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Comparison of the Debye θ Determined from Elastic Constants and Calorimetry

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INTRODUCTION

As the temperature of a solid approaches 0°K the simple Debye continuum model should be applicable and the lattice specific heat calculated from the elastic constants using this model should agree with that measured by calorimetric techniques. Now that accurate low-temperature specific heat and elastic constant data are available, it is possible to compare critically the values of the Debye characteristic temperature θ, which these two methods yield. Usually, the calorimetrically determined θ is obtained from the slope of the straight line in a plot of C/T *versus* T^2 where C is the measured specific heat and T the absolute temperature. Such a plot separates the contribution of the electrons and is a straight line only if the lattice specific heat varies with T^3 as predicted by the Debye model. To determine θ from the elastic constants requires the calculation of the three sound wave velocities as a function of direction in the crystal lattice and then the averaging of the reciprocal of each velocity cubed over all directions. It is possible to do this by hand for hexagonal materials, but cubic materials require a long and elaborate calculation which is reasonable only if an electronic computer is available. Without a computer the tables prepared by de Launay[1] or the approximate methods developed by Quimby and Sutton,[2] and by Betts *et al.*[3] may be used.

Various models have been proposed to determine the lattice specific heat in the temperature range where the Debye model is expected to become inapplicable. These models consider a discrete lattice rather than a continuum and use measured elastic constants to define the effective force constants which act upon any given lattice point. With these force constants, the dynamics of the entire lattice can be worked out and the specific heat calculated.

This paper evaluates the different methods of calculating θ from the elastic constants and compares the resulting values with the results of calorimetric measurements.

DETERMINATION OF θ_0

The necessary data for calculating the value of Debye θ at 0°K, hereafter denoted by θ_0, are shown in Table I. In this table, the low-temperature elastic constants of copper,[4] silver,[5] gold,[5] zinc,[6] magnesium,[7] and lithium fluoride[8] are extrapolated from measurements performed at 4.2°K while those of aluminum,[9] lithium,[10] sodium chloride,[11] and potassium bromide[12] are extrapolated from measurements near 77°K. The 0°K atomic volumes and densities are calculated from the lattice constants appearing in the ASTM card catalog and the following thermal expansion measurements: Nix and McNair[13] for the noble metals and aluminum, Pearson[14] for lithium, Grüneisen and Goens[15] for zinc, and Henglein[16] for potassium bromide and sodium chloride. The data for magnesium and lithium fluoride are taken from the papers cited.

Table II lists values of θ_0 as calculated from the data in Table I by various methods along with the results of calorimetric measurements. The first column shows the θ_0 obtained from de Launay's tables[1] using case 2 and the Sterling central difference interpolation formula[17] in two dimensions. A graphical interpolation may cause the results to differ by about 0.3%. These tables are

TABLE I. Constants of certain materials extrapolated to absolute zero. The elastic constants are in units of 10^{12} dyne/cm^2. Ω is the atomic volume and ρ the density at 0°K.

	C_{11}	C_{12}	C_{44}	C_{13}	C_{33}	Ω^{-1} (10^{22} cm^{-3})	ρ (g cm^{-3})
Elastic constants extrapolated from 4.2°K							
Copper	1.7620	1.2494	0.8177			8.553	9.018
Silver	1.3149	0.9733	0.5109			5.938	10.635
Gold	2.0163	1.6967	0.4544			5.953	19.488
LiF	1.246	0.424	0.649			12.292	2.646
Magnesium	0.6348	0.2594	0.1842	0.2170	0.6645	4.407	1.779
Zinc	1.7909	0.375	0.4595	0.5537	0.6880	6.708	7.279
	1.7696	0.3480	0.4589	0.528	0.6848		
Elastic constants extrapolated from the 77°K region							
Aluminum	1.230	0.708	0.3090			6.109	2.734
Lithium	0.1574	0.1333	0.1158			4.748	0.5471
NaCl	0.5750	0.0986	0.1327			4.619	2.241
KBr	0.418	0.056	0.052			2.854	2.819

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[1] J. de Launay, *Solid State Physics* (Academic Press, Inc., New York, 1956), Vol. 2, p. 286.

