X-RAY DIFFRACTION UNDER CONDITIONS OF THE SPATIALLY-INHOMOGENEOUS DYNAMIC PROBLEM

I. Sh. Slobodetskii, F. N. Chukhovskii, and V. L. Indenbom
Crystallography Institute, USSR Academy of Sciences
Submitted 25 March 1968
ZhETF Pis. Red. 8, No. 2, 90 - 94 (20 July 1968)

Analysis of the x-ray picture of lattice defects and distortion fields requires the solution of spatially-inhomogeneous problems that lie outside the scope of the known dynamic theory of propagation of x-rays. The customary formulation of the problem in this theory is limited to the case of a plane monochromatic wave incident on the surface of a semi-infinite ideal crystal [1,2]. If the crystal orientation is close to one of the Bragg positions, the wave field in the crystal is represented in the form of a superposition of two coherent plane waves, transmitted and diffracted. We shall show that the generalized two-wave approximation, in which wave packets are used in lieu of plane waves, yields solutions of a broad class of spatially-inhomogeneous problems.

1. We consider first a monochromatic spatially-inhomogeneous wave packet with frequency ω, incident on a plane surface of an ideal crystal. The wave field inside the crystal satisfies the Maxwell equation

$$\text{curl curl } \vec{E}(\omega, \vec{r}) = \kappa^2\varepsilon(\omega, \vec{r})\vec{E}(\omega, \vec{r}), \tag{1}$$

where $\kappa = \omega/c$, and the dielectric constant $\varepsilon(\omega, \vec{r})$ differs little from unity and is a periodic function of the coordinates. We expand the dielectric susceptibility $\chi = \varepsilon - 1$ in a series in the reciprocal-lattice vectors $\vec{k}_h$

$$\chi(\omega, \mathbf{r}) = \sum_h \chi_h \exp(i\mathbf{k}_h\mathbf{r}). \tag{2}$$

Near the Bragg position corresponding to the vector $\vec{k}_1$, we seek the solution of (1) in the form of a sum of two wave packets

$$\mathbf{E} = \mathbf{E}_0 \exp[i(\kappa\mathbf{r} + \kappa\frac{\chi_0}{2}\mathbf{nr})] + \mathbf{E}_1\exp\{i[(\kappa + \mathbf{k}_1)\mathbf{r} + \kappa\frac{\chi_0}{2}\mathbf{nr}]\}, \tag{3}$$

where $\vec{E}_0(\omega, \vec{r})$ and $\vec{E}_1(\omega, \vec{r})$ are slowly varying functions of the coordinates. Let us consider for simplicity the symmetrical case of Laue diffraction, when $\vec{k}_1$ is perpendicular to the normal $\vec{n}$ to the crystal surface. Going over, as usual, from the vector equations (1) to scalar ones and taking the symmetry of the problem into account, we obtain for the amplitudes $\vec{E}_0(\omega, \vec{r})$ and $\vec{E}_1(\omega, \vec{r})$ in the quasiclassical approximation

$$2i\left(\frac{\partial E_0}{\partial z} + \frac{\partial E_0}{\partial x}\right) = -\chi_1 E_1; \quad 2i\left(\frac{\partial E_1}{\partial z} - \frac{\partial E_1}{\partial x}\right) = -\chi_1 E_0 + \alpha E_1. \tag{4}$$

We have introduced here the dimensionless coordinates $z = \vec{r}\cdot\vec{n}\kappa/\cos\theta$ and $x = \vec{r}\cdot\vec{k}_1\kappa/\vec{k}_1\sin\theta$, θ is the Bragg angle, $\alpha = (2\kappa\vec{k}_1 + \vec{k}_1^2)/\kappa^2$ determines the deviation of the plane wave with wave vector κ from the Bragg condition, and χ_0 and χ_1 are the parameters of the ordinary dynamic theory, which are defined in (2). We note that in general the waves propagating in the crystal correspond to different "weak" reflections $\vec{k}_h$ with $h \neq 1$, as well as inelastically scattered waves, but the influence of these waves on the main radiation field (3) can in principle be taken into account by perturbation theory, leading only to a renormalization of of the parameters χ_0 and χ_1 (see, e.g., [3]).

Supplementing the system (4) with the boundary conditions

$$E_0(x, y, 0) = \mathcal{E}(x, y); \quad E_1(x, y, 0) = 0 \tag{5}$$

we get the general solution for the field of the diffracted wave in the form of the convolution [4]

$$E_1(\mathbf{r}) = i\,\frac{\chi_1}{2}\,\mathcal{E}(x, y) * G(x, z), \tag{6}$$

where the influence function G(x, z) differs from zero only in the region $|x| < z$, where

$$G(x, z) = \frac{1}{2}\, J_0\!\left(\frac{\chi_1}{2}\sqrt{z^2 - x^2}\right)\exp\left[-\frac{i\alpha}{4}(z - x)\right] \tag{7}$$

($J_0(\xi)$ - Bessel function of zero order).

