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EXPERIMENTAL STUDY OF ELECTRON DENSITY IN CRYSTALS:

I. ELECTRON DENSITY OF ALUMINUM

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/Tables and figures referred to herein are appended./

The method of computing electron density in a crystal lattice with the aid of Fourier's series was suggested by Bragg (1) and elaborated in its present form in the work of Duane (2).

In order to carry through the above-mentioned calculations an experimental determination of the atomic X-ray scattering factor is necessary. Contemporary methods of measuring the intensity of reflected X-rays make it possible to determine fairly accurately the atomic scattering factors and, by studying the distribution of electron density, to judge the state of atoms and the character of their combination in solid matter.

The first studies in this direction were made by Havighurst (3) on crystals of sodium chloride, sodium fluoride, and lithium fluoride. Later this method was also applied by Wollan (4) for magnesium oxide, and in the work of Grimm, Brill, Hermann and Peters (5) in the study of sodium chloride, diamond, urotropine, magnesium, and aluminum.

In order to study the small values of electron density in the zones between ions, where the outer valence electrons responsible for the chemical combination are distributed, it is necessary to determine the factors of atomic scattering with great accuracy. The study of the problem of computation of electron density in aluminum carried out at an earlier date (6), making use of documentary data concerning the F-curve of aluminum, has given indications concerning the accuracy of the method and its possibilities.

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METHOD OF DETERMINING THE F-CURVE

In our present study we shall use the photographic method of determining the intensity of X-rays, which we used previously (7) for other purposes and which has been used successfully in the work of Brindley (8), Brentano (9), and Bradley (10) for determining the F-curves. All further discussion of method will apply solely to this method of measuring intensity.

A. Choice of a Specimen Form

The first point to consider in choosing the method of measuring X-ray intensity is the question of the specimen form. A specimen of the metal under investigation was taken in a polycrystalline form, as it is possible in the case of sufficiently small crystals to eliminate the extinction completely (11), which cannot be disregarded in the case of large crystals. For an X-ray photograph, a flat specimen was chosen, which made it relatively simple to disregard the absorption factor (12).

B. Preparation of the Specimen

Extinction is completely absent, when the aluminum crystal particles have a magnitude of the order of 10^{-5} cm (11). The preparation of such a specimen offers considerable difficulty. The necessary flat, fine, crystalline specimens were obtained by condensation of aluminum vapors on a glass tablet in a high vacuum (13). The specimens used for this investigation were prepared in the laboratory of S. A. Vekshinskiy according to his own method. The prepared specimens consisted of crystals with a high degree of dispersion which could be observed by a considerable diffusion of the lines in the X-ray photograph. As a result of heating at 150°, specimens were obtained with crystals of the necessary degree of fineness, with complete absence of extinction or orientation of crystals. Due to these factors the subject specimens were considered good material for determining the atomic scattering factor in aluminum.

C. Applied Radiation

We used iron (λK_α=1.934A) and copper (λK_α=1.539A) radiations for determining the F-curve.

D. Focusing of Reflections

In photographing a flat specimen it is impossible to focus simultaneously all reflections in the X-ray picture. The focusing depends on the angle α between the plane of the specimen and the incident ray (14). In order to obtain the focusing of all reflections in the X-ray picture of aluminum, the exposure was made at two different angles α = 35° and 49° for iron radiation, and at three angles α = 30°, 65°, and 83°30' for copper radiation. The size of the angle α was determined by measuring the distance, corresponding to $2\theta - \alpha$, from the line of the known angle of Bragg to the edge of the shaded area in the X-ray photograph.

E. Taking of X-Ray Photographs and Their Processing

X-ray photographs were taken with cameras having 57.4 mm diameter, using Eastman Kodak films. In order to find the effective range of the film blackening, the blackening curves were obtaining by the mark method. The Eastman Kodak film disclosed a ratio of s = 0.9 between

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the blackening and the intensity before blackening. The exposure of the X-ray photograph was selected in such a way that the extent of blackening lay within the range 0.2 - 0.5 in relation to the undeveloped portion of the film. Composition, concentration, developer temperature and developing time were kept constant.

