less than 1° and the scattering angle was taken as read on the spectrometer.

General radiation with a spectral distribution as shown in Fig. 1 of a previous paper[1] was used.

3. Experimental Results

The results are given in Table I and in Fig. 3. Owing to experimental difficulties, we were unable to obtain a value of $(S\rho/\mu)_{\text{exp}}$ at $\phi=10^\circ$ with the $\psi=14^\circ$ crystal. We obtained the value shown for $\phi=10^\circ$ with the $\psi=90^\circ$ crystal but we feel that due to experimental error the value is too large. However, the value shown was checked by a careful repetition of the experiment at this angle.

According to Zener[4] the diffuse scattering from the valence electrons at small angles falls off as the first power of the scattering angle rather than the second power as does the scattering from the core electrons. This theoretical prediction has been obtained independently by Debye.[5] Recently Scharwächter[6] has obtained results which confirm this theoretical prediction. For a light metal at small angles this effect is measurable, but for zinc it is within the limit of our experimental error and has a negligible effect upon our experimental results.

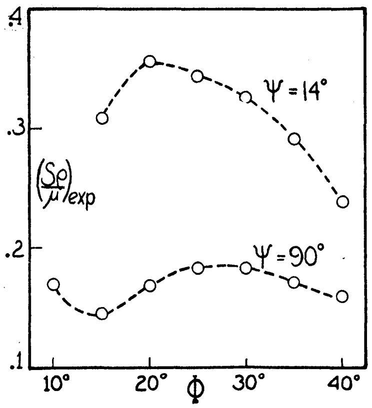

FIG. 3 Experimental values of $(S\rho/\mu)$ plotted against ϕ for $\psi=14^\circ$ and $\psi=90^\circ$.

Discussion of the results of this paper is deferred to the sixth paper of this series.

The authors wish to thank Professor G. E. M. Jauncey for his suggestion of this problem and his aid in refinement of the experimental method.

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[4] C. Zener, Phys. Rev. **48**, 573 (1935).
[5] P. Debye, Physik. Zeits. **38**, 161 (1937).
[6] W. Scharwächter, Physik. Zeits. **38**, 165 (1937).

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Atomic Structure and Vibrations in Zinc Crystals

VI. Determination of Electron Asymmetry and the Two Principal Characteristic Temperatures

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The results reported in papers by Brindley, Miller and the two previous papers of this issue of the *Physical Review* are discussed. The results show that the true atomic structure factor f (the effect of atomic vibrations having been removed) is a function of the orientation angle ψ out to $(\sin\frac{1}{2}\phi)/\lambda=0.6$. It is shown how the f values may be obtained for two values of ψ from diffuse scattering measurements alone at room temperature. The f curves for $\psi=14^\circ$ and 90° coincide for $(\sin\frac{1}{2}\phi)/\lambda$ between 0.6 and 1.0. At 0.6 the curves fork. Correcting Miller's F values ($\lambda=0.71$A) for atomic vibrations and Brindley's F values ($\lambda=1.54$A) for atomic vibrations and dispersion, f points are obtained which mostly fall between or on the f curves for $\psi=14^\circ$ (this is practically the same as the f curve for $\psi=0^\circ$) and $\psi=90^\circ$. It is shown that the difference between the two f curves is due to a reasonable asymmetry in the spatial distribution function of the valence electrons. The ΔF's between Miller's and Brindley's F values are corrected for atomic vibrations, and the resultant Δf's are all equal within experimental error. The average $\Delta f=2.35$ in good agreement with the quantum mechanical $\Delta f=2.36$. The characteristic temperatures associated with vibrations parallel and perpendicular to the principal axis have been found. The characteristic temperature for parallel vibrations decreases while that for perpendicular vibrations remains almost constant with rise of temperature in agreement with Zener's theory. The average characteristic temperature for vibrations in all directions is just slightly greater than the characteristic temperature for specific heat in agreement with Zener's theory. The decrease of the characteristic temperature with temperature appears to begin when the root mean square displacement exceeds about 0.13A.

