The theory of resonant coherent scattering of γ radiation by a regular array of nuclei in a crystal in the case of multiple diffraction

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We propose a general theory of coherent nuclear resonant and electronic scattering of Mössbauer γ radiation by a perfect crystal in the case of two or more strong reflected beams, i.e., in the case of multiple diffraction, when the Braff conditions hold simultaneously for several sets of crystal planes. The geometry of possible experiments is discussed. A general method is suggested, enabling one to calculate the energy and angular dependence of observed intensities of diffracted beams for any geometry of the experiment, any crystal thickness, and hyperfine splitting of nuclear levels. As an example of an application of the theory, we consider the case of three-beam coplanar Bragg diffraction of Mössbauer radiation of energy 14.4 KeV in $^{57}FeBO_3$ crystals.

1. INTRODUCTION

Multiple diffraction of x rays is well known in x-ray optics. The effect was predicted by Ewald in the first half of this century almost simultaneously with the prediction of diffraction itself. In recent decades, research has been mainly concentrated on two remarkable features of multiple diffraction, namely the possibility of directly measuring the phase of the x-ray scattering amplitude[1,2] and the enhancement of anomalous transmission through an absorbing crystal.[1,3–5] The latter effect is related to Bloch waves with a special spatial structure, which has the crystal symmetry and in which the points of the radiation field lattice coincide with those of the crystal lattice.[3,5] Though the effect was predicted more than a quarter of a century ago,[4,5] numerous attempts to find it, using available x-ray sources, have been unsuccessful. Convincing experimental evidence has been obtained quite recently[6] by means of a synchrotron radiation source.

Making use of the synchrotron radiation solves the main problem in experimental studies of multiple diffraction, namely the lack of intensity. In fact, to observe spectrally stable (systematic) multiple diffraction in its pure form, the incident beam should be parallel, with an angular divergence of no more than 1″ in two mutually orthogonal planes. Under laboratory conditions, the sources are separate atoms radiating a spherical wave. The intensity of the necessary plane wave component comprises only a small fraction of the total intensity, since the radiation from different atoms is incoherent. The intensity problem becomes essentially intractable for laboratory sources of Mössbauer radiation. That is why no attempts have been made thus far to observe the multiple diffraction of resonant γ radiation by crystal nuclei, while two-beam diffraction has been sufficiently well studied both theoretically[7,8] and experimentally, making use of ordinary[9,10] and synchrotron radiation[11] sources.

Only recently has it become possible to study experimentally the multiple diffraction of resonant nuclear γ radiation in perfect crystals containing Mössbauer isotopes (mainly ^{57}Fe) due to rapid progress in making use of high-intensity synchrotron sources of a new type, radiating parallel beams. As an example, we point to Ref. 12, where a diffracted beam intensity of 20,000 photons/s is reported for the nuclear 777 Bragg diffraction by a Fe_2O_3 crystal. As a source, the x-ray undulator of the TRISTAN storage ring (KEK, Tsukuba) was used.

Thus, the task of constructing a theory of multiple diffraction of resonant γ radiation becomes not only interesting, but also quite urgent, as a preliminary theoretical analysis could be very helpful in setting up fairly sophisticated experiments. From a physical standpoint, the multiple diffraction of Mössbauer γ radiation seems to be of more interest than that of x rays, since the nuclear resonant scattering depends on two additional parameters—the distance from resonance (in the case of energy resolution) or the time elapsed from the instant of radiation emission (in the case of time resolution), and the direction of the quantization axis in the case of hyperfine splitting of nuclear levels.

From the standpoint of full use of the radiation intensity, it is worth considering so-called coplanar three-beam diffraction, where the incident and two diffracted beams lie in the same plane. In this case, two-beam diffraction is impossible, and three-beam diffraction is realized instead, but we have the same requirements on the angular divergence of the incident beam as in the case of two-beam diffraction. But these cases do not exist systematically, because of the lack of free parameters to satisfy two Bragg conditions. For their realization, a certain relation between the radiation wavelength and distances between the planes for two sets of crystal planes must automatically hold, if only approximately. For a given $^{57}FeBO_3$ crystal and the Mössbauer radiation with energy 14.4 keV, several such cases have been found by van Bürck.[13]

In the present paper, the author proposes a theory and calculation methods for the multiple diffraction of resonant γ radiation, using the experience gained while studying the multiple diffraction of x rays. So far, there has only been two theoretical papers treating the problem,[14,15] where es-