[2] S. L. Quimby and P. M. Sutton, Phys. Rev. **91**, 1122 (1953), P. M. Sutton, Phys. Rev. **99**, 1826 (1955).

[3] Betts, Bhatia, and Wyman, Phys. Rev. **104**, 37 (1956).

[4] W. C. Overton and J. Gaffney, Phys. Rev. **98**, 969 (1955).

[5] J. R. Neighbours and G. A. Alers, Phys. Rev. **111**, 707 (1958).

[6] The first set of constants are from G. A. Alers and J. R. Neighbours, J. Phys. Chem. Solids, **7**, 58 (1958). The second set are the recent measurements by C. W. Garland and R. Dalven, Phys. Rev. **111**, 1232 (1958).

[7] L. J. Slutsky and C. W. Garland, Phys. Rev. **107**, 972 (1957).

[8] C. V. Briscoe and C. F. Squire, Phys. Rev. **106**, 1175 (1957).

[9] P. M. Sutton, Phys. Rev. **91**, 816 (1953).

[10] H. C. Nash and C. S. Smith, Bull. Am. Phys. Soc. Ser. II, **3**, 123 (1958).

[11] W. C. Overton and R. T. Swim, Phys. Rev. **84**, 758 (1951).

[12] J. K. Galt, Phys. Rev. **73**, 1460 (1948).

[13] F. C. Nix and D. McNair, Phys. Rev. **60**, 597 (1941); Phys. Rev. **61**, 74 (1942).

[14] W. B. Pearson, Can. J. Phys. **32**, 708 (1954).

[15] E. Grüneisen and E. Goens, Z. Physik **29**, 141 (1924).

[16] A. Henglein, Z. physik. Chem. **115**, 91 (1925).

[17] J. de Launay (private communication).

TABLE II. Debye temperature at zero degrees Kelvin.

	de Launay	Quimby and Sutton	Betts *et al.*	Numerical integration	Calorimetric	Reference
Elastic constants extrapolated from 4.2°K						
Copper	344.5	344.4	345.4	344.4	343.8 346.7 345.1	a b c
Silver	226.4	226.6	227.1	226.4	225.3 226.5 226.2	a b d
Gold	161.7	162.1	162.2	161.6	164.6 164.8 164.6	a b e
LiF	734.4	734.6	734	734.1	737 743	f g
Magnesium	···	···	385.4	385.8	406 403.3	h i
Zinc	···	···	327.1	327.1 328.8	302 309	j
Elastic constants extrapolated from 77°K						
Aluminum	427.4	428.5[k]	428.7	428.2	375 408 419	l m
Lithium	334.6		338.4	335.9	369	n
KBr	···		171.7	172.8	174	o
NaCl	···	321.6	321	321.9	320	p

[a] See reference 19.
[b] See reference 30.
[c] J. A. Rayne, Australian J. Phys. **9**, 189 (1956).
[d] J. A. Rayne, Proc. Phys. Soc. (London) **69**, 482 (1956).
[e] See reference 29.
[f] See reference 20.
[g] T. H. K. Barron and J. A. Morrison, Can. J. Phys. **35**, 799 (1957).
[h] See reference 21.
[i] See reference 28.
[j] See reference 22.
[k] The calculated value listed in reference 9 is incorrect. The corrected value calculated by Dr. Sutton is listed above.
[l] See reference 23.
[m] See reference 24.
[n] See reference 25.
[o] See reference 26.
[p] See reference 27.

based on a computer calculation and the values calculated should be exact except for errors introduced by interpolation between the tabulated values. Since the published tables apply only to cubic materials with $(C_{11}-C_{12})<2C_{44}$ there are no entries for potassium bromide and sodium chloride nor for the hexagonal metals. The second column gives the results obtained from approximating the velocity function with a six-term power series[2] and the third column shows the results obtained if a six-term expansion in cubic harmonics[3] is used. The latter expansion technique has been applied to hexagonal materials by using spherical harmonics[18] and was used to complete column three for zinc and magnesium.