F. Determination of Intensity

The X-ray photographs obtained were measured with a photometer, using a Koch-Goos microphotometer manufactured by F. Krauss, and enlarging them six times. The microphotographs were measured and converted to a semilogarithmic scale. The peaks of blackening indicated on a semilogarithmic scale were traced on compact millimetric graph paper and the proportion of their areas determined by weighing the cut-out peaks on an analytical balance. The degree of relative integral intensity of separate reflections from atomic planes was the weight (area) of the peak, traced on a semilogarithmic scale.

Comparison of intensities was made for reflections with indices 111, 002, 022, and 113 on X-ray photographs obtained with an iron radiation at angles $\alpha = 35^\circ$ and 49°, and for reflections 111, 002, 022, 113, 222, 133, 024, and 224 on X-ray photographs obtained with copper radiation at angles α equals 32°, 65°, and $83^\circ 30'$.

Comparison of intensities obtained at different angles was made with the aid of reflections which appeared in common on the X-ray photographs under comparison. In copper radiation for angles $\alpha = 32^\circ$ and 65°, such reflections were 113, and for $\alpha = 65^\circ$ and $83^\circ 30'$ a reflection of 133. The calculation of atomic scattering factors F from the value of relative intensities I of reflected rays was done on the basis of the equation

$$F = \frac{1}{4}\sqrt{\frac{I}{p \cdot A \varphi(\theta)}}$$

where A is the absorption factor determined by the method of Brindley and Spiers (12) for flat specimens; p is the recurrence factor; $\varphi(\theta)$ is the angular factor, equal to

$$\frac{1 + \cos^2 2\theta}{\sin\theta \cdot \sin 2\theta}$$

Dispersion corrections were assumed, according to Hoenl (16), for iron radiation equaling 0.21 and for copper radiation equaling 0.18.

In calculating the temperature factor, the following correction was employed, $\Delta F \cdot e^{-M}$, where M is the experimental value, determined by James and his collaborators (15) and is equal to $0.01182\ (h^2 + k^2 + l^2)$.

The transition from relative values of the atomic scattering factor to absolute values was made with the aid of the absolute value of atomic scattering for a 002 lattice of aluminum. Determined by James, Brindley, and Wood (15), by means of molybdenum radiation, this value equals 7.96, which after introducing the dispersion correction according to Hoenl will amount to 7.90.

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RESULTS OF DETERMINING THE F-CURVE

The values of atomic scattering of metallic aluminum, determined experimentally with the aid of copper radiation, are presented in Table 1 which shows the following values:

1. HKL -- indices of atomic lattices of aluminum, giving reflections on the X-ray photograph;

2. The values of $\sin\theta/\lambda$ correspond to these lattices, where θ is the Bragg's angle and λ is the wave length of the applied radiation;

3. The angle α between the specimen facet and the incident ray;

4. I -- the relative integral intensity, determined by the area of the curve peak obtained by microphotometer, constructed on a semilogarithmic scale, in relative units, standardized within the range of the determined angle α;

5. A -- absorption factor according to Brindley and Spiers (12) for a flat, fine, crystalline specimen, determined by

$$\frac{\sin(2\theta - \alpha)}{\sin(2\theta - \alpha) + \sin\alpha};$$

6. p -- recurrence factor for lattice planes of aluminum;

7. Angular factor $Q(\theta)$;

8. $F_{T\,rel}$ -- relative value of the atomic scattering factor at a temperature of 20°, calculated from the above-mentioned formula;

9. $F_{Tc/u}$ -- value of the atomic scattering factor for copper radiation at a temperature of 20°, obtained by reducing the relative values $F_{T\,rel}$ to an absolute value, using the value $F_{T\,abs}$ = 7.90 for a lattice 002 determined by James, Brindley and Wood;

10. ΔF_{e-M} -- dispersion correction for copper radiation (16), allowing for heat fluctuations;

11. $F_{T\,abs}$ -- absolute value of the atomic scattering factor of metallic aluminum at a temperature of 20°, obtained by introducing a scattering correction into values for F_{Tcu};

12. Given values of James, Brindley, and Wood for aluminum monocrystal (15), corrected for scattering and taken as absolute;

13. Values $F_{T\,abs}$, re-calculated with the aid of scattering correction from the figures of Brindley and Ridley (11), for aluminum powder with application of copper radiation.