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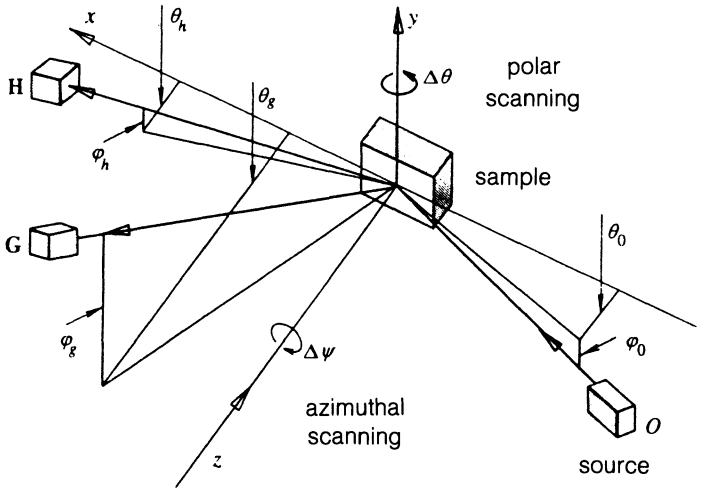

FIG. 1. Geometry of a possible experiment.

sentially the same special case of symmetric Laue diffraction with the Bragg conditions satisfied exactly has been considered, using the analytic expressions for wave fields found earlier in Refs. 4 and 5 and neglecting hyperfine splitting. The general case, which includes the Bragg geometry, hyperfine splitting, and angular dependence, can be analyzed only by robust numerical methods. In what follows we discuss the geometry of reflection-type (Bragg) diffraction, formulate the problem in a form convenient for numerical solution, and consider coplanar cases of three-beam diffraction.

2. GEOMETRIC CONDITIONS

Plane wave diffraction in a perfect crystal can be regarded as elastic scattering, with the wave vector $\mathbf{k}_0$ of the incident wave changing by an arbitrary vector $\mathbf{h}$ of the reciprocal lattice and the radiation frequency remaining the same. This means that the absolute value of the wave vector k_h of the "scattered" wave does not change, i.e.,

$$\mathbf{k}_h=\mathbf{k}_0+\mathbf{h}, \quad k_h^2=k_0^2. \tag{1}$$

In the two-beam case, this condition can be satisfied in only one way for a given vector $\mathbf{h}$. The three-beam case is realized when two vectors of the reciprocal lattice, for example $\mathbf{h}$ and $\mathbf{g}$, simultaneously satisfy the Bragg condition (1), namely

$$\begin{aligned}&\mathbf{k}_h=\mathbf{k}_0+\mathbf{h}, \quad k_h^2=k_0^2,\\ &\mathbf{k}_g=\mathbf{k}_0+\mathbf{g}, \quad k_g^2=k_0^2.\end{aligned} \tag{2}$$

Expressions (2) can be regarded as a set of equations for $\mathbf{k}_0$, which for the given radiation wavelength $\lambda=2\pi/k_0$ has only one solution and unambiguously determines the direction of $\mathbf{k}_0$ with respect to the crystal lattice.

Nevertheless, due to a high crystal symmetry, in some cases we have degeneracy, and along with the given vectors of the reciprocal lattice, Eq. (1) is satisfied by other vectors. Three-beam diffraction is then impossible and, instead, multiple diffraction with more than three beams >3 occurs. We can imagine this in the following intuitive way. Two vectors of the reciprocal lattice can be inscribed in the circle that passes through three reciprocal lattice points and comprises a cross section of the Ewald sphere. If there are other reciprocal lattice points on this circle, this is just a spectrally stable degeneracy, i.e., degeneracy is independent of the length of the wave vector $\mathbf{k}_0$, which is the Ewald sphere radius. For a certain relation between the wavelength and the crystal lattice parameter, a spectrally unstable degeneracy could occur. A special case of spectrally unstable degeneracy of the two-beam case into the three- (or more-) beam one is the coplanar case, where the vector $\mathbf{k}_0$ lies in the plane of the reciprocal lattice vectors $\mathbf{h}$ and $\mathbf{g}$.

Consider, for example, two asymmetric Bragg reflections in which all the beams are on the same side of the crystal. Figure 1 shows the standard rotation axes of the crystal line sample and direction angles for the incident and diffracted beams. The xz plane is chosen perpendicular to the crystal surface. The angles θ are formed by the x axis and the projections of the wave vectors onto the xz plane. The angles φ are the angles between these same vectors and their projections. From the point of view of setting up the experiment, the first task is to find the angles θ and φ for the given configuration. These angles relate the Cartesian coordinates of the wave vectors in the following way:

$$\begin{aligned}&\mathbf{k}_0=K[\mathbf{X}\cos\varphi_0\cos\theta_0+\mathbf{Y}\sin\varphi_0+\mathbf{Z}\cos\varphi_0\sin\theta_0],\\ &\mathbf{k}_f=K[\mathbf{X}\cos\varphi_f\cos\theta_f+\mathbf{Y}\sin\varphi_f+\mathbf{Z}\cos\varphi_f\sin\theta_f,\end{aligned} \tag{3}$$

where $f=h,g$, $K=2\pi/\lambda$, and $\mathbf{X}$, $\mathbf{Y}$, and $\mathbf{Z}$ are the unit vectors in the direction of the corresponding axes.