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1. Effect of Orientation on the Structure Factor

In a group of three papers appearing in the September 1, 1936 issue of the *Physical Review*, the evidence for the anisotropy of the atomic vibrations of zinc crystals was discussed. We shall refer to these papers[1] as I, II, and III. As pointed out by Brindley[2] the large intensity of the $(10\bar{1}0)$ reflection of Cu $K\alpha$ x-rays from powdered zinc relative to the intensity of the (0002) reflection indicates that not only is there anisotropy in the thermal vibrations of the atoms of a zinc crystal but also the electron atmospheres of the atoms are distorted. However, Brindley was reluctant to accept this explanation of the abnormally high F value for the $(10\bar{1}0)$ reflection. He preferred to ascribe the abnormality to an impurity. In this laboratory Miller and Foster, using Mo $K\alpha$ rays instead of Cu $K\alpha$ rays, confirmed Brindley's result, and also Brindley found a similar result for the $(10\bar{1}0)$ reflection of Cu $K\alpha$ rays from powdered cadmium.[3] The possibility of impurity seems to be ruled out.

According to Zener[4] the effect of the thermal vibrations may be removed from the structure factor F so as to obtain the true atomic structure f by means of

$$f = Fe^{M}, \tag{1}$$

where for hexagonal crystals like zinc

$$M = (a\cos^2\psi + b\sin^2\psi)\cdot\frac{\sin^2(\frac{1}{2}\phi)}{\lambda^2}, \tag{2}$$

ϕ is the angle of scattering and ψ is the orientation angle.

We pointed out in paper I that the f values calculated from Miller and Foster's F values for the (0002), $(10\bar{1}0)$ and $(10\bar{1}1)$ reflections indicate that when f values are plotted against $(\sin\frac{1}{2}\phi)/\lambda$ the f point for the $(10\bar{1}1)$ reflection falls between the curves which may be imagined as respectively passing through the f points for the (0002) and $(10\bar{1}0)$ reflections. This means that one way of showing the existence of asymmetry in the electron atmospheres of the atoms in zinc crystals is to correct the structure factors for thermal vibration and to plot the resulting f values against $(\sin\frac{1}{2}\phi)/\lambda$. If there is asymmetry, the f points will in general fall between two f curves, one for $\psi = 0°$ and the other for $\psi = 90°$. Such a tendency has recently been found by Miller[5] for Mo $K\alpha$ rays reflected from powdered zinc. The dependence of f on the orientation must result from the spatial distribution of the outer electrons being a function of the direction. Since probably only the two valence electrons are involved in this asymmetry and since the contribution of the valence electrons to f becomes small at large values of $(\sin\frac{1}{2}\phi)/\lambda$, the dependence of f upon ψ must vanish at a certain value of $(\sin\frac{1}{2}\phi)/\lambda$. The f curves for $\psi = 0°$ and $\psi = 90°$ will coincide for values of $(\sin\frac{1}{2}\phi)/\lambda$ greater than this value but will be separate at values less than this value. It was expected that the place of forking of the curves would be at a value of $(\sin\frac{1}{2}\phi)/\lambda$ somewhat greater than 0.240 since this is the value for the $(10\bar{1}0)$ reflection. One surprising result found by Miller[5] was the low F value for the (0004) reflection. Although, owing to the difficulty of making accurate measurements on this very weak reflection, Miller's value of $F(0004) = 10.6$ is not to be considered as accurate within ± 1.0, yet even if the value 11.6 is taken and the f value calculated, this f value is still low compared to the f values for the reflections on either side of this reflection. The (0004) reflection is for $\psi = 0°$ and occurs at $(\sin\frac{1}{2}\phi)/\lambda = 0.406$. Hence the separation of the f curves for $\psi = 0°$ and $\psi = 90°$ is considerable at $(\sin\frac{1}{2}\phi)/\lambda = 0.406$. It seems very likely that the separation continues at least as far out as $(\sin\frac{1}{2}\phi)/\lambda = 0.6$.

In the preceding two papers, IV and V, appearing in this issue of the *Physical Review*, further measurements on the diffuse scattering from single crystals of zinc are described. The results of experiments on diffuse scattering of x-rays at various angles of scattering for orientation angles $\psi = 14°$ and $\psi = 90°$ are shown as circles in Fig. 1. The measurements were made with the crystals at room temperature. The

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[1] **I.** G. E. M. Jauncey and W. A. Bruce, Phys. Rev. **50**, 408 (1936); **II.** G. E. M. Jauncey and W. A. Bruce, Phys. Rev. **50**, 413 (1936); **III.** R. D. Miller and E. S. Foster, Phys. Rev. **50**, 417 (1936).

[2] G. W. Brindley, Phil. Mag. **21**, 790 (1936).