Table 1 shows the values we obtained for the atomic scattering factor with application of copper radiation.

The values obtained with iron radiation are shown in Table 2. The symbols employed in Table 2 coincide with those in Table 1, therefore we need not examine them closely. The obtained values of atomic scattering factors of aluminum with copper and iron radiation coincide, as can be

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seen by comparing tables [illegible] factor (F-curve) of aluminum at a temperature of 20C is shown in Figure 1 in absolute units. For plotting the curve we used the values obtained for iron and copper radiation.

CALCULATION OF ELECTRON DENSITY

The F-curve obtained experimentally for aluminum makes it possible to calculate the distribution of electron density in a lattice of metallic aluminum. For the purpose of calculating the space distribution of electron density we used three-dimensional Fourier's series in the following manner:

$$\rho(x, y, z) = \sum_{h} \sum_{k}^{+\infty} \sum_{l} A_{hkl} \cos 2\pi \left(h\frac{x}{a} + k\frac{y}{a} + l\frac{z}{a}\right),$$

where hkl represents the integers from $+\infty$ to $-\infty$; a -- lattice constant for aluminum, equaling 4.041 A; A -- coefficient of resolution of Fourier's series, equaling $A_{hkl} = \frac{1}{v} F_{hkl}$, where v is the volume of the elementary nucleus, equaling $(4.041)^3$ Å^3; F -- the atomic scattering factor, determined from the F-curve. The values of F were taken on the basis of experimental measurements or by interpolation on the F-curve, Figure 1.

The zero term of resolution was calculated from the condition $F_0 = z$, in which z is the total number of atomic electrons.

As we can see from the above-mentioned formula for the electron density, the actual determination of electron density is possible with an infinite number of terms of Fourier's series. Practically, we can restrict ourselves to a finite number of terms of the series, as the experimental results obtained with a certain degree of accuracy do not make it possible to disregard very small amplitudes of the terms of Fourier's series of a higher order. Consequently, it is necessary to summarize such a number of terms of the series in order that the amplitudes of the final ones will correspond to the accuracy of the only experimentally definable value F, the atomic scattering factor. The value of the atomic scattering factor of aluminum can be determined at the present time with an accuracy up to $\pm$ 0.05. The number of terms of a series must be chosen in such a way that the coefficients of the final terms are equal to the indicated magnitude of error. The resulting number of terms of Fourier's series will depend on the number of reflections obtained on the X-ray photograph, and the latter depends on the wave length of the applied radiation.

In using FeK_α radiation it is possible to obtain 64 terms of a series; with CuK_α, 136 terms; and with MoK_α, 698 terms. Moreover, the values of F for the final terms of the series will equal, in the case of FeK_α, 5.69; CuK_α, 3.26; MoK_α, 0.85. Consequently, even when applying hard molybdenum radiation, it cannot lead to sufficiently small amplitudes of the final members of a series. The error which enters into the calculation of electron density, due to the above-mentioned limitation of the number of terms of a series, has been called the series-rupture error (17). This error increases with the degree of softness of the applied radiation (6), and can cause considerable distortions in the results of determining electron density.

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The series rupture error is eliminated with the aid of two calculating methods. One of these methods is the lengthening of the F-curve in the direction of the higher values of $\sin \theta/\lambda$, according to the method suggested by Froman (18). This procedure cannot be considered sufficiently reliable, as the curve continues beyond the range of the experimentally obtained values of F and cannot be experimentally verified. In addition, the lengthening of the F-curve leads to a considerable increase in the number of terms in the Fourier's series, which complicates the practical work of their summation. The second method was suggested by Grimm, Brill, Hermann, and Peters (5) and was termed calculation temperature.