The IBM 650 digital computer of the Ford Motor Company Research Department was programed to find the average velocity function using 120 points spread uniformly over the unit triangle for cubic materials and using a one degree interval for the single angle variable in hexagonal materials. The resulting values of θ_0 are given in the column headed "Numerical integration." The two entries for zinc are calculated from the two available sets of 4.2°K elastic constants[6] in Table I. Increasing the number of points considered in the unit triangle to 933 increased the value of θ_0 for copper by 0.17°K or 0.06% and decreased the θ_0 value for lithium by 0.49°K or 0.15%. Since the values from a 120-point calculation differ so slightly from the results of the longer calculation, and since these differences are much less than the errors expected from errors in the elastic constants, it is felt that the 120-point calculation with its consequent saving in computer time is sufficiently accurate.

Table II shows that all the foregoing methods for calculating θ_0 from elastic constants are essentially in agreement. In every case the differences are less than one percent. The columns headed "de Launay" and "Numerical integration" are results of essentially the same calculation and should agree closely, as they do. The differences between these columns are indicative of the errors introduced by interpolation and by the method of numerical integration. The large difference apparent for aluminum is presumably due to our slight extrapolation of de Launay's tables to cover the particular values of elastic constants for this metal. For lithium, the large difference (1.3°K) is not due to the inadequacy of the 120-point division of the unit triangle, but to some other unknown cause.

Roughly the ease of calculation of θ_0 by any one method is in the same order as the columns in Table II. If one uses graphical interpolation, the method of de Launay is outstanding in its simplicity. Although the two series methods are about equally involved, it is our experience that the value of θ_0 resulting from the method of Betts and co-workers is apt to be more nearly mistake-free, probably because the individual steps can be checked separately.

Since some cubic materials and all hexagonal materials fall outside the range of de Launay's published tables and since the series methods are probably poorer approximations, we take the column headed "Numerical integration" to be the best values of θ_0 calculated from elastic constants.

The uncertainty of these values is determined by the absolute accuracy of the elastic constants. With the computer program setup it is a simple matter to determine how sensitive the final θ_0 value is to errors in each individual constant. Table III shows the values of θ_0 for aluminum (low anisotropy) and for gold (average

TABLE III. Changes in Debye temperature with changes in elastic constants.

	Numerical integration	1.005 C_{11}	1.005 C_{12}	1.005 C_{44}	1.01 C_{11}
Aluminum	428.2	429.2	427.7	428.8	
Gold	161.6	162.7	160.7	161.8	
Zinc	327.1				327.3

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[18] See reference 3, p. 43.

anisotropy) which are obtained by numerical integration if only one elastic constant is increased by 0.5%. A 0.5% change in elastic constants causes θ_0 to change by less than 1%. Also listed is the θ_0 value obtained for zinc when the elastic constant C_{13} is increased by 1%. This particular constant is difficult to measure accurately so it is encouraging to observe that θ_0 is not very sensitive to its uncertainties. From pulsed ultrasonic measurements, the absolute values of the measured elastic constants are estimated to be in error by about one-half percent. Since the errors in θ_0 are about the same size as the errors in the elastic constants, the calculated Debye temperature may be expected to be accurate to about one percent. This conclusion is supported by the fact that the θ_0's calculated from the two sets of low-temperature elastic constant data available on zinc differ by only 0.7%.

