which the present method may have in the investigation of the meson spectrum at great heights (notice in this connection how the slope of the α vs. $\tau/\mu c^2$ curves increases with increasing height). An experiment of this kind by Bernardini and Scrocco was in progress in 1941, but was interrupted by a serious flying accident to the airplane which carried the apparatus. As a consequence the apparatus was gravely damaged, and for this and other reasons connected with Italian events, the experiment was given up for the time being.

Disorder Scattering of X-Rays by Local Distortions

H. EKSTEIN
Armour Research Foundation, Chicago, Illinois
(Received July 16, 1945)

The disorder scattering (background) owing to local distortions is caused mainly by the elastic strain field surrounding the distorted zone rather than by the misfit atoms in the zone of distortion. As an example, the scattering caused by a distortion of spherical symmetry is calculated. The result is extended for more general types of distortions. The background intensity increases strongly in the neighborhood of a line, and it tends toward a constant value for small scattering angles. This explains previous observations on rolled copper.

1

TO explain the plastic properties of solid bodies, it is necessary to assume local lattice distortions or irregularities. Most of the evidence for the assumed models of dislocation is indirect. Several papers have attempted to connect the observed line intensities and widths with the internal distortions.[1-6] Little attention has been given to the continuous background scattering arising from the distortions. The experimental conditions for this type of research are not easy, because other effects such as fluorescent radiation, Compton radiation, diffuse scattering by air, coherent temperature scattering and background owing to the continuous x-ray spectrum, all contribute to the observed background. Yet experiments by Guinier[7] have shown the effect of plastic deformation of copper upon the background to be appreciable. If the scattering caused by local distortions can be isolated, it will provide more useful information than the study of the lines; first, because this scattering is entirely absent in an ideal crystal, while the line intensity decreases only by a few percent when distortion is introduced, and secondly, because slowly variable internal stresses affect the line, but not the background.

The following theoretical discussion gives a correlation between local distortions and disorder scattering, which explains some of Guinier's results, and may be helpful for further experimental work.

For a simple Bravais lattice, the scattering intensity is given by:

$$I = I_e |F|^2 |\sum_n \exp (2\pi i \mathbf{R} \cdot \mathbf{r}_n)|^2, \qquad (1)$$

where I_e is the scattering intensity from one electron, F the atomic form factor,

$$\mathbf{R} = \mathbf{k} - \mathbf{k}_0, \qquad (2)$$

$\mathbf{k}$ and $\mathbf{k}_0$ the wave vectors of incident and scattered wave, and $\mathbf{r}_n$ the radius vector of the nth atom. For $\mathbf{r}_n$, we write

$$\mathbf{r}_n = \mathbf{a}_n + \mathbf{u}_n, \qquad (3)$$

[1] J. Hengstenberg and H. Mark, Zeits. f. Physik 61, 435 (1930).
[2] G. W. Brindley and F. W. Spiers, Phil. Mag. 20, 882 (1935).
[3] U. Dehlinger, Zeits. f. Krist. 65, 615 (1927).
[4] W. Boas, Zeits. f. Krist. 97, 354 (1937).
[5] U. Dehlinger and A. Kochendörfer, Zeits. f. Metallkunde 31, 231 (1939).
[6] A. Kochendörfer, Zeits. f. Krist. 101, 149 (1939).
[7] A. Guinier, Comptes rendus 208, 894 (1939).

where $\mathbf{a}_n$ is the radius vector of the nth lattice point.

In physical lattice distortions of the type usually assumed, the displacements of the atoms from the regular lattice points are of the order of magnitude of the atomic distances in the immediate neighborhood of the distortion which extends over only a few atomic distances. The number of atoms within this zone is small, and they cannot be expected to give a large contribution to the disorder scattering. Outside the distortion zone itself, the displacement of atoms is of the elastic type, i.e., the displacements are small as compared to the atomic distance. While the displacement decreases rapidly from the origin of the perturbation, the number of atoms affected is large, and we may expect an important x-ray effect from them.