The F curve, obtained experimentally at a temperature of 20°, can be reduced to any other calculation temperature by using the temperature factor

$$F_T = F_{T_1} \cdot e^{-B\Sigma h^2},$$

where F_{T1} is the atomic scattering factor at a temperature T_1; F_T - the atomic factor, determined experimentally at a temperature T, and $e^{-B\Sigma h^2}$ is the heat factor in which

$$B = \frac{6h^2}{4a^2 m k \theta} \left\{ \frac{D\left(\frac{\theta}{T_1}\right)}{\frac{\theta}{T_1}} - \frac{D\left(\frac{\theta}{T}\right)}{\frac{\theta}{T}} \right.$$

where h is Planck's constant; a, the lattice constant; m, mean weight of the atom; T, temperature, at which the experimental F-curve is determined, T_1, temperature being calculated; k, Boltzmann's constant; θ, characteristic temperature; $D\left(\frac{\theta}{T}\right)$ Debye function.

The problem in introducing a correction into the series rupture with the aid of calculation temperature consists of finding a temperature, under which the value of the atomic scattering factor, with the highest $\sin \theta/\lambda$ for a given F-curve, becomes equal to the accuracy in determining the F-curve, i.e., in the case of the aluminum F-curve, it equals ± 0.05. In order to find the necessary calculation temperature, it is sufficient to compute the changes in the minimum value range of the atomic scattering factor F (with the highest value of $\sin \theta/\lambda$) for a given F-curve, depending on the temperature according to the above formula, and to find a temperature, under which the value of F is equal to 0.05.

Figure 2 illustrates the changes, with the calculation temperature, of value F of aluminum for the last point of the F-curve, obtained with copper radiation (see Figure 1, the point where $\sin \theta/\lambda$ equals 0.60). At a temperature of 4,000° the value F becomes equal to 0.05, and therefore, this will be the calculation temperature, under which the error of series rupture will not be apparent in computing the electron density of aluminum. Figure 2 also shows that the F-curve obtained with molybdenum radiation, requires a calculation temperature of 10000.

If a calculation temperature is too low, it does not completely eliminate the error of series rupture; then the introduction of an excessively high calculation temperature will lead to an unnecessary decrease of the accuracy in computing electron density, below the limit of experimental accuracy, which can bring about discrepancies in the results obtained. Therefore, the determination of the optimum calculation temperature by the method described above is essential in determining electron density.

The computation of electron density was made on the basis of the

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F-curve, obtained experimentally with copper radiation, and reduced to a calculation temperature of 4000° (Figure 1). In order to determine the space distribution of electron density, we applied three-dimensional Fourier's series, summarizing 136 terms. The computation of electron density was made for directions 001, 011, and 111 of the elementary nucleus, shown in Figure 3. Results of computation of electron density for three directions of aluminum lattice are shown in Table 3 and in Figures 4, 5, and 6.

The electron density in all three directions 001, 011, and 111, drops abruptly from the lattice node to a distance 1.2 A; it reaches a constant value that is maintained in the entire interionic space of the aluminum lattice and equals an average of 0.20 e/A^3.

The results we received on the distribution of electron density in aluminum differ considerably from those mentioned in the work of Brill, Hermann, and Peters (5). The fluctuation mentioned by them in electron density in the interionic space is very great; which condition the authors explain by the presence of orientation, in a powdery specimen used in obtaining the F-curve, at low values of sin θ/λ.

CONSIDERATION OF RESULTS

The theoretical calculation of charge distribution in the atom, according to the method of the self-adjusted field of Hartree, made it possible to calculate the theoretical F-curve for various atoms and ions. The calculations made enable one to allow for the influence of electrons, found in various conditions in the atom on the F-curve. The figures mentioned by James (19) for K^+ ion, James, Brindley, and Wood (15) for aluminum in three ionization states Al^+, Al^{2+} and Al^{3+}, and James, Waller, and Hartree (20) for Cl^- ion, show that the influence of outer valence electrons on the F-curve is restricted to low values of sin θ/λ. With high values of sin θ/λ, the character of the F-curve is determined, fundamentally, by the inner 1s-electrons. Thus, for aluminum, the valence electrons 3s influence the F-curve up to sin $\theta/\lambda = 0.44$, in calculation of an atom in a free state. It is possible that the atom in a crystal would show some deviation from these limits, but in any case all changes in the valence condition of an atom are connected with the F-curve, at low values of sin θ/λ.

The above-mentioned theoretical calculations and considerations have enabled us, in our present work, to elaborate a method of calculating electron density for determining the distribution of valence electrons, with the aid of short F-curve, obtained by soft X-ray radiation. The application of short F-curves considerably simplifies the experimental work and cuts down the calculations in summarizing the Fourier series.

