in the foregoing method are apparent: first, it is extremely laborious, and the labor increases rapidly as higher powers of  $z$  are introduced in the representative functions;<sup>3</sup> second, no cognizance is taken of the actual range of values of the roots or of their distribution in solid angle; third, the method contains no means for ascertaining the accuracy of the result obtained. In accordance with Eq. (4), both the range and distribution of the roots depend solely on the quantity  $K$ . It is shown hereafter that if  $K > 1$ , two of the roots are negative and the third is greater than

TABLE I. Values of the constant  $K$ , and the anisotropy factor,  $A$ , for various cubic crystals.<sup>a</sup>

	$K$	$A$		$K$	$A$		$K$	$A$
Fe	2.29	2.32	Ag	1.74	2.88	Al	1.13	1.18
Ni	2.12	2.63	Pb	1.64	3.89	W	1.01	1.01
Cu	2.09	3.21	Cu <sub>2</sub> Au	1.63	2.52	NaCl	0.70	0.69
ZnS	1.98	1.16	Au	1.40	2.91	CaF <sub>2</sub>	0.60	0.57
LiF	1.93	1.69	C	1.37	1.60	KI	0.38	0.37
MgO	1.79	1.42	NaBr	1.36	1.37	KCl	0.37	0.37

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† Now at Corning Glass Works, Corning, New York.

<sup>1</sup> M. Born, *Atomtheorie des festen Zustandes*, Enc. Math. Wiss. (Teubner, Leipzig), Vol. 3, p. 648.

<sup>2</sup> L. Hopf and G. Lechner, *Verhandl. deut. physik. Ges.* **16**, 643 (1914).

<sup>a</sup> Most of these are computed with values of the elastic constants tabulated by R. F. S. Hearmon, *Revs. Modern Phys.* **18**, 409 (1946).

<sup>3</sup> Fuchs has employed an eighth degree polynomial. See *Proc. Roy. Soc. (London)* **A153**, 622 (1936) and **A157**, 444 (1936).

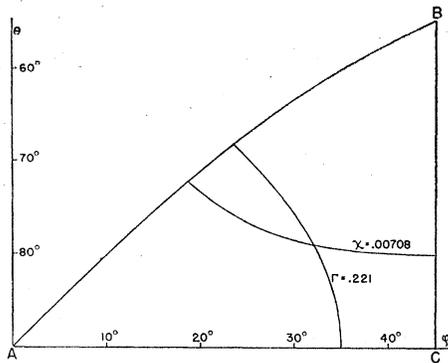


FIG. 1. The basic triangle, showing a line of constant  $\Gamma$  and a line of constant  $\chi$ .

1 for all directions in the crystal; if  $K < 1$ , all three roots lie between 0 and 1, but in general two lie close to 0 and the third close to 1. Approximate values of  $K$  for various cubic crystals are given in Table I: it will be noted that  $K > 1$  for all metals and many other crystals. Evidently, an approximation function fitted in the interval 0 to 1 is ill-suited to represent the behavior of these materials.

Obvious improvement in the method of Hopf and Lechner is gained if  $f(z)$  is represented by a polynomial in the intervals in which the roots actually lie, as suggested by Durand.<sup>4</sup> But the accuracy of the result remains uncertain, and also the optimum degree of the polynomial to be employed, and the choice of the values of  $z$  to be used in the computation of its coefficients. A means for the removal of these uncertainties is suggested by the following analysis.