If the Cartesian coordinates of the reciprocal lattice vectors $\mathbf{h}$ and $\mathbf{g}$ are known for the given coordinate system (see Fig. 1), then the six angles θ_0, φ_0, θ_h, φ_h, θ_g, and φ_g can be found from six equations following from (2). Thus, for the vector $\mathbf{h}$ we have

$$\begin{aligned}&h_x/K=\cos\varphi_h\cos\theta_h-\cos\varphi_0\cos\theta_0,\\ &h_y/K=\sin\varphi_h-\sin\varphi_0,\\ &h_z/K=-\cos\varphi_h\sin\theta_h-\cos\varphi_0\sin\theta_0.\end{aligned} \tag{4}$$

Similar equations can be written for the vector **g**.

The z axis of the Cartesian coordinate system is unambiguously given by the normal to the crystal, but in the most general case we are free to choose the x and y axes. We can rotate the crystal about the normal to the surface until the vector **h** is in the xz plane. Then $h_y=0$ and, in accordance with (4), $\varphi_h=\varphi_0$. Consider next a simple but important case, in which h_x is also zero (symmetric reflection). In this case $\theta_h=\theta_0$, and since we have the additional possibility of rotating about the vector **h**, we can set $\varphi_h=\varphi_0=0$. The other angles are determined in an invariant form as follows:

$$\sin\theta_0=h/(2K),\quad \operatorname{tg}\theta_g=A\cos\theta_0/(1-B^2),$$
$$\cos\varphi_g=A/\sin\theta_g, \tag{5}$$

where

$$A=(2\mathbf{hg}-h^2)/(2hK),\quad B^2=(2g^2+h^2-2\mathbf{hg})/(2K)^2. \tag{6}$$

The coplanar case corresponds to $\varphi_g=0$. According to (5) and (6), the condition

$$\frac{1}{(2K)^2}=\frac{h^2g^2-(\mathbf{hg})^2}{h^2g^2(\mathbf{h}-\mathbf{g})^2}=\frac{\sin^2\Phi_{hg}}{(\mathbf{h}-\mathbf{g})^2} \tag{7}$$

must be fulfilled, and we also have the formula

$$\sin\left(\frac{\theta_0+\theta_g}{2}\right)=\frac{g}{2K}. \tag{8}$$

Consider now the parameters characterizing the degree of violation of the diffraction conditions, i.e., the degree to which the Bragg conditions are not satisfied. There are two ways of doing so. Either we rotate the crystal for the given beam directions, which is usually done in an experiment, or we vary the incident beam direction. The latter is convenient when taking into account the angular divergence of the incident beam. In the first case we change the direction of the reciprocal lattice vectors **h** and **g**, while the direction of the incident beam remains constant. We have

$$\alpha_f=(k_f^2-k_0^2)/K^2\approx 2\mathbf{k}_f\Delta\mathbf{f}/K^2, \tag{9}$$

where $\mathbf{f}=\mathbf{h},\mathbf{g}$. The standard rotation axes are the y (polar angular scanning) and z axes (azimuthal scanning), as shown in Fig. 1. Using the well known formula for the variation of the vector **f** when we rotate through a small angle $\Delta\phi$ about the **l** axis, $\Delta\mathbf{f}=(\mathbf{l}\times\mathbf{f})\Delta\phi$, we obtain

$$\Delta\mathbf{h}=\mathbf{X}h_z\Delta\theta,$$
$$\Delta\mathbf{g}=\mathbf{X}(g_z\Delta\theta-g_y\Delta\psi)+\mathbf{Y}g_z\Delta\psi-\mathbf{Z}g_x\Delta\theta. \tag{10}$$

Substituting (10) into (9), we find

$$\alpha_h=-2\Delta\theta\sin 2\theta_0,$$
$$\alpha_g=-2\Delta\theta\sin(\theta_0+\theta_g)\cos\varphi_g-2\Delta\psi\cos\theta_0\sin\varphi_g. \tag{11}$$

In the coplanar case $\varphi_g=0$, and both parameters depend only on $\Delta\theta$.

