

Calculation of the Mean Debye Temperature of Cubic Crystals

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A rapid method of computing the mean Debye characteristic temperatures of anisotropic cubic crystals is described. The method employs the known relationships of the elastic moduli of single and polycrystals of the same material and gives Debye temperatures with an uncertainty of less than 1% when these values are compared with those calculated from more elaborate procedures.

INTRODUCTION

THE labor involved in the computation of the mean Debye characteristic temperature of an anisotropic cubic single crystal from the three independent moduli of elasticity, c_{ik} , can be considerably reduced by averaging the moduli over all directions in the crystal rather than the velocities of propagation of plane elastic waves. Such an averaging, in effect, gives the two independent moduli which define the elastic behavior of a polycrystal of the same material. The crystal can then be considered as isotropic elastically and the Debye temperature calculated from the appropriate equation. In this manner, the Debye temperature can be obtained from the solution of three simple equations with an uncertainty of less than 1%.

DESCRIPTION OF EQUATIONS

Huber and Schmid¹ have provided involved expressions relating the moduli which determine the elastic behavior of a single and a multiple crystal, but we suggest that the simple equations of Voigt² and Reuss³ be employed, namely,

$$\text{Voigt: } \bar{s}_{11} = \frac{2c_{11} + 3c_{12} + c_{44}}{(c_{11} - c_{12} + 3c_{44})(c_{11} + 2c_{12})};$$

$$\bar{s}_{44} = \frac{5}{(c_{11} - c_{12} + 3c_{44})},$$

$$\text{Reuss: } \bar{s}_{11} = \frac{c_{44}(3c_{11} + c_{12}) + (c_{11} - c_{12})(c_{11} + 2c_{12})}{5c_{44}(c_{11} - c_{12})(c_{11} + 2c_{12})};$$

$$\bar{s}_{44} = \frac{4c_{44} + 3(c_{11} - c_{12})}{5c_{44}(c_{11} - c_{12})},$$

where \bar{s}_{ik} are the moduli of compliance of the polycrystal. These separate expressions for the moduli of a polycrystal given by Voigt and Reuss differ in their derivation only in the manner in which the averaging of the single crystal moduli is made. Voigt considered that each randomly orientated crystallite of the polycrystal was

subjected to equal strains and he averaged the resultant stresses in all the crystallites to arrive at his equations. Reuss, on the other hand, set up equal stresses in each crystallite and found the average of the different strains or deformations present in all the crystallites.

The Debye temperature characteristic of a polycrystal, the elastic behavior of which is defined by \bar{s}_{11} and \bar{s}_{44} , is a weighted mean of the Debye temperatures associated with longitudinal and transverse elastic waves, Θ_l and Θ_t , respectively. The latter are given by

$$\Theta_l = (h/k)(3/4\pi)^{1/3}(1/V)^{1/3}(1/\rho)^{1/3}(A/\bar{s}_{44}B)^{1/3},$$

$$\Theta_t = (h/k)(3/4\pi)^{1/3}(1/V)^{1/3}(1/\rho)^{1/3}(1/\bar{s}_{44})^{1/3},$$

where V is the atomic volume, ρ the density, $A = 4\bar{s}_{11} - \bar{s}_{44}$ and $B = 3\bar{s}_{11} - \bar{s}_{44}$.

The mean Debye temperature appropriate to the specific heat theory, Θ_D , is then given by

$$3\Theta_D^{-3} = \Theta_l^{-3} + 2\Theta_t^{-3},$$

so that by substitution

$$\Theta_D = 4.289 \times 10^{-11} (1/V)^{1/3} (1/\rho)^{1/3} \left[\frac{A}{\bar{s}_{44}(2A^3 + B^3)^{1/3}} \right]^{1/3}.$$

However, the mean Debye temperature most appropriate to the temperature factor as applied to x-ray intensities, Θ_M , is given by

$$3\Theta_M^{-2} = \Theta_l^{-2} + 2\Theta_t^{-2},$$

so that by substitution

$$\Theta_M = 5.151 \times 10^{-11} (1/V)^{1/3} (1/\rho)^{1/3} \left[\frac{A}{\bar{s}_{44}(2A + B)} \right]^{1/3}.$$

TABLE I. Calculation of Debye temperature in °K with c_{ik} given in units of 10^{12} dynes cm^{-2} and \bar{s}_{ik} in units of 10^{-12} dynes $^{-1}$ cm^2 .^a

Crystal	c_{11}	c_{12}	c_{44}	F	\bar{s}_{11}	\bar{s}_{44}	Θ_D	$\Theta_D(S)$
K	0.0459	0.0372	0.0263	6.05	31.41	85.92	92.1	91.2
Cu	1.70	1.23	0.753	3.20	0.802	2.166	334	331
Si	1.67	0.65	0.80	1.57	0.612	1.498	649	646
KCl	0.370	0.081	0.079	0.55	3.938	9.934	237	235

^a The values of the moduli of elasticity, c_{ik} , for K, Cu, and KCl used in the calculations have been taken from tables compiled by C. Zener, *Elasticity and Anelasticity of Metals* (The University of Chicago Press, Chicago, 1948), Chap. II and by K. Lonsdale, *Acta Cryst.* 1, 142 (1948). The values quoted for Si are those obtained by W. P. Binnie and A. M. Liebschutz from the measurement of the x-ray diffuse scattering from a Si single crystal and presented at the Conference on Nuclear Engineering in 1953.