COMPARISON OF θ_0 WITH CALORIMETRIC RESULTS

The last column in Table II gives the values of θ_0 determined from specific heat measurements[19–27] in the 1 to 4°K temperature range. Included are several as yet unpublished results[28,29] as well as a new calculation,[30] using the 1955 temperature scale, of data already in the literature.[19] These values have been obtained by fitting the data on a C/T *versus* T^2 plot with a straight line by the method of least squares. The slope of this line defines the calorimetric θ_0. Small differences in the numerical value of the calorimetric and elastic θ_0's may arise simply because the elastic constant line is not the best least squares fit to the data. Thus the best way to compare the two results is to plot the calorimetric data and superimpose on it the line defined by the elastic constants. Since only the slope of the line is defined, it must be forced to pass through the calorimetric data at some point and disagreement is then apparent if the line and the data diverge.

Rather than plot a separate C/T *versus* T^2 graph for each material listed in Table II, the calorimetric data have been normalized to allow several sets of data to be presented in one graph. This is shown in Figs. 1 and 2 where $C\theta/T$ is plotted against $(T/\theta)^2$. On such a plot vertical lines are lines of constant T/θ. If the specific heat data are described by the sum of a linear and a cubic temperature term then, in a plot like Fig. 1, the data will define a straight line with an intercept of $\gamma\theta$ (where γ is the coefficient of the linear term) and a slope determined by the ratio of the normalizing θ to the θ which best fits the data. In constructing these figures, the values of normalizing θ were taken from the numerical integration column of Table II. The lines are drawn with the slope predicted by the Debye theory and so as to fit best the lower end of the data. We have chosen not to plot data in which there are good reasons for the large and clear differences between the calorimetric and elastic θ_0's. These are sodium chloride,[27] aluminum,[23,24] lithium,[25] and potassium bromide.[26] For sodium chloride and aluminum the specific heat data are quite scattered and can easily be described with the elastic θ_0. For lithium the lines defined by the elastic data and the calorimetric data diverge completely, but this is probably owing to the presence of a crystal structure change[31] between 77°K where the elastic constants were measured and 4°K where the specific heat was measured. In the case of potassium bromide the calorimetric measurements extend only to temperatures of the order of $\theta/50$ which is not low enough for a valid comparison.

Figure 1 shows the plot of $C\theta/T$ *versus* $(T/\theta)^2$ for the specific heat measurements of the noble metals[19] and lithium fluoride.[20] It is apparent that the elastic θ_0 defines a straight line which describes the calorimetric data for copper, silver, and lithium fluoride to within

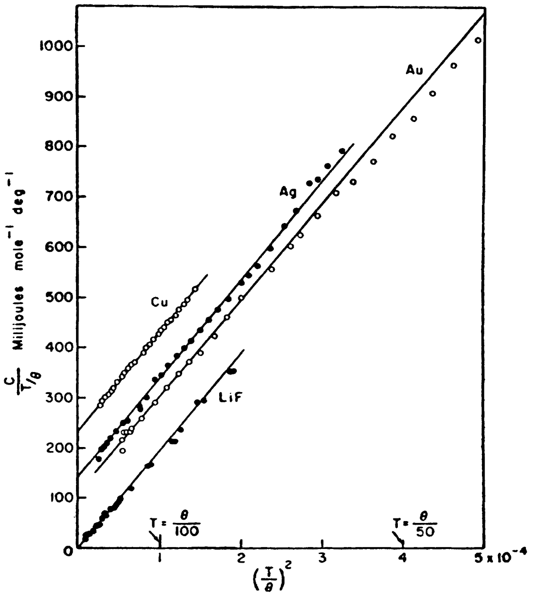

FIG. 1. Comparison of the specific heat calculated from Debye theory (solid lines) with the measured specific heats of cubic materials.

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[19] Corak, Garfunkel, Satterthwaite, and Wexler, Phys. Rev. **98**, 1699 (1955).

[20] D. L. Martin, Phil. Mag. **46**, 751 (1955).

[21] P. L. Smith, Phil. Mag. **46**, 744 (1955).