To allow for the angular divergence and nonmonochromaticity of the incident beam, it is convenient to add an increment **q** to the vector $\mathbf{k}_0(\mathbf{k}_0\to\mathbf{k}_0+\mathbf{q})$ for fixed reciprocal lattice vectors. Then

$$\alpha_f=(k_f^2-k_0^2)/K^2\approx 2\mathbf{fq}/K^2. \tag{12}$$

Introducing again the angle $\Delta\theta$ in the xz plane, the angle $\Delta\varphi$ in the $(\mathbf{k}_0,\mathbf{Y})$ plane, and the relative frequency variation $\Delta\omega/\omega$, we can write the vector **q** in the form

$$\mathbf{q}=K[(-\mathbf{X}\sin\theta_0+\mathbf{Z}\cos\theta_0)\Delta\theta-\mathbf{Y}\Delta\varphi$$
$$+(\mathbf{X}\cos\theta_0+\mathbf{Z}\sin\theta_0)(\Delta\omega/\omega)]. \tag{13}$$

Substituting (13) and (4) into (12), we find

$$\alpha_h=-2\Delta\theta\sin 2\theta_0-4(\Delta\omega/\omega)\sin^2\theta_0,$$
$$\alpha_g=-2\Delta\theta\sin(\theta_0+\theta_g)\cos\varphi_g-2\Delta\varphi\sin\varphi_g$$
$$-2(\Delta\omega/\omega)[1-\cos(\theta_0+\theta_g)\cos\varphi_g]. \tag{14}$$

Comparing (11) and (14), we see that polar scanning and horizontal beam divergence lead to the same result for α_f. Azimuthal scanning and vertical divergence lead to results which differ only by a scale factor $\cos\theta_0$.

As follows from (14), in the systematic case of diffraction ($\varphi_g\neq 0$) the variation of the radiation frequency can be compensated for by the angle variations $\Delta\theta$ and $\Delta\varphi$, and the conditions $\alpha_h=\alpha_g=0$ can be fulfilled over a wide range of wavelengths. In the coplanar case ($\varphi_g=0$), only the angle $\Delta\theta$ affects the Bragg conditions and

$$\alpha_h=-2\sin 2\theta_0[\Delta\theta+(\Delta\omega/\omega)\operatorname{tg}\theta_0],$$
$$\alpha_g=-2\sin(\theta_0+\theta_g)\left(\Delta\theta+\frac{\Delta\omega}{\omega}\operatorname{tg}\frac{\theta_0+\theta_g}{2}\right). \tag{15}$$

According to (15), vertical beam divergence does not affect the Bragg conditions, and the radiation frequency shift (or the variation of the crystal lattice parameter—for example when the temperature is changed) leads to a decomposition of three-beam diffraction into two-beam diffractions, i.e., the conditions $\alpha_h=0$ and $\alpha_g=0$ are satisfied for different values of $\Delta\theta$. This difference is given by

$$\Delta\theta_h-\Delta\theta_g=\left(\operatorname{tg}\frac{\theta_0+\theta_g}{2}-\operatorname{tg}\theta_0\right)\frac{\Delta\omega}{\omega}. \tag{16}$$

From an experimental standpoint, the coplanar cases are also of interest, in that although the condition (7) is not satisfied exactly and the three-beam case is not feasible, it is possible nevertheless, to get two different cases of two-beam diffrection in one experimental setup and with one angular scan.

3. GENERAL THEORY

To formulate the theory, we use the approach suggested by Kagan and Afanas'ev.[16] The electromagnetic field in a crystal is described by Maxwell's equation for the Fourier component $\mathbf{E}(\mathbf{k},\omega)$ of the electric field:

$$(k^2-K^2)\mathbf{E}(\mathbf{k},\omega)-\mathbf{k}[\mathbf{kE}(\mathbf{k},\omega)]=(4\pi i\omega/c^2)\mathbf{j}(\mathbf{k},\omega), \tag{17}$$

where $K=\omega/c=2\pi/\lambda$, λ is the wavelength of the radiation, c is the speed of light, and $\mathbf{j}(\mathbf{k},\omega)$ is the Fourier component of the induced current density, equal to a quantum mechanical average of the Fourier component of the current density operator over the ground state of the crystal in the presence of an external magnetic field. Allowing for the crystal lattice periodicity, in the linear approximation, in $\mathbf{E}$ we have in the most general case

$$j^i(\mathbf{k}_0,\omega)=(c^2K^2/4\pi\, i\omega)\sum_{mj} g_\omega^{ij}(\mathbf{k}_0,\mathbf{k}_m)E^j(\mathbf{k}_m,\omega), \tag{18}$$

where $\mathbf{k}_m=\mathbf{k}_0+\mathbf{h}_m$, $\mathbf{h}_m$ is the reciprocal lattice vector multiplied by 2π, and $g_\omega^{ij}(\mathbf{k}_0,\mathbf{k}_m)$ is the Fourier component of the polarizability tensor multiplied by 4π, in which all possible processes, both of resonant interaction of γ radiation with nuclei and of interaction with atomic electrons, are taken into account.