[3] G. W. Brindley, Proc. Leeds Phil. Soc. **3**, 200 (1936).

[4] C. Zener, Phys. Rev. **49**, 122 (1936).

[5] R. D. Miller, Phys. Rev. **51**, 959 (1937).

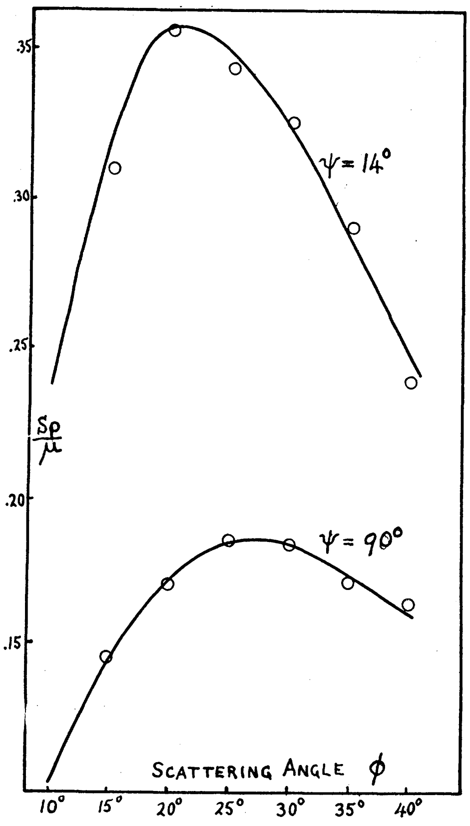

FIG. 1. The experimental values of $(S\rho/\mu)$ are shown in the circles. The curves are obtained from the theoretical equations using the f's given in Table IV and $g=2.27\cos^2\psi+0.64\sin^2\psi$.

spectral distribution of the energy in the primary x-rays is shown in Fig. 2. We shall show that from the values given in Table I, paper V or shown in Fig. 1 we can obtain values of a and b in Zener's formula for M and also f values for $\psi=14°$ and $\psi=90°$.

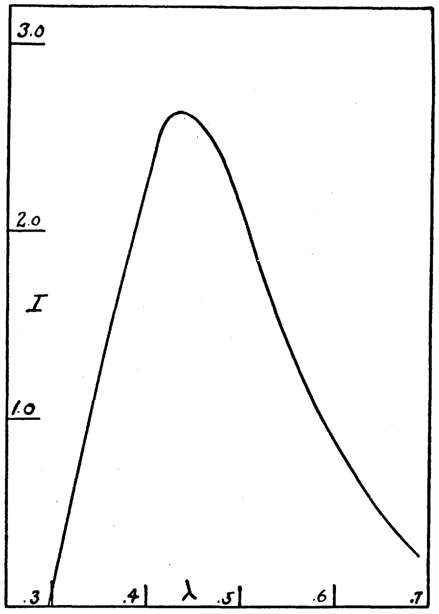

FIG. 2. Spectral distribution curve for the x-rays falling upon the crystal.

Because the largest angle of scattering is 40°, we shall neglect the effect of the Compton change of wave-length on the incoherent part of the diffuse scattering. From (9) and (10) of paper II we have

$$(S\rho/\mu)_{\text{exp}}=\int(S_{\text{coh}}+S_{\text{inc}})\cdot(\rho/\mu)Id\lambda, \qquad (3)$$

where

$$S_{\text{coh}}=f^2(1-e^{-2M})/Z, \qquad (4)$$

$$S_{\text{inc}}=1-(1/Z)\Sigma E_r^2 \qquad (5)$$

and the spectral distribution $I(\lambda)$ is normalized so that

$$\int Id\lambda=1. \qquad (6)$$

We may consider the quantity on the left as an experimental quantity whose value is calculated by means of (8) of paper II. We shall show later that S_{inc} is very insensitive to the value of the orientation angle ψ and we shall therefore assume that S_{inc} is independent of ψ. The values of ΣE_r^2 for zinc shown in Table I are interpolated from a table given by Compton and Allison.[6] From Table I and Fig. 2 we have calculated Table II. Subtracting these from the corresponding values in Table I of paper V, we obtain Table III.