[22] G. Seidel and P. H. Keesom, Bull. Am. Phys. Soc. Ser. II, **3**, 17 (1958). By assuming that θ is temperature dependent between 1 and 4°, Seidel finds that a least squares fit to his data would give $\theta_0=309$°K. We are indebted to Mr. Seidel for communicating this result to us. See also Phys. Rev. **112**, 1083 (1958).

[23] Howling, Mendoza, and Zimmerman, Proc. Roy. Soc. (London) **A229**, 86 (1955).

[24] J. A. Kok and W. H. Keesom, Physica **4**, 835 (1937).

[25] L. M. Roberts, Proc. Phys. Soc. (London) **E70**, 744 (1957).

[26] Barron, Berg, and Morrison, Proc. Roy. Soc. (London) **242**, 472 (1957).

[27] Morrison, Patterson, and Dugsdale, Can. J. Chem. **33**, 375 (1955).

[28] J. Rayne, J. Phys. Chem. Solids (to be published).

[29] J. E. Zimmerman (unpublished data, 1958).

[30] J. Skalyo and A. Arrott (to be published). These results are based on the data of reference 19 but are recalculated using the 1955 temperature scale and a least squares fit to the data.

[31] C. S. Barrett, Acta Cryst. **9**, 671 (1956).

the experimental scatter of the data. For gold, the elastic line is clearly not the best straight line fit to the data. This difference is just outside the experimental errors arising from elastic constant errors. It may be that simple Debye theory is not appropriate over the whole temperature range given in the figure in which case the elastic constant line should fit the data only below a certain temperature. From this point of view, it may be concluded that the elastic θ_0 and Debye theory successfully describe the calorimetric data below temperatures of approximately $\theta/60$.

The disagreement between calorimetric and elastic θ_0's is more explicit for the hexagonal metals since both cases examined show large deviations. Figure 2 shows a $C\theta/T$ *versus* $(T/\theta)^2$ plot of the specific heat measurements on magnesium[28] and zinc.[22] Superimposed on these data are the straight lines predicted by the elastic constant measurements with the lines chosen to pass through the data at the low-temperature end. It is obvious that the line based on elastic data is not the best straight-line fit to the data and that a good description of the data occurs only below temperatures of about $\theta/150$ where we have required it to fit. In these cases, the elastic constants would have to be in error by about 4% in order to account for the difference in results. Such a difference is far outside experimental error for all the constants except C_{13}. Table III shows that if this one constant is changed by 1%, the value of θ is only changed by 0.1% which makes it unlikely that the inaccuracy of C_{13} could account for the discrepancy in θ values. It may be argued that the true Debye region has not been reached for these hexagonal metals even though the temperature is below $\theta/100$. However, the magnesium specific heat data does fall on a straight line which indicates that it can be well described with a T^3 dependence. The zinc data deviate slightly from a T^3 law and Seidel[22] has made a least squares fit to his heat capacity data assuming a temperature dependent θ. From this he extrapolates to $T=0$°K to obtain a value of $\theta_0=309$°K which is still 5% below the elastic constant value.

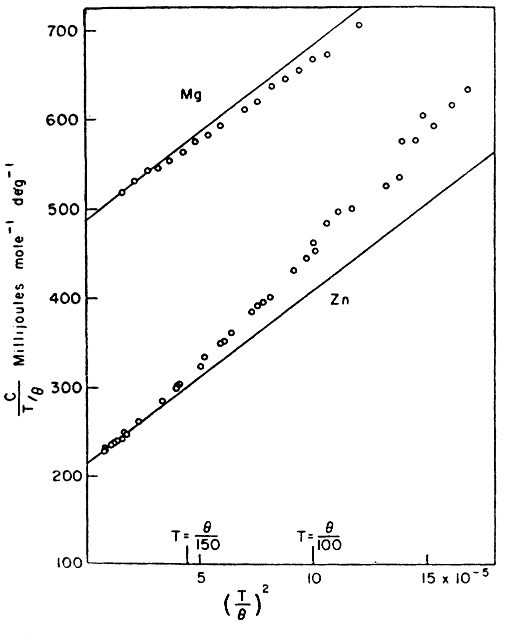

FIG. 2. Comparison of the specific heat calculated from Debye theory (solid line) with the measured specific heats of hexagonal metals.