Let the integral in Eq. (5) be denoted by  $Y$  and written in the form

$$Y = \frac{1}{4\pi} \sum_i \int_{z_i} \frac{1}{(C+z_i)^{\frac{1}{2}}} \frac{d\Omega_i}{dz_i} dz_i, \quad (6)$$

where, now,  $(d\Omega_i/dz_i)dz_i$  is the element of solid angle associated with values of the  $i$ th root lying between  $z_i$  and  $z_i+dz_i$ . Evidently, the values of  $z$  chosen for computation of the representative function should include those at which maxima in the functions  $d\Omega_i/dz_i$  occur. Furthermore, if the three distribution functions,  $d\Omega_i/dz_i$ , are known, a direct measure of the accuracy of the approximate method follows from comparison of values of  $Y$  obtained when the true and representative functions are, respectively, inserted in the integrand. The optimum degree of the representative polynomial is then the lowest that yields a desired accuracy. Accordingly, the matters of immediate interest are, first, the specification of the ranges of the roots in terms of  $K$ , and second, the determination of the functions  $d\Omega_i/dz_i$ . Analytical expressions for the distribution functions in terms of  $K$  have not been obtained (otherwise no

approximation would be necessary), but a numerical evaluation thereof for a particular crystal permits a satisfactory resolution of the questions raised in the foregoing.

#### DESCRIPTION OF THE METHOD

Consider a unit vector drawn from the origin of a rectangular coordinate system whose axes lie parallel to the principal crystal axes. The direction of this vector may be specified by the polar coordinates,  $\theta$ ,  $\varphi$ , of its point of intersection with a unit sphere centered on the origin. In consequence of the crystal symmetry, the value of  $Y$  is 48 times the value of the integrals in Eq. (5) extended over the solid angle subtended by the right spherical triangle whose vertices lie at the points  $\theta=90^\circ$ ,  $\varphi=0^\circ$ ;  $\theta=54^\circ 45'$  ( $\cos^2\theta=\frac{1}{3}$ ),  $\varphi=45^\circ$ ;  $\theta=90^\circ$ ,  $\varphi=45^\circ$ . Figure 1 is a plan drawing of this triangle, in which the abscissas are proportional to  $\varphi$  and the ordinates to the complement of  $\theta$ . Goens<sup>5</sup> has given closed expressions for the three roots of Eq. (4) at all points on the boundary of the triangle. Expressed in terms of  $K$ , these are as follows.

For the boundary  $AC$ ,

$$z_1, z_2 = \frac{1}{2} \{1 \pm (\cos^2 2\varphi + K^2 \sin^2 2\varphi)^{\frac{1}{2}}\}, \quad z_3 = 0; \quad (7)$$

for the boundary  $AB$ ,

$$z_1, z_2 = \frac{1}{4} \{ (K-1) \sin^2 \psi + 2[1 \pm F(K)] \}, \\ z_3 = \frac{1}{2} (1-K) \sin^2 \psi, \quad (8)$$

where

$$F(K) = \left\{ -\frac{3}{4}(5K+3)(K-1) \sin^4 \psi \right. \\ \left. + (4K+3)(K-1) \sin^2 \psi + 1 \right\}^{\frac{1}{2}},$$

and  $\psi$  is the polar angle measured along  $AB$  from  $A$ .

For the boundary  $BC$  the formulas are those of the boundary  $AB$  with  $\theta$  substituted for  $\psi$  and  $z_2, z_3$  interchanged. In these expressions  $z_1$  is the root corresponding to the longitudinal wave, is always positive, and  $z_1 \geq 1$  according as  $K \geq 1$ . The roots  $z_2$  and  $z_3$  correspond to transverse waves, are negative or positive according as  $K \geq 1$ , and  $|z_2| \geq |z_3|$ .

The values of the roots at the points  $A, B$  and  $C$  are given in Table II. It will appear presently that these values determine the ranges of the roots. If  $K > 1$ , the negative roots lie between  $\frac{1}{2}(1-K)$  and 0, and the

TABLE II. Values of the roots of Eq. (4) at the vertices of the basic triangle, Fig. 1.

	A	B	C
$\Gamma$	0	1/3	1/4
$\chi$	0	1/27	0
$z_1$	1	$\frac{1}{2}(1+2K)$	$\frac{1}{2}(1+K)$
$z_2$	0	$\frac{1}{2}(1-K)$	$\frac{1}{2}(1-K)$
$z_3$	0	$\frac{1}{2}(1-K)$	0

<sup>4</sup> M. A. Durand, Phys. Rev. **50**, 449 (1936).