For a first approximation we shall assume that the primary rays consist of monochromatic rays of $\lambda=0.44$A (half-value absorption in aluminum). This assumption gives fairly good results so long as the calculations are made for the scattering at angles greater than the angles at which the humps of the respective curves occur in Fig. 1. The values of $(\sin\frac{1}{2}\phi)/\lambda$ are then 0.6 and 0.78 for

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[6] A. H. Compton and S. K. Allison, *X-Rays in Theory and Experiment*, p. 782.

30° and 40° respectively. At a given angle of scattering

$$\frac{S_{\mathrm{coh}}(\psi=\psi_1)}{S_{\mathrm{coh}}(\psi=\psi_2)}=\frac{1-e^{-2g_1x^2}}{1-e^{-2g_2x^2}}, \tag{7}$$

where $x=(\sin\frac{1}{2}\phi)/\lambda$ and

$$g=a\cos^2\psi+b\sin^2\psi. \tag{8}$$

Then from the values of the ratio $S_{\mathrm{coh}}(14°)/S_{\mathrm{coh}}(90°)$ at $\phi=30°$ and $\phi=40°$ we obtain two equations containing the two unknowns g_1 and g_2. From these two values of g, values of a and b are obtained by means of (8). The μ/ρ for $\lambda=0.44\mathrm{A}$ in zinc is 14.5 g^{-1} and we calculate values of S_{coh} from the values given in Table III. Knowing a and b we then calculate f values and plot a curve of f against $(\sin\frac{1}{2}\phi)/\lambda$. Using this f curve, the spectral distribution curve, and the values of a and b we have found values of

$$\int(S_{\mathrm{coh}}\rho/\mu)Id\lambda \tag{9}$$

graphically. These values differ slightly from the values shown in Table III. Then by successive approximations it is possible to find values of a and b and of f that will make the values of (9) fit best with the values of Table III. We finally obtained

$$a=2.27\mathrm{A}^2 \quad\text{and}\quad b=0.64\mathrm{A}^2$$

and the f values shown in Table IV. The graphs of these f values are shown in Fig. 3. Using these values together with the values of a and b given above, we have plotted the curves in Fig. 1. Since we have been able to make the curves pass very nearly through the experimental points, we have a considerable degree of confidence in the values of a and b and in the f values of Table IV. Two f curves—one for $\psi=14°$ and the other for $\psi=90°$—are definitely required for values of $(\sin\frac{1}{2}\phi)/\lambda$ not greater than 0.6, the fork occurring at this value.

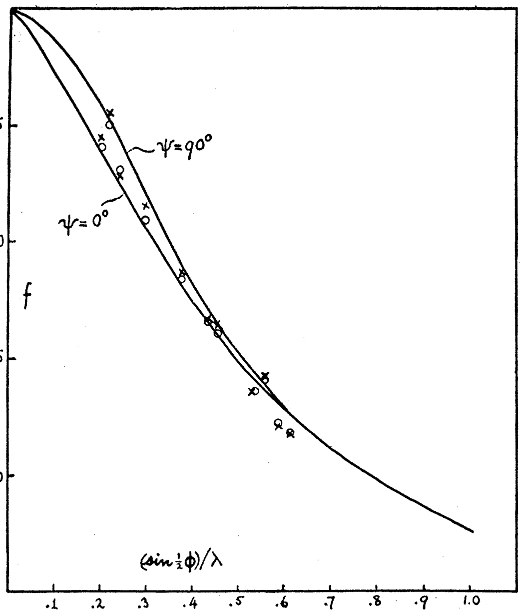

FIG. 3. The f curves are obtained from diffuse scattering experiments and the points are f values obtained from powder crystal F values through the formula $f=Fe^M$.

TABLE I. *Values of* ΣE_r^2 *for zinc.*

$(\sin\frac{1}{2}\phi)/\lambda$	ΣE_r^2	$(\sin\frac{1}{2}\phi)/\lambda$	ΣE_r^2
0.0	30	0.6	9.4
.1	24.8	.7	7.3
.2	19.0	.8	6.3
.3	14.7	.9	6.2
.4	12.5	1.0	5.2
.5	10.4	1.1	4.2

It should be noted that a and b and the f values have been determined by diffuse scattering measurements at room temperature for two orientation angles at various scattering angles. We have however, assumed the quantum mechanical values of S_{inc} and the absence of any effect due to electron asymmetry at $\phi=30°$. Still we need not make this latter assumption since if for instance we assume no asymmetry effects beyond $\phi=25°$ we are unable to obtain curves which pass so nearly through the experimental points as do the curves of Fig. 1.