Let a plane wave with the wave vector $\mathbf{k}_0$ satisfy the multiple diffraction conditions. In a crystal having the shape of a plate the vector $\mathbf{k}_0$ can change only its z component (along the normal to the surface):

$$\mathbf{k}_0\to\mathbf{k}_0+K\frac{\varepsilon}{2\gamma_0}Z,\quad \gamma_0=\frac{k_{0z}}{K}. \tag{19}$$

Since the interaction of γ radiation with the crystal is small, in the linear approximation the electric field remains transverse. This enables us to introduce two scalar amplitudes for each beam:

$$\mathbf{E}(\mathbf{k}_m,\omega)=\sum_s E_{ms}\mathbf{e}_{ms}, \tag{20}$$

where the subscript $s=\pi,\sigma$ gives the polarization state, $\mathbf{e}_{ms}$ is the polarization unit vector, the vectors $\mathbf{e}_{m\pi}$, $\mathbf{e}_{m\sigma}$ and $\mathbf{s}_m=\mathbf{k}_m/K$ form a right-hand rectangular basis, and the index $m=0,h,g,\ldots$ labels only strong waves satisfying the Bragg conditions (1).

Substituting (18) and (19) into (17), allowing for (20) and neglecting all weak waves, the problem reduces to finding the eigenvalues and eigenvectors of the matrix whose elements are the amplitudes of kinematic scattering:

$$\varepsilon E_{ms}=\sum_{m's'} G^{ss'}_{mm'}E_{m's'}, \tag{21}$$

where

$$G^{ss'}_{mm'}=\beta_m[g^{ss'}_{mm'}-\alpha_m\delta^{ss'}_{mm'}],\quad \beta_m=\gamma_0/\gamma_m,$$
$$\gamma_m=k_{mz}/K, \tag{22}$$
$$g^{ss'}_{mm'}=\sum_{ij} e^i_{ms}g_\omega^{ij}(\mathbf{k}_m,\mathbf{k}_{m'})e^j_{m's'}=p^{ss'}_{mm'}(\omega)+\chi^{ss'}_{mm'},$$

$\delta^{ss'}_{mm'}$ is the Kronecker delta, and the parameters α_m giving the degree to which the Bragg conditions are not satisfied were considered in the previous section.

The matrix $p^{ss'}_{mm'}(\omega)$ describes the resonant scattering of γ rays. For the hyperfine splitting of the ground and excited nuclear levels,

$$p^{ss'}_{mm'}(\omega)=\sum_{ge} A^{ss'}_{mm'}(ge)\frac{\Gamma/2}{\hbar(\omega-\omega_{eg})+i\Gamma/2}, \tag{23}$$

where

$$A^{ss'}_{mm'}(ge)=\frac{8\pi\eta}{\omega^2V_0\Gamma_0(2I_0+1)}\sum_a \times\exp\{i(\mathbf{k}_{m'}-\mathbf{k}_m)\mathbf{r}_a\}f^{1/2}_{am}f^{1/2}_{am'} \times\langle g|\hat{j}^s_a(\mathbf{k}_m)|e\rangle\langle e|\hat{j}^{*s'}_a(\mathbf{k}_{m'})|g\rangle. \tag{24}$$

Here the index g labels the levels of the ground state, while the index e labels those of the excited state; I_0 is the nuclear spin in the ground state, ω_{eg} are the frequencies of allowed transitions between the ground and excited states, Γ is the total line width allowing for inhomogeneous broadening, Γ_0 is the natural line width, V_0 is the unit cell volume, the subscript a denotes atoms inside the unit cell, $\mathbf{r}_a$ is the displacement of the ath atom, $f_{am}=\exp[-\langle(\mathbf{u}_a\mathbf{k}_m)^2\rangle]$ is the temperature-dependent Lamb–Mössbauer factor, $\mathbf{j}_a(\mathbf{k})$ is the Fourier component of the current density operator for the ath atom, and η is the concentration of the resonant isotope.

To calculate the matrix elements of the current density operator, we usually need to expand them in a multipole series. For the transitions from low-lying excited states, as a rule, the first term of the expansion is sufficient. In what follows we will consider only $M1$ transitions. In this case the current density operator has the form

$$\hat{\mathbf{j}}(\mathbf{k})=ic[\mathbf{k}\hat{\mathbf{m}}], \tag{25}$$

where $\hat{\mathbf{m}}$ is the operator of the magnetic dipole moment, whose matrix elements are[17]

$$\langle g|\hat{\mathbf{m}}|e\rangle=-i\left[\frac{3(2I+1)\Gamma_1}{4K^3}\right]^{1/2} \times(-1)^M\begin{pmatrix} I_0 & 1 & I \\ -M_g & M & M_e\end{pmatrix}\mathbf{n}_M. \tag{26}$$