<sup>5</sup> E. Goens, Ann. phys. **29**, 279 (1937). Formulas appropriate to crystals of the tetragonal and hexagonal systems are also given.

positive root between 1 and  $\frac{1}{3}(1+2K)$ . If  $K < 1$ , the smaller roots lie between 0 and  $\frac{1}{2}(1-K)$ , and the larger between  $\frac{1}{3}(1+2K)$  and 1.

The computation of  $d\Omega/dz$  for each of the three roots is based upon a graphical method for the solution of the cubic Eq. (4).<sup>6</sup> The substitution  $z = y + \frac{1}{3}$  reduces this equation to the form

$$y^3 + py + q = 0, \tag{9}$$

where

$$\begin{aligned} p &= (1-K^2)\Gamma - \frac{1}{3}, \\ q &= \frac{1}{3}(1-K^2)\Gamma - (1-3K^2+2K^3)\chi - 2/27. \end{aligned} \tag{10}$$

In accordance with Eq. (9),  $p$  varies linearly with  $q$  for constant  $y$ . If  $p, q$  are regarded as the orthogonal coordinates of a point, then the curve  $y = \text{real constant}$  is a straight line, such as the line  $AC$  of Fig. 2, which corresponds to  $y = -\frac{1}{3}$  ( $z = 0$ ). The envelope of this family of lines is the discriminant curve of the cubic, the equation of which is

$$4p^3 = -27q^2. \tag{11}$$

The discriminant is shown as the curve  $NOM$  of Fig. 2. All points corresponding to values of  $p$  and  $q$  that yield real roots of Eq. (9) lie on, or within the cusp of, this curve. Associated with a point on either branch of the discriminant is a double root corresponding to the tangent to that branch, and a single root corresponding to the tangent to the other branch, both tangents being drawn through the point. The three real roots associated with a given point within the cusp are those associated with the three tangents to the discriminant, drawn through the point. They are

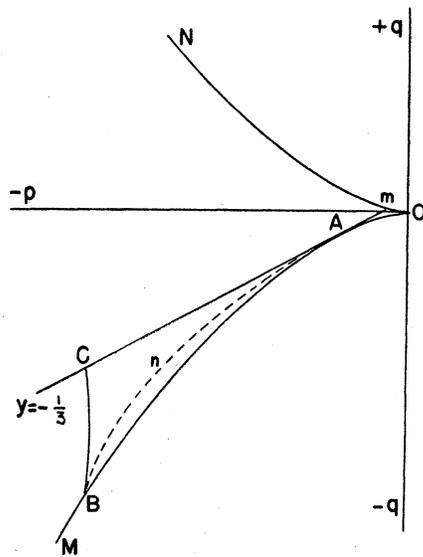


Fig. 2. Graphical solution of the reduced cubic, Eq. (9) (schematic).

<sup>6</sup> C. Runge, *Graphical Methods* (Columbia University Press, New York, 1912), p. 59.

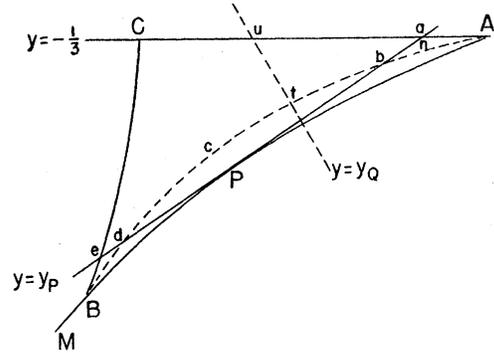


FIG. 3. Detail of Fig. 2 (schematic).

the respective double roots associated with the three tangent points on the discriminant. The values of the double roots at points on the discriminant are given by the expression

$$y = \pm (-p/3)^{1/2}, \tag{12}$$

where  $p$  is the abscissa of the point and the sign of  $y$  is same as that of the ordinate,  $q$ . It follows that, for different points within the cusp, the absolute values of the real roots are monotonically increasing functions of the absolute values of the abscissas of the points of tangency with the discriminant.