TABLE II. *Values of* $\int(S_{\mathrm{inc}}\rho/\mu)Id\lambda$.

10°	15°	20°	25°	30°	35°	40°
0.025	0.034	0.039	0.044	0.047	0.050	0.058

TABLE III. *Values of* $\int(S_{\mathrm{coh}}\rho/\mu)Id\lambda$.

ψ \ φ	15°	20°	25°	30°	35°	40°
14°	0.274	0.316	0.299	0.278	0.240	0.180
90°	0.111	0.130	0.137	0.136	0.121	0.102

2. Comparison with Powdered Crystal Results

The circles in Fig. 3 represent the f values calculated from Miller's F values when the above values of a and b are used in M, while the crosses represent the values of $(f+2.36)$ where f has been calculated from Brindley's F values in a similar way. The addition of 2.36 is due to dispersion. The f points fall very well between the $\psi=0°$ (more correctly the $\psi=14°$ curve but the difference between the $\psi=0°$ and $\psi=14°$ curves must be small) and the $\psi=90°$ curve. Only at the larger values of $(\sin\frac{1}{2}\phi)/\lambda$ do the f points fall outside the area between the two curves but owing to the method of approximation used some disagreement might be expected at the larger angles. However, we feel that the small disagreement may be due to error in the F values.

Although the accuracy is not very great it is interesting to calculate the difference Δf between Brindley's and Miller's f values from the difference ΔF between their F values by means of

$$\Delta f=\Delta F\cdot e^{M} \tag{10}$$

and the above values of a and b. The Δf values are given in Table V, from which it is seen that Δf has values which scatter about the average value 2.35. The amount of departure from the average value is in no case greater than that due to experimental error in ΔF. The results support the view that Δf is constant with respect to $(\sin\frac{1}{2}\phi)/\lambda$ as quantum mechanics requires that it should be according to Hönl.[7] The average Δf is 2.35. The quantum-mechanical value for Δf when $\lambda(\text{Mo } K\alpha)=0.71\text{A}$, $\lambda\ (\text{Cu } K\alpha)=1.54\text{A}$ and Zn $K=1.28\text{A}$ is 2.36. This agreement indicates that the values of a and b have been well chosen.

3. The Two Principal Characteristic Temperatures

We next consider the results reported in paper IV. The diffuse scattering was measured at a scattering angle $\phi=30°$ in all cases. The values of $(S\rho/\mu)_{\text{exp}}$ for $\psi=3°$ and 90° and for $T=100°$, 200°, 298°, 370°K are given in Table I of paper IV. Using the f values given in Table IV and the spectral distribution given in Fig. 2, we have calculated a and b for each temperature. These values are shown in Table VI. The quantity a is related to the characteristic temperature $\Theta_{||}$ associated with displacements parallel to the c axis by the Debye formula

$$a=\frac{6h^2T}{mk\Theta_{||}^2}Q\left(\frac{\Theta_{||}}{T}\right), \tag{11}$$

where Q is what Zener calls the quantization factor. A similar formula connects b with $\Theta_{\perp}$. The values of the two characteristic temperatures are shown in Table VI. It is to be noted that, excepting at low temperatures, $\Theta_{||}$ falls with rise of temperature. This is exactly the same effect that James and Firth[8] working with NaCl, and James and Brindley[9] working with KCl, have observed at temperatures from 600° to 900°. This deviation from a constant characteristic temperature can be explained by assuming that the Debye model is no longer valid because the very large atomic vibrations introduce third and fourth order terms into the expression for the potential energy. This approach has been investigated by Waller[10] but even for simple cubic crystals the problem is so complicated that no quantitative results are available. On the other hand, Zener and Bilinsky,[11] using the Debye model, have found that (11) is valid provided that the characteristic temperature is itself considered to be a function of tem-

Table IV. *Structure factors for zinc.*

$(\sin\frac{1}{2}\phi)/\lambda$	0.0	0.1	0.2	0.3	0.4	0.5	0.6	0.8	1.0
$\psi=14°$	30.0	27.3	23.8	20.5	17.3	14.7	12.8	9.8	7.6
$\psi=90°$	30.0	28.7	25.9	21.8	18.2	15.2			

Table V. *Effect of dispersion.*

Reflection	ΔF	Δf	Reflection	ΔF	Δf
0002	2.2	2.4	2021	1.8	2.1
1010	1.9	2.1	2023	2.2	2.1
1011	2.6	2.7	1015	1.3	2.2
1012	1.9	2.2	1124		
1013	2.3	2.7	2131	2.1	2.7
1120			0006	1.55	2.4
1122	1.9	2.3	2132		

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[7] H. Hönl, Zeits. f. Physik **84**, 1 (1933).