In the following the atoms within the distorted zone in this sense are disregarded, and only the indirect effect of the distortion, through its elastic strain field, is taken into account.

Consequently, we may assume that in Eq. (3) $\mathbf{u}_n$ is small in comparison to the interatomic distance. With the notation

$$G = \sum_n \exp (2\pi i \mathbf{R} \cdot \mathbf{r}_n), \qquad (4)$$

the Taylor expansion yields:

$$G = \sum_n \exp (2\pi i \mathbf{R} \cdot \mathbf{a}_n)$$
$$+ 2\pi i \mathbf{R} \cdot (\sum_n \mathbf{u}_n \exp (2\pi i \mathbf{R} \cdot \mathbf{a}_n))$$
$$+ \cdots = G_0 + G_1 \cdots \qquad (5)$$

The first term of (5) represents the ordinary scattering by a regular crystal and can be disregarded here. As we are interested only in the scattering outside the lines, the second term may be treated separately.

In order to bring the second term of (5) into a more convenient form, we use a transformation formula given by Ewald.[8] If $\mathbf{A}_h$ are the lattice vectors of the reciprocal lattice and v the volume of the unit cell, then

$$\sum_n u_n \exp (2\pi i \mathbf{R} \cdot \mathbf{a}_n) = \frac{1}{v} \sum_h U(\mathbf{R} - \mathbf{A}_h), \qquad (6)$$

where $U(\mathbf{R})$ is the Fourier transform of a function

$u(\mathbf{r})$ which interpolates the values u_n at the lattice points:

$$U(\mathbf{R}) = \int u(\mathbf{r}) \exp (2\pi i \mathbf{R} \cdot \mathbf{r}) dv, \qquad (7)$$

and

$$u(\mathbf{r} = \mathbf{a}_n) = u_n. \qquad (8)$$

This transformation may be considered as a three-dimensional generalization of Poisson's sum formula. Patterson's representation of the interference function of perfect crystals[9] can be recognized as a special application of the generalized Poisson formula.

The Eqs. (6)–(8) are evidently still applicable if the quantities u_n are vectors, $\mathbf{u}_n$, if only the functions $u(\mathbf{r})$ and $U(\mathbf{R})$ are replaced by vector functions $\mathbf{u}(\mathbf{r})$ and $\mathbf{U}(\mathbf{R})$. Equations (6)–(8) become:

$$\sum_n \mathbf{u}_n \exp (2\pi i \mathbf{R} \cdot \mathbf{a}_n) = \frac{1}{v} \sum_h \mathbf{U}(\mathbf{R} - \mathbf{A}_h), \qquad (6a)$$

$$\mathbf{U}(\mathbf{R}) = \int \mathbf{u}(\mathbf{r}) \exp (2\pi i \mathbf{R} \cdot \mathbf{r}) dv, \qquad (7a)$$

$$\mathbf{u}(\mathbf{r} = \mathbf{a}_n) = \mathbf{u}_n. \qquad (8a)$$

The Eqs. (7) and (8) do not determine uniquely the function $\mathbf{U}$ because any function which interpolates the values $\mathbf{u}_n$ is acceptable for $\mathbf{u}(\mathbf{r})$.

The disorder scattering function G_1 is built up of a number of identical functions having their respective origins at lattice points of the reciprocal lattice. The advantage of this transformation is that the function $\mathbf{U}(\mathbf{R})$ often decreases so rapidly from $\mathbf{R} = 0$, that near a lattice point $\mathbf{A}_i$ of the reciprocal lattice, all terms of the sum (6) can be neglected except the term $\mathbf{U}(\mathbf{R} - \mathbf{A}_i)$.

2

As an example, the case of spherical dilatation will be considered. If one or several atoms are inserted into the lattice in addition to the regular atoms or if a larger atom is substituted for a regular one, then the neighboring atoms will be pushed radially outwards. In most metal crystals each atom is surrounded by a sizable number of equidistant atoms so that it is reasonable to replace the central perturbation by a spherical cavity with a pressure p_1. Furthermore, the resultant displacements will be calculated as if

---

[8] P. P. Ewald, Göttinger Nachrichten 55 (1938).