In virtue of Eqs. (10), the triangle of Fig. 1 can be mapped on the  $p$ - $q$  space of Fig. 2. The  $p, q$  values corresponding to points  $A$  and  $B$  satisfy Eq. (11) and  $q$  is negative, hence both lie on  $OM$ . One root corresponding to point  $C$  and, by Eq. (7) to all points on  $AC$ , is  $y = -\frac{1}{3}$  ( $z = 0$ ). Hence the line  $AC$  of Fig. 1 maps as the tangent  $AC$  of Fig. 2. The boundary  $AB$  of Fig. 1 maps as the dotted curve  $AnB$  of Fig. 2. (Not all values of  $p$  and  $q$  that yield real roots of Eq. (9) are consistent with Eqs. (10), because the ranges of possible values of  $\Gamma$  and  $\chi$  are limited to  $\frac{1}{3}$  and  $1/27$ , respectively.) Now  $\Gamma$  and  $\chi$  may be regarded as curvilinear coordinates of points in the triangle  $ABC$  of Fig. 1. Hence, through Eqs. (10), every point in this triangle can be mapped in the triangular area  $AnBC$  of Fig. 2, and vice versa.

It should be noted that the triangle  $AnBC$  of Fig. 2 corresponds to  $K > 1$ . If  $K < 1$ , the point  $A$  remains unaltered, but point  $C$  lies on  $Am$  and point  $B$  on  $AO$ . If  $K = 0$ ,  $C$  coincides with  $m$  and  $B$  with  $O$ ; if  $K = \frac{1}{3}$ ,  $C$  lies on the  $p$ -axis.

Earlier remarks concerning the signs of the roots and their ranges are immediate deductions from Fig. 2. For example, it is evident that, for  $K > 1$ , the maximum positive root corresponds to the tangent to  $ON$  through  $B$ , and the negative root of greatest absolute value corresponds to the tangent through  $C$  to  $OM$  prolonged.

The reader should now imagine that Fig. 1 is modified by the addition, within the triangle, of a grid of coordinate lines of constant  $\Gamma$  and constant  $\chi$ . (One each is shown in the figure.) It follows from the foregoing that to any area within the triangle  $AnBC$  of Fig. 2 there

corresponds an area in the triangle  $ABC$  of Fig. 1, which can be mapped with the aid of this coordinate grid. The value of this area is proportional to  $\int d\theta d\varphi$ . Suppose, next, that the abscissa of every point of the grid is reduced in the ratio  $\sin\theta:1$ . Then any area mapped on the shrunken grid is proportional to  $\int \sin\theta d\theta d\varphi$ , i.e. to the solid angle associated with that area. Hence to any area in the triangle of Fig. 2 there corresponds a solid angle measurable with a planimeter. This is the basis of the present method for measuring  $d\Omega/dz$ , which will now be described.

A portion of Fig. 2 is redrawn, schematically, in Fig. 3. Here  $ae$  is the line corresponding to the (negative) double root  $y_P$  on  $AM$ . It must be recalled that, in accordance with the present convention regarding the negative roots,  $|z_2| > |z_3|$ . Now for all points in the area  $AnbaA$ , tangent points of both tangents to  $AM$  lie between  $A$  and  $P$ , hence, by Eq. (12), both negative roots corresponding to such points are less than  $y_P$ . But for all points in the area  $abcdeCa$  the tangent point of only one tangent, namely that corresponding to the smaller root, lies between  $A$  and  $P$ , i.e., only the root  $z_3$  is less than  $y_P$ . Thus the solid angle,  $\Omega$ , associated with roots  $z_2$  less than  $y_P$  is that corresponding to the area  $AnbaA$ , while the solid angle associated with roots  $z_3$  less than  $y_P$  is that corresponding to the area  $AnbcdeCA$ . Furthermore, let the dashed line,  $ut$ , be the tangent to  $ON$  corresponding to the (positive) double root  $y_Q$ . Then the solid angle associated with roots  $z_1$  less than  $y_Q$  is that corresponding to the area  $AntuA$ .

