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# Elastic Constants of Iron from 4.2 to 300°K

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The zero-field elastic constants of iron have been measured from 4.2 to 300°K using the ultrasonic pulse technique. Extrapolation of the data to absolute zero gives $c_{11}=2.431\pm0.008$, $c_{12}=1.381\pm0.004$, and $c_{44}=1.219\pm0.004$, all expressed in units of $10^{12}$ dyne cm$^{-2}$. The corresponding limiting value of the Debye temperature is $\theta_0=(477\pm2)$°K. Using this figure, the low-temperature heat capacity data for iron have been reanalyzed assuming the presence of a spin-wave contribution to the specific heat, i.e., the heat capacity is assumed to follow the relation $C=\gamma T+\beta T^3+\alpha T^{\frac{3}{2}}$. A least squares fit of $(C-\beta T^3)/T$ versus $T^{\frac{1}{2}}$ gives $\gamma=(11.7\pm0.1)\times10^{-4}$ cal mole$^{-1}$ deg$^{-2}$, $\alpha=(2\pm1)\times10^{-5}$ cal mole$^{-1}$ deg$^{-5/2}$. There is agreement, within experimental error, between the latter figure and the theoretical estimate of $\alpha=0.8\times10^{-5}$ cal mole$^{-1}$ deg$^{-5/2}$ obtained from the low-temperature magnetization data of Fallot. From the room temperature elastic constants, the compressibility of iron is found to be $K=(5.95\pm0.02)\times10^{-13}$ cm$^2$ dyne$^{-1}$, which agrees exactly with the static value obtained by Bridgman.

## I. INTRODUCTION

IT is well known[1] that, at low temperatures, there should be a spin-wave contribution to the specific heat of iron. Owing to the attendant high electronic heat capacity, it is not possible to obtain any information about the magnitude of this contribution from specific heat data alone. This situation arises from the circumstance that, over the temperate range available, a spin-wave term in the heat capacity cannot be distinguished from a change in the lattice heat capacity with the accuracy currently available in low-temperature calorimetry. If, however, an independent estimate of the lattice term can be obtained, this contribution can be subtracted from the total specific heat and the remainder can be analyzed in a fairly unambiguous way to obtain the spin-wave term. The magnitude of the low-temperature lattice heat capacity can, as has been demonstrated in numerous cases,[2] be obtained quite accurately from a knowledge of the elastic constants extrapolated to absolute zero, since only long-wavelength phonons are thermally excited at low temperatures. In this paper the results of elastic constant measurements on iron from 4.2° to 300°K are described. The limiting value of Debye temperature $\Theta_0$ has been calculated from these data; it has then been used in a re-evaluation of the available low-temperature heat capacity data on iron.[3] This re-evaluation reveals a spin-wave contribution to the specific heat in reasonable agreement with that expected from theory. A slight alteration in the value of $\gamma$, the coefficient of the electronic term in the heat capacity, results from the present analysis. The contribution to the elastic constants of iron, arising from the compressibility of the electron gas, is also discussed. The low magnitude of this contribution suggests that the number of conduction electrons having an *s* character is quite small.

## II. EXPERIMENTAL DETAILS

The single crystal of iron, used in the present work, was grown in this Laboratory by the strain-anneal method.[4] After orientation by the usual Laue back-reflection technique, two parallel flat surfaces perpendicular to the [110] direction were ground on the crystal. The distance between these surfaces was approximately 1.9 cm. Elastic constant measurements were made at 10 Mc/sec by the ultrasonic pulse technique using unrectified pulses to eliminate transit time errors. Details of the measuring technique have been described elsewhere.[5] In the present experimental arrangement, an electronic regulator has been added to enable the specimen temperature to be regulated to one one-hundredth of a degree at any temperature between 4.2° and 300°K. Glycerine was found to give a satisfactory bond for all propagation modes below room temperature. The thermal expansion data of Nix and MacNair[6] were used to obtain the elastic moduli from the observed propagation velocities. Since their results extend only down to 92°K, it was necessary to extrapolate in order to cover the range down to liquid helium temperatures. Little error is involved in this procedure. however, since the total expansion in the range 4.2° to 90°K is quite small. The density of iron at absolute zero was taken to be $\rho_0=7.9240$ gm cm$^{-3}$, which value was obtained using the lattice parameter $a=2.86645$ A at 293°K, as given by Pearson.[7]