¹ A. Huber and E. Schmid, *Helv. Phys. Acta* 7, 620 (1934).

² W. Voigt, *Lehrbuch der Kristallphysik* (B. G. Teubner, Leipzig, 1910), p. 962.

³ A. Reuss, *Z. angew. Math. u. Mech.* 9, 49 (1929).

This difference between the Debye temperatures, Θ_D and Θ_M , has been pointed out by Zener and Bilinsky⁴ who show that Θ_M is always the larger by a few percent.

APPLICATION OF EQUATIONS

For crystals with an anisotropic factor of less than 2, Reuss' equations for \bar{s}_{ik} give Debye temperatures differing by less than 1% from the values obtained from the elaborate procedure recommended by Sutton.⁵ When the anisotropic factor is greater than 2, the average values of \bar{s}_{11} and \bar{s}_{44} given by both Voigt's and

Reuss' equations give better agreement than either alone, the Debye temperatures, at least for the metals where $c_{11} - c_{12} < 2c_{44}$, lying between the values calculated by Sutton's expressions and by Hopf and Lechner's method as modified by Keesom and Pearlman.⁶

Table I shows values of the Debye temperature, Θ_D , for a number of crystals of varying anisotropic factor, F , the Debye temperatures having been calculated from the average moduli of compliance as given by both Voigt's and Reuss' equations. The corresponding values obtained from Sutton's method are given in the final column headed $\Theta_D(S)$.

⁴ C. Zener and S. Bilinsky, Phys. Rev. **50**, 101 (1936).

⁵ P. M. Sutton, Phys. Rev. **99**, 1826 (1955).

⁶ N. Pearlman and P. H. Keesom, Phys. Rev. **88**, 398 (1952).

Long-Time Components in the Emission of Luminescent Materials*

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The decay of light emission in the time range from 150 microseconds to 20 milliseconds, caused by excitation by single high-energy electrons and alpha particles at room temperature, was studied for several different types of phosphors. The zinc cadmium sulfides investigated were found to exhibit emission under alpha particle excitation longer than can be accounted for by the bimolecular decay theory, indicating that traps are of importance even with this kind of excitation. Several alkali halides also emit a considerable part of their total light in this interval when excited by alpha particles. Of the organic phosphors studied, only diphenylacetylene showed measurable emission in this time range, and only when excited by alpha particles. A phosphor with a very large number of traps (Standard 7) had practically no emission in the time range investigated.

1. INTRODUCTION

THE influence of traps on the light emission of various phosphors from 2.5 milliseconds after the beginning of excitation to hours was discussed in a previous publication.¹ The shapes of the rise of fluorescence curves presented there were due to the cooperative effects of the many electrons excited by high-energy radiation. Additional information on the light emission will be given here, in particular, on the amount of light emitted up to various times in the range from 150 microseconds to 20 milliseconds due to excitation by single high-energy electrons and alpha particles at room temperature. There have been many investigations² of

long-time emission induced by high-energy particles and quanta, cathode rays, and light. It is difficult to correlate the results of the latter two with the present results where high-energy particles were used to excite the phosphors, because such particles produce an appreciable excitation in a very short interval of time and within a relatively small area.¹

2. EXPERIMENTAL PROCEDURE

(a) Excitation

Since the intensity of the light emission due to a single fast electron is low, particularly several hundred microseconds after excitation, excitation was furnished by a burst of high-energy electrons, about 1500 in number, in a time interval of about 150 microseconds (or about 100 alpha particles in the same interval). The observed emission was equivalent to that of the sum of 1500 (or 100) single particles, since other measurements¹ showed that with these numbers there is little overlap of the areas excited by different particles when the sample is de-excited prior to excitation. This excitation by a burst instead of by a single particle introduces an uncertainty of ± 75 microseconds in the emission time.

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¹ H. Kallmann and G. M. Spruch, Phys. Rev. **103**, 94 (1956).

² H. W. Leverenz, *An Introduction to Luminescence of Solids* (John Wiley & Sons, Inc., New York, 1950), p. 263 ff; see P. Pringsheim, *Fluorescence and Phosphorescence* (Interscience Publishers, Inc., New York, 1949) for an extensive bibliography. Some of the more recent papers are: J. Bonanomi and J. Rossel, Helv. Phys. Acta **25**, 725 (1952); I. Broser and C. Reuber, Z. Naturforsch. **9a**, 689 (1954); J. R. Cook and K. A. Mahmoud, Proc. Phys. Soc. (London) **B67**, 817 (1954); C. R. Emigh and L. R. Megill, Phys. Rev. **93**, 1190 (1954); Williams, Usiskin, and Dekker, Phys. Rev. **92**, 1398 (1953); F. B. Harrison, Nucleonics **12**, 24 (1954); J. A. Jackson and F. B. Harrison, Phys. Rev. **89**, 322 (1953).