As a result of using short F-curves, it is necessary to make considerable use of an optimum calculation temperature, amounting to several thousand degrees. Our calculations with an introduction of a different calculation temperature have shown that the results obtained with regard to the distribution of electron density are not disturbed by the above-mentioned temperature correction.

Table 4 shows the results of calculation of F-curves for various temperatures in the case of aluminum, which were obtained through multiplication by the temperature factor, of the F-curve obtained experimentally

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from 20°, with iron, copper and molybdenum radiations. On the basis of the F-curves obtained for aluminum at different temperatures, calculation was made of the distribution of electron density for direction 001 of the aluminum lattice AB on Figure 3. The results are indicated in Table 5 and, more specifically, in Table 7, where the change of electron density for certain points of direction 001 is shown in relation to the calculation temperature. The points are chosen in such a way that point 1 (see Figure 7, right side) is situated in a lattice node, point 2 and the following through one tenth of a period of identity, in the direction 001, and point 5, is halfway between the nodes of the lattice.

The diagram shows that the greatest change in electron density, with the introduction of calculation temperature, occurs at the point corresponding to the lattice node (ionic center) and there is no change whatever at points sufficiently distant from the lattice node, i.e., situated in the interionic space. The calculation temperature, therefore, will cause considerable distortion in the distribution of electron density in the lattice nodes. In the interionic space, where the valence electrons are located, the distribution of electron density will not be distorted by the calculation temperature.

The curves of the change in electron density with temperature (Figure 7) show smooth paths at temperatures over 1,000° (with lower calculation temperatures there is a dispersion of points), which makes it possible to carry out reverse extrapolation to room temperature. The results obtained in this case are shown in Figure 7 by numbers indicated opposite each curve in the diagram. A construction of this kind was made for points in the direction 001, passing through 0.20 A, and the results are shown in the form of a diagram (Figure 8, upper part). Consequently, we may say that the calculation temperature does not cause any distortion in the results of determining the distribution of valence electrons and, in addition, the method of reverse extrapolation makes it possible to show the distribution of electron density, corresponding to the temperature of the experiment.

DETERMINATION OF THE DEGREE OF ATOMIC IONIZATION

The distribution of electron density in interionic space in direction 001 of the aluminum lattice is shown on an enlarged scale (Figure 8, lower part).

Making use of Figure 8, we can assume the ion radius of aluminum to equal 1.20 A, since beyond this limit the electron density becomes constant and equals, on the average, 0.20 el/A^3. After determining the volume of the elementary nucleus from the aluminum lattice constant and deducting the volume occupied by the four ions, one can determine the volume pertaining to the conductivity electrons. In dividing the number of valence electrons by the volume occupied by them in the nucleus, one can determine the average electron density of the valence electrons in the lattice. This calculation gives the following values of electron density: in the case of complete ionization of aluminum (Al^{3+}) 0.24 el/A^3; in the case of a bivalent ion of aluminum (Al^{2+}) 0.16 el/A^3; and for a monovalent ion of aluminum (Al^{+}) 0.08 el/A^3.

The value obtained experimentally corresponds, on the average, to 0.20 el/A^3, and the distribution of the separate points is shown in Figure 8 (lower part). The points obtained experimentally and the mean

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[illegible] with a varied degree of ionization, or by the possibility, considering the metallic character of the combination of atoms in the lattice, of an uninterrupted change in the degree of ionization as opposed to the distinct change, which is characteristic for ionization in ion lattices. The second assumption appears to be more plausible, taking into consideration the principles of the structure of atoms in a metallic state. In any event, the incomplete ionization of the atom in a crystal lattice of metallic aluminum is apparent.

CONCLUSIONS

1. An experimental determination of the F-curve of aluminum has been made by the photographic method, with iron and copper radiations, using a flat specimen obtained by condensation in a vacuum.

2. A method has been suggested for finding the optimum "calculation temperature" and it has been determined that for an aluminum F-curve, obtained with molybdenum radiation, a calculation temperature of 1,000° is necessary; for copper radiation, 4,000°, and for iron radiation, 6,300°.