Therefore, to obtain the solid angles  $\Omega_1, \Omega_2, \Omega_3$  associated, respectively, with roots  $z_1, z_2, z_3$ , less than preassigned values it is necessary only to plot the corresponding straight lines  $ae$  and  $ut$  on the shrunken grid of Fig. 1 and planimeter the appropriate areas. Curves

$$\begin{aligned} a_5 &= (1/x^2)\{2.25m_1/bd - 9m_2/bcg + 40.5m_3/cdf - 9m_4/bcf + 20.25m_5/ceg\}, \\ a_4 + (2 + \frac{2}{3}x)a_5 &= (1/x)\{3m_1/bd + 3m_2/xbc - 40.5m_3/xd - 3m_4/bcf\}, \\ a_3 + 2a_4 + (x^2 - x + 3)a_5 &= (1/x)\{m_1/b + (m_2 - m_4)/bc\}, \\ a_2 + (2 - x)a_3 + (x^2 - 3x + 3)a_4 + (2 - x)(x^2 - 2x + 2)a_5 &= (1/x)\{m_1 - (m_4/b)\}, \\ a_1 + a_2 + a_3 + a_4 + a_5 &= m_1, \\ a_0 &= m_0, \end{aligned}$$

where

$$\begin{array}{llll} m_0 = f(0), & m_3 = f(\frac{2}{3}x) - m_0, & x = \frac{1}{2}(1 - K), & d = 3 - 2x, \\ m_1 = f(1) - m_0, & m_4 = f(1 - x) - m_0, & b = 1 - x, & e = 3 - 4x, \\ m_2 = f(x) - m_0, & m_5 = f(1 - 4x/3) - m_0, & c = 1 - 2x, & f = 3 - 5x, \\ & & & g = 3 - 7x. \end{array}$$

Furthermore,

$$\begin{aligned} Y_R &= -5a_5(16x^3be)/385 + (5a_5 + 2a_4)(16x^2b^2)/21 \\ &+ (5a_5 + 4a_4 + 3a_3)(4x^2e)/105 \\ &- (5a_5 + 4a_4 + 3a_3 + 2a_2)(4xb)/5 + m_1 + 3m_0. \end{aligned} \quad (14)$$

The curves of Fig. 4 appertain specifically to a crystal for which  $K = 2.29$ . However, certain characteristics of

of  $\Omega_i$  as function of  $z_i$  are plotted, and graphical differentiation yields the functions  $d\Omega_i/dz_i$ .

The procedure described in the foregoing has been completed for the value  $K = 2.29$  of crystalline iron, with the result shown in Fig. 4. With regard to  $d\Omega_3/dz_3$ , separate analysis shows that, in the neighborhood of  $z_3 = 0$ ,

$$\frac{d\Omega_3}{dz_3} = \frac{\pi}{8} \left\{ \frac{1 + K}{(1 + 2K)(1 - K)z_3} \right\}^{\frac{1}{2}}.$$

Hence the contribution of this region to the quantity  $Y$  remains finite and computable.

The curves of Fig. 4 suggest that if a fifth degree polynomial is adopted to represent  $f(z)$ , then suitable values of  $z$  to be used for computing the coefficients of this polynomial are  $\frac{1}{2}(1 - K)$ ,  $\frac{1}{3}(1 - K)$ ,  $0$ ,  $1$ ,  $\frac{1}{2}(1 + K)$  and  $\frac{1}{3}(1 + 2K)$ . These lie at the termini of the resultant distribution function  $\sum_i d\Omega_i/dz_i$ , and at or near its three maxima. A significant computational advantage accrues from this choice of  $z$  values, for then an analytical solution of the resulting five simultaneous equations yields closed expressions for the polynomial coefficients and, with the aid of the averages of the appropriate functions of  $\Gamma$  and  $\chi$  previously mentioned, a closed expression for the approximate value of  $Y$  itself, all in terms of the single parameter  $K$ . Thus, let  $[f(z)]_R$  denote the representative polynomial given by the expression

$$[f(z)]_R = a_0 + a_1z + a_2z^2 + a_3z^3 + a_4z^4 + a_5z^5,$$

and

$$Y_R = \int_0^{4\pi} \left\{ \sum_i [f(z_i)]_R \right\} d\Omega/4\pi. \quad (13)$$