## III. DISCUSSION AND RESULTS

The results of the experiments are given graphically in Figs. 1 to 3. Smoothed values of the elastic constants

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[1] N. F. Mott and H. Jones, *The Theory of the Properties of Metals and Alloys* (Oxford University Press, New York, 1936).

[2] For a review, see G. A. Alers and J. R. Neighbours, Revs. Modern Phys. **31**, 673 (1959).

[3] C. H. Cheng, C. T. Wei, and P. A. Beck, Phys. Rev. **120**, 426 (1960).

[4] H. Sato, Research Report 8-0107-R3, Westinghouse Research Laboratories, 1956 (unpublished).

[5] J. A. Rayne, Phys. Rev. **115**, 63 (1959).

[6] F. C. Nix and D. MacNair, Phys. Rev. **60**, 597 (1941).

[7] W. B. Pearson, *A Handbook of Lattice Spacings and Structures of Metals and Alloys* (Pergamon Press, New York, 1958).

TABLE I. Smoothed values for zero-field elastic constants of iron, in units of $10^{12}$ dyne cm$^{-2}$.

| Temperature (°K) | $\frac{1}{2}(c_{11}+c_{12})+c_{44}$ | $c_{44}$ | $\frac{1}{2}(c_{11}-c_{12})$ |
|---|---|---|---|
| 4.2 | 3.125±0.015 | 1.2190±0.005 | 0.5250±0.0003 |
| 20 | 3.125 | 1.2190 | 0.5250 |
| 40 | 3.122 | 1.2183 | 0.5242 |
| 60 | 3.118 | 1.2168 | 0.5228 |
| 80 | 3.110 | 1.2148 | 0.5212 |
| 100 | 3.102 | 1.2125 | 0.5190 |
| 120 | 3.093 | 1.2100 | 0.5167 |
| 140 | 3.085 | 1.2070 | 0.5142 |
| 160 | 3.077 | 1.2040 | 0.5113 |
| 180 | 3.069 | 1.2005 | 0.5084 |
| 200 | 3.060 | 1.1970 | 0.5053 |
| 220 | 3.053 | 1.1938 | 0.5020 |
| 240 | 3.045 | 1.1900 | 0.4992 |
| 260 | 3.037 | 1.1862 | 0.4953 |
| 280 | 3.029 | 1.1825 | 0.4918 |
| 300 | 3.021 | 1.1783 | 0.4883 |

are given in Table I. The error in these values is estimated conservatively at about one-half percent, although the internal consistency of the data is somewhat better. As noted previously no correction has been applied for so-called transit time errors, since it is felt that measurements on unrectified pulses, using the beginning of the first cycle, are free from such uncertainties. From the graphs it may be seen that there is reasonable agreement between the present work and that of Goens and Schmidt,[8] the maximum discrepancy being approximately $1\frac{1}{2}\%$. The value of the compressibility of iron at 300°K calculated from our elastic data is $K=5.95\times10^{-13}$ cm$^2$ dyne$^{-1}$, which agrees exactly with the static value of Bridgman.[9]