3. A calculation of the distribution of electron density has been made, in directions 001, 011 and 111 of the aluminum lattice, using the method of three-dimensional Fourier's series with a calculation temperature of 4,000°.

4. The possibility has been shown of using a short F-curve, obtained with soft X-ray radiation, in calculating electron density, and the absence of distortions has been made evident when introducing the optimum temperature correction in calculating the distribution of valence electrons.

5. A method of reverse extrapolation has been suggested for reducing the distribution of electron density to the temperature of the experiment, which makes it possible to obtain a curve of the distribution of electron density without temperature correction.

6. A curve has been obtained for the distribution of electron density for direction 001 of the aluminum lattice of 20°.

7. It has been shown that the atom is incompletely ionized in metallic aluminum and the degree of ionization is between Al^{2+} and Al^{3+}.

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[Appended tables and figures follow.]

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Table 1. Atomic Scattering Factor of Aluminum (Copper Radiation)

hkl	$\sin\theta/\lambda$	α	I	A	p	$\rho(\theta)$	$F_{T_{rel}}$	$F_{T_{cu}}$	ΔF_{e-M}	$F_{T_{abs}}$	$F_{T_{abs}}$ [11]	$F_{T_{abs}}$ [11]
1	2	3	4	5	6	7	8	9	10	11	12	13
111	0.214	30°00'	142.7	0.228	8	7.84	0.790	8.62	0.17	8.45	8.40	8.45
002	0.247	30°00'	100.0	0.338	6	5.61	0.740	8.07	0.17	7.90	7.90	7.81
022	0.350	30°00'	94.0	0.532	12	2.41	0.615	6.71	0.16	6.55	- -	6.52
113	0.410	30°00'	112.0	0.599	24	1.68	0.550	5.85	0.16	5.69	- -	5.69
113	0.410	65°00'	100.0	0.202	24	1.68	0.873	5.85	0.16	5.69	- -	5.69
222	0.429	65°00'	34.8	0.249	8	1.55	0.840	5.61	0.16	5.45	5.46	5.51
133	0.539	65°00'	100.0	0.435	24	1.48	0.635	4.27	0.14	4.13	- -	4.02
133	0.539	83°30'	100.0	0.324	24	1.48	0.737	4.27	0.14	4.13	- -	4.02
024	0.553	83°30'	101.3	0.357	24	1.58	0.682	3.96	0.14	3.82	- -	3.88
224	0.606	83°30'	146.0	0.452	24	2.46	0.585	3.40	0.14	3.26	- -	3.27

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Table 2. Atomic Scattering Factor of Aluminum (Iron Radiation)

hkl	$\sin\theta/\lambda$	α		I		A		p	$Q(\theta)$	$f_{T\,rel}$		$f_{T\,Fe}$			Δf_{c-M}	$f_{T\,abs}$
1	2	3		4		5		6	7	8		9			10	11
				35°	49°	35°	49°			35°	49°	35°	49°	mean		
111	0.214		35°00'	172.3	--	0.298	--	8	4.56	0.995	--	8.61	--	8.61	0.20	8.41
002	0.247	35°00'	49°00'	106.2	58.0	0.398	0.161	6	3.20	0.935	1.082	8.10	8.16	8.13	0.20	7.93
022	0.350	35°00'	49°00'	100.0	100.0	0.572	0.437	12	1.50	0.773	0.892	6.74	6.74	6.74	0.19	6.55
113	0.410	35°00'	49°00'	151.9	--	0.621	--	24	1.40	0.675	--	5.85	--	5.85	0.18	5.67

Table 3. Electron Density of Aluminum in Directions 001, 011, 111; 136 Term Series; Calculated Temperature 4,000°

Direction 001

Distance from lattice node	A	0	0.20	0.40	0.61	0.81	1.01	1.21	1.41	1.62	1.82	2.02
Electron density	Elec/A³	8.41	7.53	5.43	3.16	1.46	0.65	0.36	0.21	0.18	0.17	0.21

Direction 011

Distance from lattice node	A	0	0.29	0.57	0.85	0.97	1.14	1.28	1.43	1.57	1.71	1.85	2.00	2.28	2.56	2.8[illegible]
Electron density	Elec/A³	8.41	6.76	3.53	1.24	0.68	0.41	0.28	0.25	0.28	0.41	0.68	1.24	3.53	6.76	8.4[illegible]