TEMPERATURE DEPENDENCE OF θ

The previous section has shown the degree to which Debye theory describes experimental specific heat measurements near absolute zero. In order to calculate the lattice specific heat above $T=0$ using elastic constant data, it is necessary to modify Debye theory to include effects which arise because the solid is not a continuum but a lattice of discrete atoms. This requires considering a model in which the solid consists of mass points held in equilibrium by forces which are expressable in terms of the elastic constants. For convenience, the results of these modifications are usually expressed in terms of an effective θ which can be compared with the Debye θ. This modified θ is expected to vary with temperature and its temperature dependence can be calculated assuming a particular force constant model. From this, the lattice specific heat can be determined and compared to the calorimetric measurements in order to judge the validity of the model chosen. It is also possible to calculate a calorimetric θ from specific heat measurements and compare it with the modified θ predicted by the lattice theory. But unless very precise calorimetric measurements are used, the resulting values of θ may show considerable scatter and make a judgment of the theoretical model very difficult. We have chosen to compare the specific heat values themselves since these are of more technical interest and since it is then obvious how much error can be expected from using elastic constant models to estimate lattice specific heats.

Figure 3 shows the experimental data for copper,[32] silver,[33] and gold[34] plotted as C/T *versus* T^2. The solid curves labeled D show the variation of the specific heat predicted by the unmodified Debye theory which has the constant value of $\theta=\theta_0$. Gold, which shows deviations from the elastic constant θ_0 at temperatures of $\theta/60$, follows this theory to remarkably high temperatures ($T\sim\theta/7$) even though silver and copper deviate considerably from it at temperatures of the order of $\theta/20$. The curves marked L are based on the model of de Launay[1] who assumes a central force connecting nearest and next-nearest neighbor atoms

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[32] W. F. Giauque and P. F. Meads, J. Am. Chem. Soc. **63**, 1897 (1941).

[33] Meads, Forsythe, and Giauque, J. Am. Chem. Soc. **63**, 1902 (1941).

[34] T. H. Geballe and W. F. Giauque, J. Am. Chem. Soc. **74**, 2368 (1952).

and a third force arising from the compressibility of the electron gas. This model does not describe the lattice specific heat for gold and copper over the temperature range in which data are available but seems to describe the silver data up to temperatures of approximately $\theta/10$.

The curves marked *H* are the predictions of the model of Horton and Schiff[35] which are based on assuming a three-force constant noncentral interaction between nearest neighbor atoms only. This model is in better agreement with the measurements for copper and gold, but not enough to be significant. None of the models gives a really satisfactory description of the specific heat in the range where measurements are available. However, this apparent failure may not be serious since these theories are expected to apply only up to temperatures of $\theta/20$ and the available data do not cover this range. A critical evaluation of the models must wait for accurate specific heat data between 4 and 15°K.

A model applicable to hexagonal metals has been calculated by Garland and Slutsky.[36] Using central forces between the first three nearest neighbors and a force due to the compressibility of the electron gas they find that θ decreases with increasing temperature but not as rapidly as is observed. They also find that zinc with its high c/a ratio cannot be described well with their model and do not attempt a comparison with the specific heat values.