### A. Limiting Value of Debye Temperature

Using de Launay's formula[10] and the values of elastic constants extrapolated to absolute zero, the Debye temperature $\Theta$ for iron was calculated to be

$$\Theta=477-0.05T^2. \qquad (1)$$

The limiting value of Debye temperature is $\Theta_0=477$°K, which differs considerably from the figure of 445°K obtained by Cheng *et al.*[3] Since the dispersive term in Eq. (1) is negligible in the liquid helium range, it is believed that this discrepancy may be attributed to the presence of a spin-wave contribution to the specific heat. The presence of such a term would not, with the presently available accuracy of specific heat measurements, be distinguishable from an apparent change in the lattice heat capacity. Accordingly, the calorimetric data have been reanalyzed assuming a heat capacity of the form

$$C=\gamma T+\beta T^3+\alpha T^{\frac{3}{2}}, \qquad (2)$$

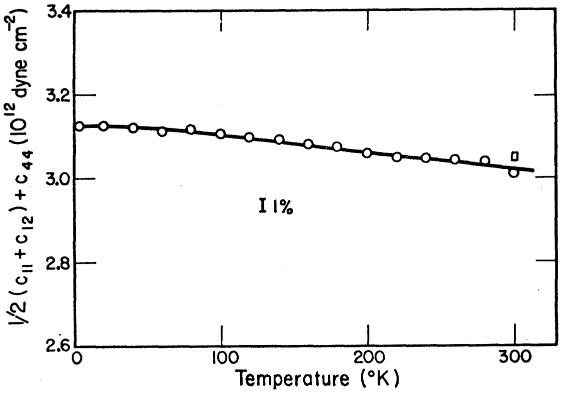

FIG. 1. Temperature variation of the elastic constant $\frac{1}{2}(c_{11}+c_{12})+c_{44}$ for iron. The point marked with a square is the room temperature value of Goens and Schmidt.

where the last term represents the spin-wave contribution and where $\beta$ is known from the value of $\Theta_0$ calculated from the elastic data. A least-squares fit of $(C-\beta T^3)/T$ vs $T^{\frac{1}{2}}$ yields

$$\begin{aligned}\gamma&=(11.7\pm0.1)\times10^{-4}\text{ cal mole}^{-1}\text{ deg}^{-2},\\ \alpha&=(2\pm1)\times10^{-5}\text{ cal mole}^{-1}\text{ deg}^{-\frac{5}{2}}.\end{aligned} \qquad (3)$$

Now from spin-wave theory, the magnetic contribution to the specific heat for a cubic metal is given by

$$C=1.18R(\sigma_0-\sigma)/\sigma_0, \qquad (4)$$

where $\sigma_0$ is the saturation magnetization at absolute zero. At low temperatures the magnetization obeys the relation

$$\sigma=\sigma_0(1-AT^{\frac{3}{2}}), \qquad (5)$$

the value of $A$ for iron being $3.3\times10^{-6}$.[11] From (4) and (5) we obtain

$$\alpha=0.8\times10^{-5}\text{ cal mole}^{-1}\text{ deg}^{-\frac{5}{2}}, \qquad (6)$$

which must be considered to be in reasonable agreement

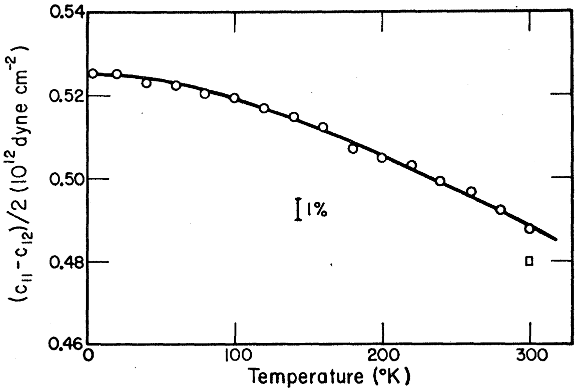

FIG. 2. Temperature variation of the elastic constant $c_{44}$ for iron. The point marked with a square is the room temperature value of Goens and Schmidt.

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[8] E. Goens and E. Schmidt, Naturwissenschaften **19**, 520 (1931).

[9] P. W. Bridgman, Proc. Am. Acad. Arts Sci. **77**, 187 (1949).