Direction 111

Distance from lattice node	A	0	0.35	0.70	1.05	1.40	1.75	2.10	2.44	2.80	3.14	3.49
Electron density	Elec/A³	8.41	6.07	2.31	0.60	0.25	0.21	0.20	0.18	0.15	0.15	0.20

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Table 4. Atomic Scattering Factors of Aluminum for Various Temperatures

hkl	$\sin\theta/\lambda$	20°	500°	600°	700°	900°	1000°	2500°	4000°	4750°	5500°	6500°
111	0.214	8.45	7.95	7.87	7.77	7.57	7.48	6.20	5.12	4.66	4.24	3.73
002	0.247	7.90	7.30	7.20	7.08	6.84	6.71	5.21	4.06	3.56	3.20	2.65
022	0.350	6.55	5.60	5.40	5.26	4.88	4.72	2.84	1.72	1.34	1.04	0.75
113	0.410	5.63	4.61	4.38	4.20	3.81	3.65	1.81	0.91	0.65	0.46	0.29
222	0.429	5.35	4.32	4.10	3.92	3.53	3.35	1.58	0.74	0.51	0.35	0.21
004	0.495	4.60	3.38	3.15	2.96	2.58	2.40	0.89	0.32	0.19	0.12	0.06
133	0.539	4.13	2.85	2.61	2.41	2.06	1.90	0.58	0.17	0.08	0.05	--
024	0.553	3.82	2.60	2.39	2.20	1.86	1.71	0.49	0.14	0.07	0.04	--
224	0.606	3.36	2.06	1.86	1.68	1.36	1.24	0.27	0.06	0.03	--	--
333	0.636	2.95	1.76	1.57	1.40	1.12	0.99	0.18	--	--	--	--
006	0.738	2.20	1.10	0.94	0.81	0.60	0.51	0.05	--	--	--	--
444	0.860	1.54	0.60	0.49	0.40	0.27	0.22	--	--	--	--	--
008	0.982	1.05	0.30	0.23	0.18	0.10	0.10	--	--	--	--	--
555	0.067	0.85	0.22	0.16	0.12	0.06	0.05	--	--	--	--	--

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Table 5. Electron Density of Aluminum for Various Calculation Temperatures. Direction CCI

Calculation Temperature in °C	Distance From Lattice Node in Å											No. of Terms in Series
	0	0.20	0.40	0.61	0.81	1.01	1.21	1.41	1.62	1.82	2.02	
20	94.36	54.16	7.06	2.13	2.26	0.02	-0.07	-0.38	0.20	-0.49	-1.06	635
20	41.91	34.43	15.13	0.81	-2.98	-0.55	0.82	0.00	0.45	2.06	4.26	136
20	25.43	22.09	14.17	5.94	0.81	-0.83	-0.45	-0.20	0.12	0.30	0.37	54
500	53.92	35.56	9.80	1.77	0.56	0.42	0.34	0.09	0.16	0.04	0.02	638
700	44.01	30.52	10.24	2.29	0.56	0.21	0.22	0.13	0.27	0.16	0.03	[illegible]
900	36.85	27.03	10.18	2.59	0.[illegible]	0.23	0.27	0.16	0.25	0.26	0.19	898
1000	34.08	25.04	9.58	2.83	0.57	0.24	0.24	0.20	0.24	0.10	0.07	698
2500	13.07	11.98	7.38	3.34	1.23	0.48	0.23	0.18	0.26	0.31	0.32	258
4000	8.40	7.53	5.43	3.16	1.46	0.65	0.36	0.21	0.18	0.17	0.21	156
4750	6.90	6.26	4.60	2.92	1.54	0.74	0.36	0.21	0.19	0.22	0.24	136
5500	5.82	5.36	4.16	2.75	1.56	0.82	0.44	0.28	0.21	0.19	0.18	112
6500	4.65	4.36	3.58	2.49	1.53	0.85	0.46	0.28	0.21	0.19	0.17	84