Then

these curves are independent of the value of  $K$ , and these both justify the application of Eq. (14) to crystals of arbitrary  $K$  and permit a facile computation of approximate distribution functions for such crystals. Thus, the maximum of  $d\Omega_1/dz_1$  always lies at the value of  $z_1$  corresponding to  $\frac{3}{4}$  of the interval of  $z_1$ ; the maximum of  $d\Omega_2/dz_2$  always lies slightly beyond the value of

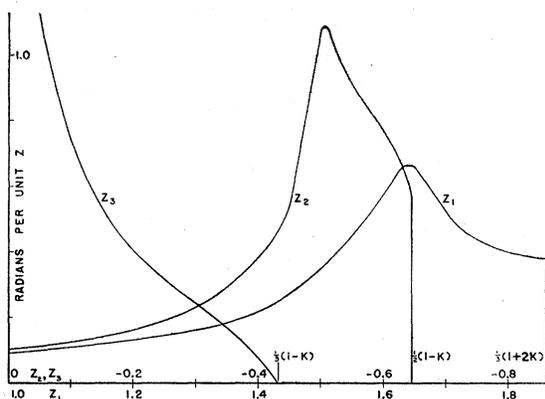


FIG. 4. The distribution functions for  $K=2.29$ .

$z_2$  corresponding to  $\frac{2}{3}$  of the interval to  $z_2$ ; the maximum of  $d\Omega_3/dz_3$  always lies at  $z_3=0$ , and its minimum, which is zero, always lies at the value of  $z_3$  corresponding to  $\frac{2}{3}$  of the interval of  $z_2$ . Furthermore, the interval of  $z_1$  is  $4/3$  that of  $z_2$ , irrespective of the value of  $K$ , and all three intervals are proportional to  $|K-1|$ . Lastly, the areas under all three curves must always equal  $4\pi/48$ . Hence the distribution curves for any cubic crystal are approximately those obtainable from Fig. 4 by altering the abscissas of all points in the ratio  $|K-1|/(2.29-1)$  and altering their ordinates in the inverse ratio.

If the curves of Fig. 4 are replotted with a single scale of abscissas, so that those for  $z_2$  and  $z_3$  lie to the left of  $z=0$ , and that for  $z_1$  lies to the right of  $z=1$ , then the distribution functions for crystals with  $K<1$  are similar, in the above sense, to those obtained by reflection of the  $z_2$  and  $z_3$  curves in the plane  $z=0$  and reflection of the  $z_1$  curve in the plane  $z=1$ . The remarks of the preceding paragraph are applicable without modification to these curves.

#### IMPROVEMENT OF THE ACCURACY OF THE METHOD

The accuracy of a tentative set of distribution functions can be readily ascertained as follows. Consider the two expressions

$$(a) \quad \frac{1}{4\pi} \sum_i \int_{z_i} [f(z_i)]_R (d\Omega_i/dz_i) dz_i,$$

and

$$(b) \quad \frac{48}{4\pi} \sum_i \int_{z_i} [f(z_i)]_R (d\Omega_i/dz_i)_C dz_i. \quad (15)$$

Here the range of each integral is the range of values of the indicated root of the cubic Eq. (4),  $(d\Omega_i/dz_i)$  is the *true* distribution function for this root, and  $(d\Omega_i/dz_i)_C$  the computed distribution function. Then (a) is identical with the quantity  $Y_R$  and is evaluated exactly by Eq. (14). The accuracy of the computed function follows by comparison of this figure with that obtained from expression (b) with the aid of a planim-

eter. The observed discrepancy is 0.23 percent for the functions of Fig. 4, and this is a reasonable estimate of the intrinsic inaccuracy of the graphical method employed. The procedure for obtaining the approximate distribution functions of other crystals from those of iron, described at the end of the preceding section, is verified by application of formulas (a) and (b) to the data of lead ( $K=1.64$ ). The discrepancy is 3.3 percent.