[9] A. L. Patterson, Phys. Rev. 56, 972 (1939).

the crystal were isotropic, because the results will be interesting mainly for their order of magnitude. According to Love,[10] the radial displacement u in a shell bounded by concentric spherical surfaces of radii r_0 and $r_1(r_0 > r_1)$ is given by

$$u = \frac{1}{3\lambda+2\mu} \frac{p_1 r_1^3}{r_0^3 - r_1^3} \cdot r + \frac{1}{4\mu} \frac{r_0^3 r_1^3 p_1}{r_0^3 - r_1^3} \cdot \frac{1}{r^2}. \qquad (9)$$

In our case the crystal size r_0 is large as compared to the radius of the distortion r_1 so that the first term in Eq. (9) can be neglected. Similarly, we disregard the term r_1^3 in the denominator of the second term of (9). The displacement u_1 at the inner surface is

$$u_1 = (r_1/4\mu)p_1, \qquad (10)$$

and we get instead of (9)

$$u = u_1(r_1^2/r^2). \qquad (11)$$

Inserting (11) into (7a), we obtain

$$\mathbf{U} = u_1 r_1^2 \int \frac{\mathbf{r}}{r^3} \exp(2\pi i \mathbf{R} \cdot \mathbf{r}) dv. \qquad (12)$$

Because of the spherical symmetry of the displacement, $\mathbf{U}$ must be parallel to $\mathbf{R}$:

$$U_R = u_1 r_1^2 \int \frac{\cos(\mathbf{r}, \mathbf{R})}{r^2} \exp(2\pi i \mathbf{R} \cdot \mathbf{r}) dv,$$

$$= \frac{2i u_1 r_1^2}{R} \left(\frac{\sin 2\pi r_1 R}{2\pi r_1 R} - \frac{\sin 2\pi r_0 R}{2\pi r_0 R} \right). \qquad (13)$$

This function vanishes at $R=0$, but beyond a maximum at $R=1/2r_0$, the first term rapidly becomes predominant. Now, the central spot of the interference function G_0 which gives rise to the x-ray line itself, extends to about $R=2/r_0$. As the disorder scattering cannot be measured in the immediate neighborhood of the line, we may limit ourselves to such points which are well outside the line. In the following, this domain will be called "near the lattice point" (of the reciprocal lattice) or, "near the line." With this restriction, U_R becomes

$$U_R = i u_1 r_1 \frac{\sin 2\pi r_1 R}{\pi R^2}, \qquad (14)$$

and, by Eqs. (6a) and (5)

$$G_1 = \frac{-2u_1 r_1}{v} R \sum_h \cos(\mathbf{R}, \mathbf{R} - \mathbf{A}_h)$$

$$\times \frac{\sin 2\pi r_1 |\mathbf{R} - \mathbf{A}_h|}{|\mathbf{R} - \mathbf{A}_h|^2}. \qquad (15)$$

Now, the distance between two neighboring lattice points of the reciprocal lattice is of the order of the inverse interatomic distance. As r_1 is of the order of this latter quantity, it may be seen from (14) and (5) that the bulk of the function which constitutes the contribution of a particular lattice point $\mathbf{A}_i$ will be contained in the space between $\mathbf{A}_i$ and its immediate neighbors. Near any lattice point, we may disregard the contributions of all other lattice points, because of the rapid increase of the individual function $\mathbf{U}(\mathbf{R} - \mathbf{A}_i)$.