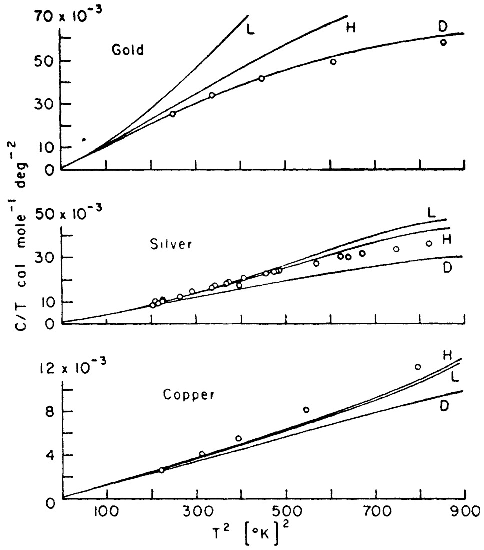

FIG. 3. Comparison of the specific heat calculated from several different models with the measurements in the 15 to 30°K range. The curves marked *D* are based on Debye's continuum model while those marked *L* and *H* refer to the lattice models proposed by de Launay and by Horton and Schiff, respectively.

CONCLUSIONS

For the cubic materials considered, the value of θ_0 calculated from elastic constants measured at 4°K by direct numerical integration is in very good agreement (except possibly for gold) with the low-temperature specific heat measurements. The tables of de Launay yield results which agree with the integration to within the accuracy of reading the table and is by far the easiest to apply. The two expansion methods of Betts *et al.* and of Quimby and Sutton appear to give θ_0 accurately to 1% even for the most anisotropic case but the method of Quimby and Sutton seems laborious and more susceptible to mistakes. Considering the differences in the results of the series approximation, and the errors in interpolation and extending de Launay's tables, we advance the values listed under the Numerical integration column in Table II to be the best available values calculated from elastic constants.

Since the lattice specific heat predicted by Debye theory from elastic constants is consistent with the calorimetric measurements to the extent shown in Fig. 1, it seems possible to conclude that the simple Debye model of lattice heat capacity is a very good approximation at low temperatures in cubic substances. In materials where the lattice specific heat cannot clearly be separated from other contributions (i.e., when there are large electronic specific heats, low-temperature phase transitions, or magnetic interactions) the elastic constants can be used to define the lattice contribution without introducing appreciable error.

For the hexagonal metals and gold there seems to be a definite difference between the calorimetric θ_0 and the elastic constant value. The reason for this is not certain. It is not likely that errors in elastic constants will account for the difference. Furthermore, for zinc two independently measured sets of elastic constants result in nearly the same θ_0 value. It is possible that small systematic errors in the specific heat measurements or uncertainties in the temperature scale would account for the difference.

It may be that temperatures of $\theta/60$ are not sufficiently low for the simple Debye model to apply to these metals. This may imply that dispersion of the elastic waves is an important effect at these temperatures. Simple reasoning indicates that for an isotropic medium deviations down from the straight line in a C/T *vs* T^2 plot are a result of an upward bending of the $\omega(k)$ curve and conversely for an upward deviation. Although not strictly applicable to anisotropic media, such reasoning would indicate that the $\omega(k)$ curve for gold and magnesium tends to bend upward away from the Debye approximation while for zinc it bends downward. However, examination of Figs. 1 and 2 indicates that the data need not be considered as "curving away" from the theoretical straight line since it can be fitted by a straight line of different slope. Thus the dispersion must be of a rather special nature.

There may be effects which modify the measured

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[35] G. K. Horton and H. Schiff, Can. J. Phys. **36**, 1127 (1958).

[36] C. W. Garland and L. J. Slutsky, J. Chem. Phys. **28**, 331 (1958).

elastic constants and could therefore cause the observed differences. If dislocations contribute to the measured elastic constants, the resulting value of θ_0 would be lower than the calorimetric value. This might be the case for gold and magnesium, but the deviation for zinc is in the other direction. Furthermore, the excellent agreement for copper and silver must then be considered as somewhat fortuitous.