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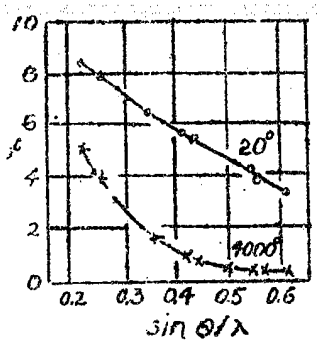

Figure 1. Curve of Atomic Scattering of Aluminum

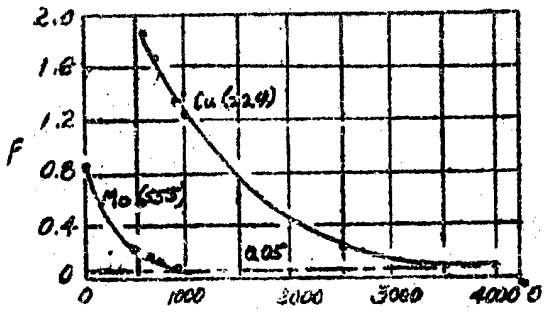

Figure 2. Determination of Calculated Temperature

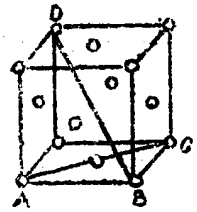

Figure 3. Elementary Nucleus of Aluminum

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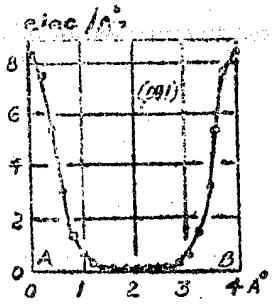

Figure 4. Electron Density of Aluminum; Direction 001; Calculation Temperature 4,000°

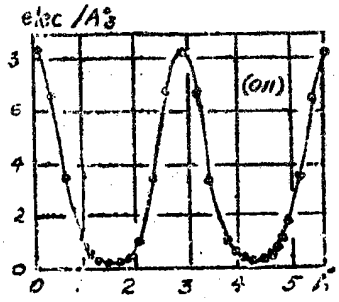

Figure 5. Electron Density of Aluminum; Direction 011; Calculation Temperature 4,000°

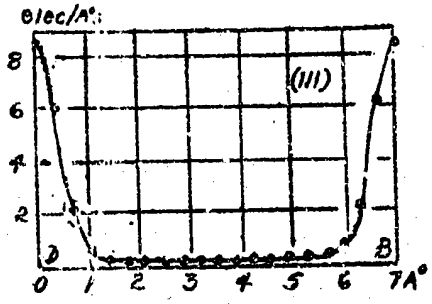

Figure 6. Electron Density of Aluminum; Direction 111; Calculation Temperature 4,000°

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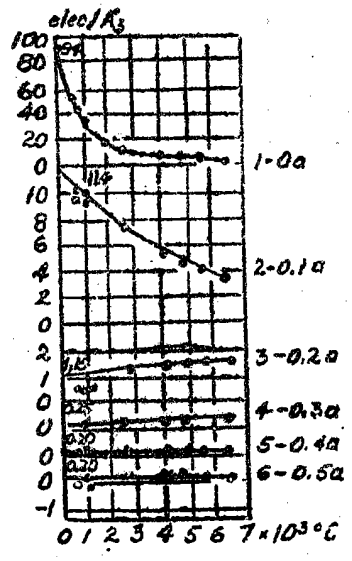

Figure 7. Electron Density of Aluminum in Relation to Temperature for Direction 001

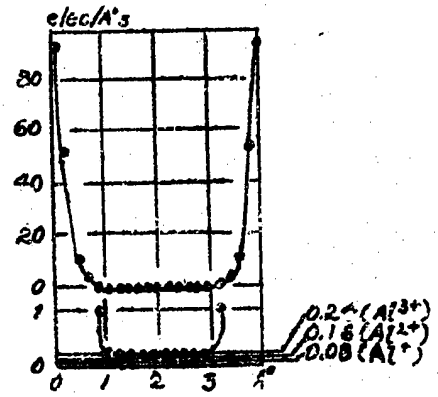

Figure 8. Electron Density of Aluminum in Direction 001 at 20° C and Degree of Atom Ionization

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