The percent error in the computed mean  $\Theta_D$  introduced by the substitution of  $Y_R$  for  $Y$  in Eq. (5) is one third of the percent difference between these two quantities. The difference itself is given by the expression

$$\frac{48}{4\pi} \sum_i \int_{z_i} \{f(z_i) - [f(z_i)]_R\} (d\Omega_i/dz_i)_C dz_i, \quad (16)$$

evaluated with a planimeter. Clearly approximate distribution functions, such as those of lead cited in the preceding paragraph, are entirely adequate for use in the formula (16), since the error so computed is a few percent at most. A means is therefore available whereby the approximate value,  $Y_R$ , of  $Y$  for whatever crystal can be *corrected*, so that the residual error in the computed mean  $\Theta_D$  due to the approximation is entirely negligible.

As  $z$  approaches  $-C$ , the function  $f(z)$  approaches infinity, hence the representation afforded by  $[f(z)]_R$  and the accuracy of the approximation become poorer. Now the minimum value of  $z$ ,  $z(\min)$ , is  $\frac{1}{2}(1-K)$  and  $1+z(\min)/C = (c_{11}-c_{12})/2c_{44} = 1/A$ , where  $A$  is the anisotropy factor of the crystal. The correction, computed as a function of  $1/A$  with formula (16), which is to be *added* to the value of  $Y_R$  obtained with Eq. (14), is given in Fig. 5. When the value of  $Y_R$  thus corrected is substituted for the integral in Eq. (5), the associated residual uncertainty in the computed mean  $\Theta_D$  is of the order 0.1 percent, which is at least an order of magnitude less than that introduced by the experimental uncertainty in the difference factor  $(c_{11}-c_{44})$  of Eq. (5).

#### APPLICATIONS OF THE METHOD

Grüneisen and Goens<sup>7</sup> devised an alternative method for the evaluation of  $v_m$ . In this method the vertices of the basic triangle are the points  $\theta=0$ ;  $\theta=90^\circ$ ,  $\varphi=0$ ;

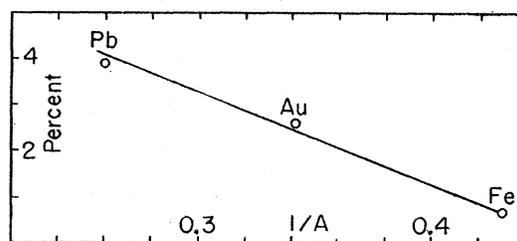


FIG. 5. Correction to be added to the value of  $Y_R$  computed with Eq. (14).

<sup>7</sup> E. Grüneisen and E. Goens, Z. Physik 26, 255 (1924).

$\theta=90^\circ$ ,  $\varphi=45^\circ$ . Values of  $z_i$  at angular intervals of  $15^\circ$  on the boundary are computed with Eqs. (7) and (8); values at the same intervals on the meridians  $\varphi=15^\circ$ ,  $\varphi=30^\circ$  are obtained by solution of the cubic Eq. (4).<sup>8</sup> The corresponding mean velocities  $v_{mi}$  are computed with the trapezoidal formula, and then  $v_m$  with Eq. (2).

<sup>8</sup> A. Zavrotsky, *Tablas para la Resolucion de las Ecuaciones Cubicas* (Editorial Standard, Caracas, 1945), contains the real and complex roots of the reduced cubic [Eq. (9)] to six figures, for  $-100 < p, q < +100$ , with the interval unity.