Here I is the spin of the excited state, $\Gamma_1=\Gamma_0/(1+\alpha)$ is the line width related to the radiative transition, α is the conversion coefficient, $M=-1,0,1$ is the radiation "magnetic" quantum number, M_g and M_e are the quantum numbers of the projection of the nuclear spins in the ground and excited states onto the quantization axis (according to selection rules, only those transitions for which $M_g=M_e+M$ are allowed), $\mathbf{n}_0=\mathbf{n}_z$ is the unit vector in the direction of the quantum axis (internal magnetic field at nuclei), $\mathbf{n}_\pm=\mp(\mathbf{n}_x\pm i\mathbf{n}_y)/\sqrt{2}$ are mutually orthogonal unit vectors in the plane perpendicular to the quantization axis, and

$$\begin{pmatrix} I_0 & 1 & I \\ -M_g & M & M_e\end{pmatrix}$$

are $3j$ symbols.[18]

Substituting Eqs. (25) and (26) into (24), we find

$$A^{ss'}_{mm'}(ge)=-\frac{6\pi\eta}{(1+\alpha)V_0K^3}\frac{(2I+1)}{(2I_0+1)}\begin{pmatrix}I_0 & 1 & I\\ -M_g & M & M_e\end{pmatrix}^2$$

$$\times\sum_a \exp\{i(\mathbf{k}_{m'}-\mathbf{k}_m)\mathbf{r}_a\}f^{1/2}_{am}f^{1/2}_{am'}P^{ss'}_{mm'}(aM), \tag{27}$$

where

$$P^{ss'}_{mm'}(aM)=(\mathbf{m}_{ms}\mathbf{n}_M)(\mathbf{m}_{m's'}\mathbf{n}_M)^*,\quad \mathbf{m}_{ms}=[\mathbf{s}_m\mathbf{e}_{ms}]. \tag{28}$$

Here we use unit vectors $\mathbf{m}_{ms}$ of the magnetic field polarization, and the a-dependence is due to the fact that the directions of the quantization axis at different atoms may differ. It is convenient to express the polarization matrix in terms of the magnetic field direction at the nuclei. It is easily verified that[19]

$$P^{ss'}_{mm'}(aM)=\begin{cases}(\mathbf{m}_{ms}\mathbf{n}_0)(\mathbf{m}_{m's'}\mathbf{n}_0), & M=0\\ \{(\mathbf{m}_{ms}\mathbf{m}_{m's'})-(\mathbf{m}_{ms}\mathbf{n}_0)(\mathbf{m}_{m's'}\mathbf{n}_0)\\ \quad \mp i([\mathbf{m}_{ms}\mathbf{m}_{m's'}]\mathbf{n}_0)\}/2, & M=\pm 1.\end{cases} \tag{29}$$

The matrix $\chi^{ss'}_{mm'}$ describes the scattering of γ rays by atomic electrons. It depends only on the "momentum transfer" $\mathbf{k}_{m'}-\mathbf{k}_m$, which is equal to the reciprocal lattice vector $\mathbf{h}_{m'm}$. The dominant contribution comes from $E1$ scattering. In this case, as is well-known from x-ray scattering theory,[3]

$$\chi^{ss'}_{mm'}=(\mathbf{e}_{ms}\mathbf{e}_{m's'})\sum_a\left\{-\frac{4\pi r_0}{V_0K^2}[f_a(\mathbf{h}_{m'm})+\Delta f'_a]\right.$$

$$\left.+i\frac{1}{V_0K}\sigma^D_a\right\}\exp\{-i\mathbf{h}_{m'm}\mathbf{r}_a-W_a(\mathbf{h}_{m'm})\}. \tag{30}$$

Here $r_0=e^2/mc^2$, f_a is the form factor (the Fourier component of the atomic electron density), $\Delta f'_a$ is the dispersion correction to the form factor, σ^D_a is the dipole contribution to the photoabsorption cross section, $\exp(-W_a)$ is the Debye–Waller factor, and $W_a(\mathbf{h})=0.5\langle(\mathbf{u}_a\mathbf{h})^2\rangle$.

Consider now the problem of $N=$beam diffraction by a plate-shaped crystal in the most general case. Let the upper crystal surface diffract Laue-type plane waves for which $\gamma_m>0$, and the lower surface Bragg-type waves for which $\gamma_m<0$, with the amplitudes of these waves being known. Let us construct a vector D_{ms} from them. As a result of diffraction, the outgoing waves at the upper crystal surface are of the Bragg type, while the waves at the lower surface of the Laue type, and the amplitudes of these waves are to be found. Let us construct a vector R_{ms} from them, for which we need to find the matrix that transforms the vector $\mathbf{D}$ into the vector $\mathbf{R}$. The this end, as a first step, it is necessary to find all the solutions of the problem (21). In the N-beam case the matrix has the rank $2N$, and by $N=3$ this problem can only be solved numerically. As is well known, a matrix of rank $2N$ has $2N$ eigenvalues ε_j and eigenvectors E^j_{ms}.