It has been predicted[37] that the calorimetric θ_0 should be larger than the elastic θ_0 because the measured elastic constants include a contribution due to a relaxation mechanism of the electrons. The available low-temperature elastic constant data do not indicate any such relaxation mechanism of the required magnitude and the values of θ_0 which are predicted are in good agreement with the calorimetric θ_0's for metals with presumably the same free electron structure as gold.

The attempts to describe the specific heat at temperatures where Debye theory fails by using a lattice model are satisfying only in a qualitative way, but are unsatisfactory in predicting the detailed temperature dependence of θ. However, before a critical comparison can be attempted, accurate specific heat measurements must be made in the 4° to 20°K range.

ACKNOWLEDGMENTS

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ADDENDUM

Since submitting this article, more elastic constant and calorimetric data have become available. Calorimetric measurements by Phillips[38] down to $\theta/1000$ (0.3°K) gives $\theta_0=426°$ for aluminum which compares favorably with the calculated value of $\theta_0=428.2$ shown in Table II. New calorimetric measurement on LiF[39] down to $\theta/80$ give $\theta_0=722°$K which is in disagreement with the calculated value in Table II. However, these latter calorimetric data are somewhat scattered and, in fact, can be reasonably well described by a line corresponding to $\theta_0=734.1°$K.

TABLE I. Additions.

	C_{11}	C_{12}	C_{44}	Ω^{-1}	ρ	Reference
Elastic constants extrapolated from 4.2°K						
KCl	0.483	0.054	0.0663	3.294	2.038	a
Nickel	2.612	1.507	1.317	9.206	8.968	b
Elastic constants extrapolated from 77°K						
KI	0.338	0.022	0.0368	2.321	3.197	a
Thorium	0.780	0.482	0.513	3.058	11.787	c

[a] M. H. Norwood and C. V. Briscoe, Phys. Rev. **112**, 45 (1958).
[b] Alers, Neighbours, and Sato (to be published).
[c] Armstrong, Carlson, and Smith, J. Appl. Phys. **30**, 36 (1959).

TABLE II. Additions.

	de Launay	Numerical integration	Calorimetric	Reference
Elastic constants extrapolated from 4.2°K				
KCl	236.3[c]	237.1	235.1	a
Nickel	476.3	476.2	441	b
Elastic constants extrapolated from 77°K				
KI	130.9[c]	131.5	132.3	a
			128	d
Thorium		164.2	170	e

[a] See reference 40.
[b] J. A. Rayne and W. G. Kemp, Phil. Mag. 1, 918 (1956).
[c] These values were calculated using tables prepared by J. de Launay which are to be published in J. Chem. Phys.
[d] See reference 39.
[e] P. L. Smith, Proc. Conf. de Phys. des Basses Temp., Paris, p. 283 (1955)

Other new data are shown in the added tables. Additions to Table I shows the recent elastic constant data. The values of atomic volume and density are taken from the reference cited. Additions to Table II shows the resulting calculated values of θ_0.

As before, the calculated values of θ_0 are in good agreement with each other. The results of calorimetric measurements are also listed. For thorium, although the calorimetric θ_0 seems to be in disagreement, the calorimetric data up to $\theta/50$ is well described by choosing $\theta_0=164.2°$K. The calorimetric and elastic constant values for nickel are apparently in disagreement but the calorimetric data are quite scattered so that critical comparison is not possible.

For the two alkali halides listed, the calculated and calorimetric values are in apparent agreement. However, on a plot like Fig. 1 the elastic constant line through the origin does not fit the calorimetric data, which extends down to almost $\theta/100$. Dispersion effects can explain this failure as shown by Barron, Berg, and Morrison[40] who obtained the values of θ_0 listed above by extrapolating calorimetric data to $T=0$. This result indicates that deviations from the Debye approximation occur at relatively lower reduced temperatures for the alkali halides than for the cubic metals. If dispersion is to account for the discrepancies in the hexagonal metals, it must be concluded that the Debye approximation is inapplicable at reduced temperatures much lower than those which are suitable even for the alkali halides.

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