The surrounding of the lattice point (000), i.e., of the direct transmitted beam, assumes a special place. By Eq. (5), the disorder scattering is proportional to R, and furthermore $\sum u_n$ vanishes because the center of gravity is at rest, so that we should expect the disorder scattering to tend toward zero near the direct beam. The physical significance of this fact was explained by Ewald[11] by the observation that even an asphalt road makes a fairly good mirror when observed at a very oblique angle. Yet, according to Eq. (15), the predominant term of the sum is that which corresponds to $\mathbf{A}_h = 0$; $\mathbf{R}$ becomes equal to $(\mathbf{R} - \mathbf{A}_h)$:

$$G_1 \cong -\frac{2u_1 r_1}{v} \frac{\sin 2\pi r_1 R}{R}, \qquad (16)$$

and G_1 tends toward a constant value at $R=0$. This is true, as explained above, only for points not too close to the line (000) itself, but it describes the experimental form of the disorder scattering curve. Indeed, Guinier's experiments show that the background intensity of cold worked copper becomes constant near the scattering angle zero. As the Compton radiation as well as the temperature scattering tends toward zero at small angles, it is probable that the effect is caused by a perturbation similar to that considered here.

[10] A. E. H. Love, *Mathematical Theory of Elasticity* (Cambridge University Press, New York, 1934), p. 142.

[11] P. P. Ewald, *Handbuch der Physik* (Berlin, 1927), Vol. 24, p. 271.

Equation (14) predicts a strong increase of intensity near a reciprocal lattice point. This, too, is in agreement with Guinier's observations. The exact form of the intensity curve for a polycrystalline aggregate would be given by the average of $|G_1|^2$ over all crystal orientations, the absolute value $|R|$ being fixed for a given scattering angle. But this integration would not have a result comparable to Guinier's experiments. Indeed, G_1 is proportional to the cosine of the angle between R and $(R-A_h)$ in the example under consideration, and this is owing to the spherical symmetry of the perturbation assumed in this section. We cannot expect the local perturbation created by plastic deformation to have a spherical symmetry, so that our example would not be typical for the general case.

3

The results of the preceding section are susceptible of considerable generalization. In this section, an infinitely extended body with a local perturbation of general character and no forces at infinity will be considered. The action of the local distortion will be replaced by a system of volume forces $f(r)$, confined within a volume of atomic order of magnitude. The resultant force,

$$\int f(r)dv,$$

must vanish if there are no boundary stresses. The laws of isotropic elasticity will again be used.

This method differs from that of Section 2, where the distorted zone was replaced by a cavity, in that the atomic configuration within the distorted zone is replaced by one which is formally in agreement with elastic equilibrium and the fictitious volume force. However, because of the small number of these atoms, no appreciable difference between the two methods should arise.

If the displacement $u(r)$ is represented by a Fourier integral

$$u(r) = \int U(R) \exp(-2\pi iR \cdot r)dV, \quad (17)$$

then the inversion of Eq. (17) is Eq. (6a). By differentiating under the integral sign, we obtain

from Eq. (17):

$$\Delta u = -4\pi^2 \int R^2 U \exp(-2\pi iR \cdot r)dV, \quad (18)$$

grad div u

$$= -4\pi^2 \int R \cdot (R \cdot U) \exp(-2\pi iR \cdot r)dV. \quad (19)$$

The force function $f(r)$ will also be represented by a Fourier integral:

$$f(r) = \int F(R) \exp(2\pi iR \cdot r)dV, \quad (20)$$

with the inversion:

$$F(R) = \int f(r) \exp(-2\pi iR \cdot r)dv. \quad (21)$$

The equation of elastic equilibrium:

$$\mu\Delta u + (\lambda+\mu) \text{ grad div } u + \rho f = 0, \quad (22)$$

becomes, by Eqs. (18)–(20):

$$\int \exp(-2\pi iR \cdot r)$$

$$\times [-4\pi^2\mu R^2 U - 4\pi^2 R \cdot (R \cdot U) + \rho F]dV = 0. \quad (23)$$

By virtue of a general theorem, the transform must vanish:

$$\mu R^2 U + (\lambda+\mu)R \cdot (R \cdot U) = \frac{\rho}{4\pi^2}F. \quad (24)$$