A real field in the crystal is a superposition of these solutions with weights λ_j, which can be found from the boundary conditions. The latter, if we take into account the definitions introduced above, can be written in the form

$$\sum_j E^j_{ms}\exp(i\varepsilon_j l_m)\lambda_j=D_{ms}, \tag{31}$$

where $l_m=0$, if γ_m is positive, $l_m=Kt/2\gamma_0$ if γ_m is negative, and t is the crystal thickness. Upon calculating the degrees of excitation for the eigensolutions (Bloch waves), we can find the amplitudes of the diffracted waves:

$$R_{ms}=\sum_j E^j_{ms}\exp(i\varepsilon_j b_m)\lambda_j, \tag{32}$$

where $b_m=0$ if γ_m is negative, and $b_m=Kt/2\gamma_0$ if γ_m is positive.

These formulas give the solution of the problem implicitly. We find the explicit solution using matrix algebra. To make the notation simpler, we assume that the subscript m subsumes both the beam number and polarization, and instead of ms we will simply write m. The eigenvectors form the matrix E_{mj} of rank $2N$, and the amplitudes λ_j, D_m, and R_m are vectors in the same space. If we write them without subscripts, all additions and multiplications are understood to be generalized to a $2N$-dimensional-space. Equations (21), (31), and (32) can be written as follows:

$$E\cdot\varepsilon=G\cdot E,\quad X\cdot\lambda=D,\quad R=Y\cdot\lambda, \tag{33}$$

where $\varepsilon_{jj'}=\varepsilon_j\delta_{jj'}$ is a diagonal matrix. The explicit solution is now easily found in the form containing an inverse matrix:

$$R=Y\cdot X^{-1}\cdot D=M\cdot D,\quad M=Y\cdot X^{-1}. \tag{34}$$

Let us call $M_{mm'}$ the dynamic scattering matrix. Unlike the kinematic scattering matrix $G_{mm'}$, it depends on the crystal thickness. Obviously, in the limit $t=0$ we have $X=Y$ and $M=I$, where I is the identity matrix. It can be shown that for small crystal thickness

$$M_{mm'}\approx\delta_{mm'}+i\frac{Kt}{2\gamma_0}\operatorname{sign}(\gamma_m)G_{mm'}, \tag{35}$$

i.e., the dynamic matrix is simply proportional to the kinematic one.

Equation (34) yields a satisfactory solution only in the case of pure Laue geometry, with the Bragg beams being absent. If we have mixed Bragg–Laue diffraction, the expression (34) is not suited to numerical solution even in the case of relatively thin crystals, let alone the case with $t\to\infty$. The point there is that when Bragg reflection takes place, some eigenvalues have a negative imaginary component ε''_j. Moreover, if the number of Bragg beams is N_B, the number of such solutions is exactly $2N_B$. The physics behind these solutions is fairly simple. To each eigenvalue there corresponds a Bloch wave with a definite direction of the energy flux. In solutions with $\varepsilon''_j<0$, the energy flux has a negative z component, and these waves are damped for upward motion. These solutions can sensibly be called

Bragg-type Bloch waves, while the other solutions, with positive ε_j'', can be called Laue type Bloch waves.

A solution appropriate for numerical calculations should not contain increasing exponents. To find such a solution, we order the subscript m according to decreasing γ_m and the subscript j according to decreasing ε_j''. For the sake of simplicity, we denote all Laue-type indices by L and all Bragg-type indices by B. We also introduce diagonal matrices

$$C_{LL}=\exp\left(i\frac{Kt}{2\gamma_0}\varepsilon_j\right)\delta_{jj'},\quad j\in L,$$
$$C_{BB}=\exp\left(i\frac{Kt}{2\gamma_0}\varepsilon_j\right)\delta_{jj'},\quad j\in B. \tag{36}$$

In the new notation, the set of equations (31) split into two subsets, and can be written in the form

$$E_{LL}\cdot\lambda_L+E_{LB}\cdot\lambda_B=D_L,$$
$$E_{BL}\cdot C_{LL}\cdot\lambda_L+E_{BB}\cdot C_{BB}\cdot\lambda_B=D_B. \tag{37}$$