[8] R. W. James and E. M. Firth, Proc. Roy. Soc. **A117**, 62 (1928).

[9] R. W. James and G. W. Brindley, Proc. Roy. Soc. **A121**, 155 (1928).

[10] I. Waller, Ann. d. Physik **83**, 153 (1927).

[11] C. Zener and S. Bilinsky, Phys. Rev. **50**, 101 (1936).

TABLE VI. *Calculated values of a, b, and the characteristic temperatures.*

T	a	b	a/b	$\Theta_{\|\|}$	$\Theta_{\perp}$	$(2\Theta_{\perp}+\Theta_{\|\|})/3$
100°K	0.68A^2	0.26A^2	2.6	169°K	281°K	244°K
200	1.25	.44	2.8	170	290°	250°K
298	2.36	.64	3.7	150	290°	243°K
370	3.80	.84	4.5	130	276°	227°K
550	6.20			122		

perature. Zener and Bilinsky give the formula

$$\Theta(T)=\Theta(0)e^{-KH(T)}, \tag{12}$$

where $\Theta(0)$ is the characteristic temperature obtained by means of the Debye specific heat formula from C_v measured at low temperatures and $KH(T)$ is a quantity depending upon the thermal expansion coefficient and the compressibility of the crystal. Let us write M in the form $g\cdot(\sin^2 \frac{1}{2}\phi)/\lambda^2$. From the curves given by Zener and Bilinsky it is seen that the characteristic temperature for KCl or NaCl is constant for the range $g=0$ to $g=1.0$, but decreases for values of g greater than 1.0. By reference to our Table VI, it is seen that $\Theta_{||}$ begins to decrease when $a>1.25$. Our a corresponds to the g for KCl or NaCl. So our results for the vibrations parallel to the c axis of a zinc crystal are in qualitative agreement with the results for KCl and NaCl. Next we may point out that no approach to this problem through higher terms in the potential energy could predict a lower value of $\Theta_{\perp}$ at 100°K than at 200°K. Zener has called it to our attention that this effect may be due to the change in the sign of the linear thermal expansion coefficient for a direction perpendicular to the c axis of a zinc crystal[12] which occurs in the region of 100°K.

For the purpose of calculating the specific heat of a hexagonal crystal it is necessary to use an average characteristic temperature given by

$$\Theta_{\text{Av}}=(2\Theta_{\perp}+\Theta_{||})/3. \tag{13}$$

Values of this average are given in Table VI. It is interesting to note that Θ_{Av} for room temperature is 243°K. The Θ which is used for specific heat purposes is 235°K. According to Zener and Bilinsky the Θ for x-rays should be somewhat larger than that for specific heat. In the case of cubic crystals with a Poisson ratio of 0.25, the Θ for x-rays should be 2.5 percent greater than the Θ for specific heat. Our result for the hexagonal crystal zinc is thus in qualitative agreement with Zener and Bilinsky's theoretical prediction.

According to Zener[4] the ratio a/b should be 1.8. It is interesting to note that our value of a/b is considerably greater than this at all temperatures.

In paper IV we described how the ratio a/b could be measured without a knowledge of the spectral distribution $I(\lambda)$. The value found was 2.96. Strictly speaking, the method used in paper IV is only applicable when a/b is independent of the temperature, and this is so when $\Theta(T)$ may be taken as equal to $\Theta(0)$ and the quantization factor is nearly unity. But, when a is greater than 1.25A^2 or the root mean square displacement parallel to the c axis is greater than 0.126A, $\Theta(T)$ falls below $\Theta(0)$ and the method begins to fail. Since the temperatures used in the method were 106° and 314°K, the method really gives a value which is between the true value of a/b for 106° and a/b for 314° and this it does as seen by reference to Table VI.