Röhl obtained by this method the mean Debye temperatures  $158^\circ\text{K}$  for gold and  $212^\circ\text{K}$  for silver at room temperature.<sup>9</sup> The present method *applied to Röhl's data*, yields the values  $157.6^\circ\text{K}$  and  $211.3^\circ\text{K}$ , respectively.

In conclusion, the authors gratefully acknowledge their indebtedness to the Watson Scientific Computing Laboratory of Columbia University for an especially prepared, six-place, differenced table of values of  $x^{-\frac{1}{2}}$ .

<sup>9</sup> H. Röhl, *Ann. phys.* **16**, 887 (1933).

## Deflection of High-Energy Electrons in Magnetized Iron\*

STEPHAN BERKO AND FRANK L. HEREFORD  
*University of Virginia, Charlottesville, Virginia*

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High-energy electrons are scattered in magnetized iron. From a shift in the multiple scattering curves due to the reversal of the magnetic field, the effective field  $b_{\text{eff}}$  acting on electrons traversing ferromagnetic media is computed. Such an effective field is dependent on the short range forces between beam electrons and spin-aligned ferromagnetic electrons. The measurements show an effective field equal to the macroscopically measured flux density  $B$ .

THE question as to the effective magnetic field acting on charged particles traversing a ferromagnetic medium was first raised in connection with cosmic-ray deflection experiments.<sup>1</sup> The most complete theoretical discussion of the problem is given by Wannier,<sup>2</sup> who translated into quantum-mechanical language the objections, first raised by Swann<sup>3</sup> in classical terms, against the supposition that the effective field is necessarily equal to the macroscopically defined flux density  $B$ . Wannier's theoretical conclusions can be summed up as follows.

Since the magnetization in a ferromagnet is due to the electron spin, the macroscopically defined flux density  $B$  is the result of an average over all elementary dipoles (spin-aligned electrons). If a fast charged particle traverses the magnet, it is influenced at each point by a

force due to the "true" field at this point. This true field, however, varies over a very wide range of magnitudes within regions of the order of a Compton wavelength around the spin-aligned electrons. The effective field  $b_{\text{eff}}$  is defined as an average field acting on the particle along its path. It can be shown that, although rare, close range interactions (corresponding to classical "head-on collisions") between the beam particle and the ferromagnetic electrons are decisive in determining this average. Only if all points in the magnet can be given equal statistical weight, will  $b_{\text{eff}}=B$ . Should short-range forces exist between beam particle and electrons, the effective field will be changed accordingly. This effect is described by introducing a "coincidence probability,"

$$p(r) = \frac{\text{(chance of finding the electron at } r \text{ if beam particle is also at } r\text{)}}{\text{(chance of finding the electron at } r \text{ if beam particle is far away)}}$$

The average of the magnetization along the path of the beam particle is taken by first weighting the true magnetization at each point with this coincidence probability  $p(r)$ , a quantity dependent on the force between beam particle and electrons. Wannier has com-

puted  $p(r)$  for the case of Coulomb forces. The final result is expressed by  $b_{\text{eff}}=B+2\pi M(p-1)$ .

In this formula  $p>1$  means attractive forces (for example positrons)  $p<1$ , repulsive ones. It is seen that  $b_{\text{eff}}$  can be larger than  $B$  for the attractive case. The deviation of  $p$  from 1 occurs, however, at such low beam energies that it would be hardly verifiable experimentally. Should, however, short-range forces exist, the deviation of  $b_{\text{eff}}$  from  $B$  could be more pronounced than for the pure Coulomb case. An experiment on the effect-

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<sup>1</sup> B. Rossi, *Atti acad. Lincei* **11**, 478 (1930); L. M. Mott-Smith, *Phys. Rev.* **39**, 403 (1932); B. Rossi, *Nature* **128**, 300 (1931).

<sup>2</sup> G. H. Wannier, *Phys. Rev.* **72**, 304 (1947).

<sup>3</sup> W. F. G. Swann, *Phys. Rev.* **49**, 574 (1936).