The solution of this vector equation is:

$$U = \frac{\rho}{4\pi^2 R^4}\left(\frac{R \times (F \times R)}{\mu} + \frac{R \cdot (F \cdot R)}{\lambda+2\mu}\right). \quad (25)$$

We are interested in the behavior of U at small values of $|R|$. Expansion of Eq. (21) yields:

$$F = \int f dv + 2\pi i \int (R \cdot r)f dv + \cdots. \quad (26)$$

The first term is the resultant force, and therefore, vanishes. Introducing the expansion (26) into Eq. (25), it can be seen that U behaves like $1/R$ for small values of R.

This is the generalization of the result of Section 2. In particular, it can be seen from

Eqs. (5) and (6a) that near the lattice point (000), the scattering amplitude and consequently the intensity tend toward a constant value, in agreement with Guinier's observations.

The results of this section are valid only for infinitely extended crystal grains. When the grain is finite, but large enough to give rise to sharp lines, the statements of this section remain valid only for points well outside the line, as was shown in Section 2.

Near a lattice point A_h, the scattering amplitude will be given by

$$G_1 = \frac{2\pi i}{v} |A_h| \cos (A_h, U) \cdot |U(R - A_h)|. \qquad (27)$$

Now, if the force system f has a privileged crystallographic direction, then we must expect to obtain different scattering near different lattice points of similar absolute distance $|A_h|$, because of the direction cosine appearing in Eq. (27). Conversely, observations of the disorder scattering near different lines should be able to show the crystallographic symmetry of distortions.

A disorder scattering of the type under consideration must affect the measured line intensity and line width. However, conditions are more complex within the line itself, because the grain size and the slowly variable stresses account for part of the line broadening.[6]

Special Cases of Predissociation

B. ROSEN

Department of Astrophysics, University of Liége, Liége, Belgium

(Received July 27, 1945)

A study of the AlO spectrum indicates that a predissociation of the type one b takes place in the lower electronic state of the green system. It is suggested that the γ- and ϵ-bands of NO do not belong to a single system; the γ system shows a strong perturbation of the $v'=4$ level. An accidental predissociation of the vibrational type is found in the spectrum of Te_2, and the analogy of the three molecules S_2, Se_2, and Te_2 is strengthened.

AlO

ONLY a few examples of predissociation involving the lower state of a molecule are known, among which the best studied case is that of HgH. However, in the type III of predissociation (by rotation) exhibited by HgH the widening of the predissociated levels is such that they cannot be observed. Holst[1] has reported predissociation effects in two systems of emission bands of AlH due to transitions ending on the unstable $^1\Pi$ level. But, so far as we know, this example has not been studied in detail. The observation of the predissociated lines in the above-mentioned examples is difficult on high dispersion spectrograms, on account of the intensity drop in the centers of the lines.

It is well known that, as a result of the rise in total absorption in the incompletely resolved

predissociated lines (Loomis and Fuller),[2] predissociation may, under certain conditions be observed in absorption even with low dispersion. This criterion has been applied previously to the investigation of induced predissociation. In the case of natural predissociation, the criterion was first applied to the H_2 spectrum by Beutler, Deubner, and Jünger,[3] and to the S_2 spectrum by Rosen and Neven.[4] The latter example has recently been investigated in detail by Herzberg and Mundie.[5]

In emission, the widening of the lines of incompletely resolved bands manifests itself in different manners according to the position of

[1] W. Holst, Thesis (Trondheim, 1936).

[2] F. Loomis and H. Fuller, Phys. Rev. **39**, 180 (1932).

[3] H. Beutler, A. Deubner, and H. O. Jünger, Zeits. f. Physik **98**, 181 (1935).

[4] B. Rosen and L. Neven, Comptes rendus **203**, 662 (1936); J. Chim. Phys. **35**, 58 (1938).

[5] G. Herzberg and L. C. Mundie, Phys. Rev. **8**, 263 (1940).