It should be noted that the method of diffuse scattering has a distinct advantage over other methods in that the characteristic temperatures $\Theta_{||}$ and $\Theta_{\perp}$ can be measured at a single temperature T. Some methods give the average characteristic temperatures between two temperatures. The reason for this is that the diffuse scattering can be measured at the same scattering angle and the same temperature for two values of ψ. We thus obtain two equations containing a and b and we can solve for these two quantities. However, the diffuse scattering measurements must be made at a scattering angle large enough to be beyond the effect of the structure asymmetry of the valence electrons. In powdered crystal work each reflection is for a fixed value of ψ and ϕ and the experimenter must take what nature gives him; whereas in the case of diffuse scattering the experimenter can arrange the ϕ's and ψ's at will, taking care only to evade the Laue spots.

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[12] In the derivation of M by Debye and Waller and by Zener and Jauncey, no account was taken of the effect the change in the separation of the lattice due to thermal expansion has on the mean square displacement.

4. Asymmetry of the Electron Atmosphere

The two valence electrons may be considered as having a spatial distribution something like that of the electron of a hydrogen atom. According to quantum mechanics the probability of a hydrogen electron being in a volume element *dv* at a distance *r* from the nucleus is

$$(1/\pi a^3)e^{-2r/\gamma}dv,$$

where γ is the radius of the first Bohr orbit in hydrogen. From this it follows that the structure factors for the hydrogen electron are given by

$$E=1/(1+4\pi^2\gamma^2x^2)^2, \tag{14}$$

where $x=(\sin\frac{1}{2}\phi)/\lambda$. In order to introduce asymmetry we shall suppose that γ^2 in (14) is replaced by

$$p^2\cos^2\psi+q^2\sin^2\psi. \tag{15}$$

We shall represent E for a given value of x and ψ by $E(x, \psi)$. Using the values

$$p=0.7\text{A} \quad \text{and} \quad q=0.3\text{A}$$

we have calculated values of $2\delta E$, where $\delta E=E(x, 90°)-E(x, 0°)$. These values are shown in Table VII. The δf values in this table are values of $f(x, 90°)-f(x, 14°)$ which are obtained from Table IV. It is probable that $f(x, 14°)$ is very nearly equal to $f(x, 0°)$. There is no attempt in Table VII to show that $\delta f=2\delta E$, but merely to show that a valence electron asymmetry designated by the above values of p and q does have an effect out to $(\sin\frac{1}{2}\phi)/\lambda=0.6$ and that the effect of the asymmetry is of the proper order. Further, the values $p=0.7\text{A}$ and $q=0.3\text{A}$ are not unreasonable in view of the fact that γ for the hydrogen atom in (14) is 0.53A. A more accurate agreement between $2\delta E$ and δf can probably be obtained by using another formula than (14) for E and another way than (15) of taking care of the asymmetry. However, the δf at $(\sin\frac{1}{2}\phi)/\lambda=0.2$ is so large, being apparently larger than 2, that perhaps the asymmetry extends to electrons beneath the valence electrons.

Table VII.

$(\sin\frac{1}{2}\phi)/\lambda$	$2\delta E$	δf
0.1	0.46	1.4
.2	.90	2.1
.3	.88	1.3
.4	.70	0.9
.5	.48	.5
.6	.17	.0

In Section 1 of this paper we said that S_{inc} was insensitive to change of ψ. At $(\sin\frac{1}{2}\phi)/\lambda=0.3$, we have $\Sigma E_r^2=14.7$ from Table I. If we take the two valence electrons to be hydrogen-like, we have E for each of these equal to 0.25. The ΣE_r^2 for the core electrons is therefore $14.7-2\times 0.25^2=14.57$. Now $E(0.3, 90°)=0.57$ and $E(0.3, 0°)=0.13$. Hence, including the valence electrons, we have $\Sigma E_r^2(0.3, 0°)=14.65+2\times 0.13^2=14.68$ and $\Sigma E_r^2(0.3, 90°)=14.65+2\times 0.57^2=15.3$. Hence

$$S_{\text{inc}}(0.3, 0°)-S_{\text{inc}}(0.3, 90°)=0.02.$$

Now the experimental value of $S_{\text{coh}}+S_{\text{inc}}$ for $(\sin\frac{1}{2}\phi)/\lambda=0.3$ and $\psi=90°$ is 2.1. The change in S_{inc} due to going from $\psi=0°$ to $\psi=90°$ is thus one percent of the experimental value of S. The error introduced into our theoretical calculations by not taking account of the change in S_{inc} due to a change in ψ is therefore no greater than our experimental error, which is about 1 or 2 percent.