[10] J. de Launay, *Solid-State Physics*, edited by F. Seitz and D. Turnbull (Academic Press, Inc., New York, 1956), Vol. 2, pp. 285, 277.

[11] M. Fallot, Ann. phys. **6**, 305 (1936).

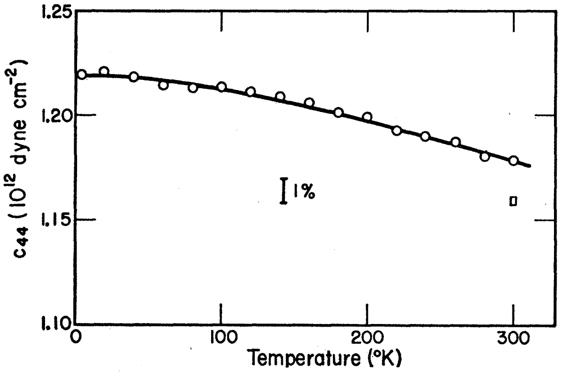

FIG. 3. Temperature variation of the elastic constant $\frac{1}{2}(c_{11}-c_{12})$ for iron. The point marked with a square is the room temperature value of Goens and Schmidt.

with the estimate obtained from the calorimetric data in view of the considerable uncertainty of the latter figure. It is to be noted that the coefficient $\gamma$ of the electronic heat capacity of iron is slightly lower than that given by Cheng *et al.*

### B. Deviation from the Cauchy Relation

As has been discussed by de Launay,[10] the difference $c_{12}-c_{44}$ can be attributed in a metal to the bulk modulus of the valence electrons. For a parabolic band of width $\zeta$ the electronic contribution to the bulk modulus is easily shown to be

$$K_e=\tfrac{2}{3}n\zeta, \tag{7}$$

$n$ being the density of valence electrons. By making the reasonable assumption that $\zeta=7$ ev for Cu, Ni, and Fe, we can use the relation (7) to calculate the electron concentration necessary to explain the observed difference between $c_{12}$ and $c_{44}$. The results of these calculations are shown in Table II, together with the actual number of $s$ electrons.[12] It can be seen that there is a rough correlation between the last two columns, which suggests that in the case of iron and nickel, the unfilled $d$ band does not contribute to the bulk modulus of the electron gas. This situation is to be contrasted with palladium, where recent work[13] has indicated that the $d$ band does indeed make a large contribution to the bulk modulus. The reason for the difference in the present case is somewhat difficult to understand, unless it is assumed that all the $d$ band electrons in iron and nickel are fairly localized.

TABLE II. Calculated electron density corresponding to the difference $c_{12}-c_{44}$.

| Metal | $c_{12}-c_{44}$ ($10^{12}$ dyne cm$^{-2}$) | $n_{\text{calc}}$ (electron/atom) | $n^{\text{b}}$ (electron/atom) |
|---|---|---|---|
| Cu | 0.46[a] | 0.72 | 1 |
| Ni | 0.42[a] | 0.70 | 0.6 |
| Fe | 0.25 | 0.39 | 0.6 |

[a] See reference 10.
[b] See reference 12.

## IV. CONCLUSION

The zero-field elastic constants of iron have been measured from 4.2° to 300°K and the limiting value of the Debye temperature for iron calculated therefrom. This value of Debye temperature has been used to re-evaluate the low-temperature specific heat data on iron. It is concluded that there is a spin-wave contribution to the heat capacity in approximate agreement with theory. The difference between $c_{12}$ and $c_{44}$ is shown to be consistent with the bulk modulus of the $s$ electrons in iron, thus suggesting that there is no contribution due to the unfilled $d$ band.

## ACKNOWLEDGMENTS

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[12] R. M. Bozorth, *Ferromagnetism* (D. Van Nostrand Company, Inc., Princeton, New Jersey, 1951), p. 436.

[13] J. A. Rayne, Phys. Rev. **118**, 1545 (1960).