The field of the transmitted wave is determined from the second equation of (4).

2. Slit image. Let a plane monochromatic wave of unit amplitude be incident on a crystal having on its surface a slit $|x| \le a$. In this case it follows from (6) and (7) that

$$E_1(x, z) = \frac{i\chi_1}{4}\int\limits_{\max(x-z,\,-a)}^{\min(x+z,\,a)} d\xi\, J_0\!\left(\frac{\chi_1}{2}\sqrt{z^2 - (x - \xi)^2}\right)\exp\left[-\frac{i\alpha}{4}(z - x + \xi)\right]. \tag{8}$$

When $a \to \infty$ formula (8) goes over naturally into the usual solution of the dynamic problem

$$E_1(z) = i\left\{\sin\!\left(\frac{\chi_1 z}{2}\sqrt{1 + (\alpha/2\chi_1)^2}\right) \Big/ \sqrt{1 + (\alpha/2\chi_1)^2}\right\}\exp\!\left(-i\frac{\alpha z}{4}\right). \tag{9}$$

If the slit half-width a is larger than the crystal thickness t, then the solution (9) is valid only for the central "uniformly illuminated" region $|x| < a - t$, and in the "half-shadow" fringes at the edges of the image, $a + t > |x| > a - t$, there should be observed intensity oscillations that are symmetrical about the center of the slit. Figure 1 shows examples of the intensity distribution at the edge of the image of the slit for $\alpha = 0$ and for different values of the parameter $\chi_1 t$, which determines the intensity at the central section.

If the slit half-width is smaller than the crystal thickness, the uniformly illuminated region vanishes, and the regions of intensity oscillations become superimposed, the intensity maxima shifting towards the edge of the image with decreasing slit width or with increasing crystal thickness (Fig. 2). In the limiting case $\chi_1\sqrt{ta} \ll 1$ and $\alpha a \ll 1$ the image of the slit is closely described by the square of the Bessel function $J_0(\chi_1/2\sqrt{t^2 - x^2})$, which agrees with the results of Kata [5], who calculated the image of an infinitesimally narrow slit in the approximation of spherical wave emerging from the slit. We note that the slit-image details illustrated in Fig. 2 have been lost sight of in a paper by Authier et al. [6], who solved the system (4) numerically.

3. Image of a real crystal. The influence function (7) can be used to construct in the

Born approximation a general solution of the dynamic problem of propagation of x-rays in a distorted crystal, when the dielectric susceptibility is no longer a periodic function of the coordinates. Assuming that the crystal is only slightly distorted, we replace χ_h by $\chi_h \exp(i\vec{u}\cdot\vec{k}_h)$, where $\vec{u}(\vec{r})$ is the slowly-varying dispacement field. Then Eq. (4) remains formally valid if α is replaced by $\alpha + 2(\partial/\partial z - \partial/\partial x)(\vec{k}_1\cdot\vec{u})$, but becomes an equation with variable coefficients. In the first approximation $E_1 = (E_1^0 + E_1') \exp(i\vec{k}_1\cdot\vec{u})$, where $E_1^0(z)$ is

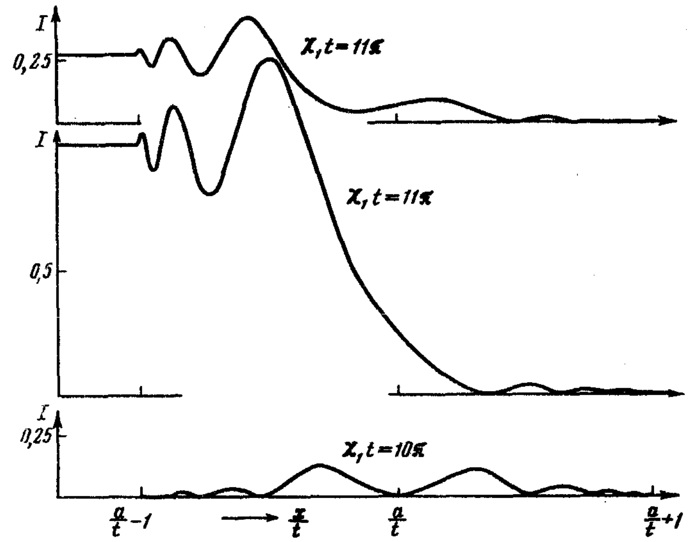

Fig. 1. Diffraction image of broad slit $a > t$ at the exact Bragg position of the non-absorbing crystal, $\alpha = 0$, as a function of the quantity $\chi_1 t$.

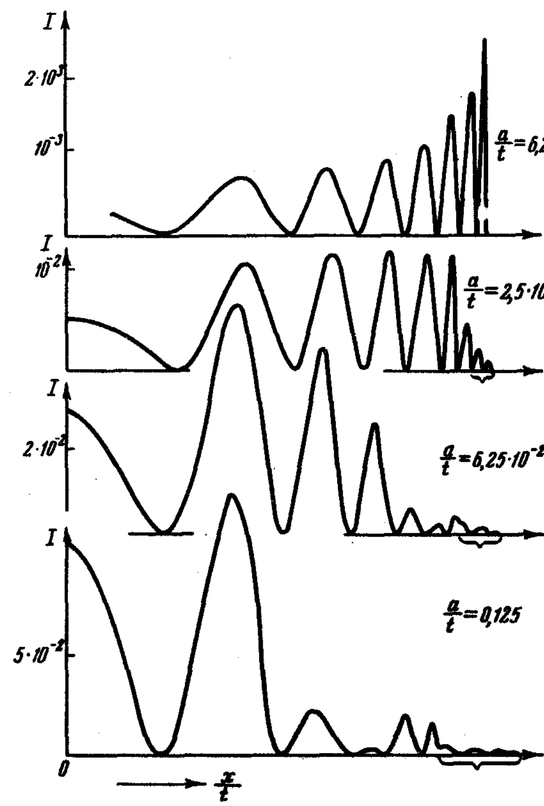

Fig. 2. Diffraction image of narrow slit $a < t$ at the exact Bragg position of the non-absorbing crystal, $\alpha = 0$, as a function of the ratio a/t. The braces in the figure denote the region

the solution of the ordinary dynamic problem, and $E_1'(\vec{r})$ is given by the convolution

$$E_1'(\mathbf{r}) = -i\left\{\left(\frac{\partial}{\partial z}+\frac{\partial}{\partial x}\right) E_1^{\circ}\left(\frac{\partial}{\partial z}-\frac{\partial}{\partial x}\right)(\mathbf{k}_1 \mathbf{u})\right\} * G(x,\ z). \tag{10}$$

As expected, unlike the well-known case of diffraction electron-microscope images, the connection between the displacement field $\vec{u}(\vec{r})$ and its x-ray image $E_1'(\vec{r})$ is nonlocal. It is not surprising that different attempts at a local interpretation of the x-ray images of distortion fields were unsuccessful.

The authors are grateful to Professor Z. G. Pinsker for continous interest in the work, valuable remarks, and a discussion of the results.

[1] R. W. James, Solid State Physics 15, N. Y., 1963.
[2] B. W. Batterman and H. Cole, Revs. Modern Phys. 36, 681 (1964).
[3] A. M. Afanas'ev and Yu. M. Kagan, Zh. Eksp. Teor. Fiz. 52, 191 (1967) [Sov. Phys.-JETP 25, 124 (1967)].
[4] R. Courant, Partial Differential Equations, Wiley, 1962.
[5] N. Kato, Acta Cryst. 14, 627 (1961).
[6] A. Authier, C. Malgrange, and M. Tournarie, Acta Cryst. A24, 126 (1968).

NEUTRINOS IN ANISOTROPIC COSMOLOGICAL SOLUTIONS

A. G. Doroshkevich, Ya. B. Zel'dovich, and I. D. Novikov
Applied Mathematics Institute, USSR Academy of Sciences
Submitted 21 May 1968
ZhETF Pis. Red. 8, No. 2, 95 - 99 (20 July 1968)

The singular behavior of the weakly-interacting neutrinos in anisotropic and homogeneous cosmological models and the appreciable influence of these particles on the dynamics of the models themselves were noted in [1, 2].

The hypothesis was advanced that the evolution is naturally subdivided into the following stages: 1) practically total equilibrium of all particles, including the neutrinos, and 2) the stage of free neutrinos, the momentum of which increases by virtue of the "blue shift" produced by compression along one of the axes.

Misner [3, 4] proposes that the equilibrium period is followed by a stage in which the neutrino influence can be described by using the concept of viscosity.

For this purpose it is obviously necessary that the neutrino mean free path not be too large; the characteristic length is ct, where the time t is reckoned from the singularity. Misner arrives at the conclusion that the viscosity, causing heating (entropy growth) of the matter, eliminates the second stage of free neutrinos in the strongly anisotropic expansion phase. According to Misner, the neutrinos become free when the expansion anisotropy is no longer large.

The two different points of view, Misner's (M) and ours (O), lead to different laws for the time variations of such quantities as the temperature (M: $T \sim t^{-1/5}$, O - $T \sim t^{-5/18}$), the entropy (M: $S \sim t^{2/5}$, O: $S \sim t^{1/6}$), and particularly the energy of one neutrino (M: $E_1 \sim T \sim t^{-1/5}$, O: $E_1 \sim t^{1/9}$. The total energy density of the neutrinos is proportional in both cases to the energy density of the strongly-interacting particles