Here E_{LL} and E_{BB} are square $2N_L\times 2N_L$ and $2N_B\times 2N_B$ matrices, where $N_L=N-N_B$, and the matrices E_{LB} and E_{BL} are in general rectangular. This set is used to find the vectors λ_L and λ_B. The solution must be written in a form containing only decreasing exponents, i.e., instead of the matrix C_{BB}, the inverse matrix C_{BB}^{-1} should be used. Simple calculations yield

$$\lambda_L=Z_{LL}^{-1}\cdot(D_L-E_{LB}\cdot C_{BB}^{-1}\cdot E_{BB}^{-1}\cdot D_B),$$
$$\lambda_B=C_{BB}^{-1}\cdot Z_{BB}^{-1}\cdot(D_B-E_{BL}\cdot C_{LL}\cdot E_{LL}^{-1}\cdot D_L), \tag{38}$$

where

$$Z_{LL}=E_{LL}-E_{LB}\cdot C_{BB}^{-1}\cdot E_{BB}^{-1}\cdot E_{BL}\cdot C_{LL},$$
$$Z_{BB}=E_{BB}-E_{BL}\cdot C_{LL}\cdot E_{LL}^{-1}\cdot E_{LB}\cdot C_{BB}^{-1}. \tag{39}$$

In new notation, (32) takes the form

$$R_L=E_{LL}\cdot C_{LL}\cdot\lambda_L+E_{LB}\cdot C_{BB}\cdot\lambda_B,$$
$$R_B=E_{BL}\cdot\lambda_L+E_{BB}\cdot\lambda_B. \tag{40}$$

Substituting the solution (38) for the vector λ into Eq. (40), we finally obtain

$$R_L=M_{LL}\cdot D_L+M_{LB}\cdot D_B,$$
$$R_B=M_{BL}\cdot D_L+M_{BB}\cdot D_B, \tag{41}$$

where the blocks of the dynamic scattering matrix have the form

$$M_{LL}=E_{LL}\cdot C_{LL}\cdot Z_{LL}^{-1}-E_{LB}\cdot Z_{BB}^{-1}\cdot E_{BL}\cdot C_{LL}\cdot E_{LL}^{-1},$$
$$M_{LB}=E_{LB}\cdot Z_{BB}^{-1}-E_{LL}\cdot C_{LL}\cdot Z_{LL}^{-1}\cdot E_{LB}\cdot C_{BB}^{-1}\cdot E_{BB}^{-1},$$
$$M_{BL}=E_{BL}\cdot Z_{LL}^{-1}-E_{BB}\cdot C_{BB}^{-1}\cdot Z_{BB}^{-1}\cdot E_{BL}\cdot C_{LL}\cdot E_{LL}^{-1},$$
$$M_{BB}=E_{BB}\cdot C_{BB}^{-1}\cdot Z_{BB}^{-1}-E_{BL}\cdot Z_{LL}^{-1}\cdot E_{LB}\cdot C_{BB}^{-1}\cdot E_{BB}^{-1}. \tag{42}$$

It is easy to check that, in spite of a relatively cumbersome form, these formulas are very convenient for numerical calculations irrespective of the crystal thickness and, particularly, in the limit $t\to\infty$.

In a standard reflection-type geometry, a beam with wave vector $\mathbf{k}_0$ strikes the crystal and the Bragg beams are measured (see Fig. 1). This case is described by the block M_{BL}. In zeroth-order perturbation theory in the small exponents we have

$$(M_{BL})_{t\to\infty}\approx E_{BL}\cdot E_{LL}^{-1}. \tag{43}$$

This result in the theory of multiple x-ray diffraction was first reported in Refs. 20 and 21.

When the suppression of nuclear reaction inelastic channels is observed directly, the intensity of Laue beams at the lower face of a thick crystal is of interest. This situation is described by the block M_{LL}. In first-order perturbation theory, (42) yields

$$(M_{LL})_{t\to\infty}\approx(E_{LL}-E_{LB}\cdot E_{BB}^{-1}\cdot E_{BL})\cdot C_{LL}\cdot E_{LL}^{-1}. \tag{44}$$

This result was first reported in Ref. 22.

In contrast to approximate formulas, the general expressions (42) can be used to calculate multilayer crystalline systems. The corresponding recurrence relations for x-ray diffraction theory were first found in Ref. 23. However, in the case of diffraction of Mössbauer γ rays, this problem is not so urgent due to the lack of samples. The only situation that might conceivably be simulated is that of crystals with a temperature gradient normal to the surface.

Once the reflection amplitudes have been found, the reflection coefficient of the ms wave into the $m's'$ wave can be written as

$$J(m's',ms)=\frac{|\gamma_{m'}|}{|\gamma_m|}\frac{|R_{m's'}|^2}{|D_{ms}|^2}. \tag{45}$$

Under standard conditions, this quantity is to be summed over the index s' and, in the case of unpolarized radiation, averaged over the index s.

4. SCATTERING IN AN $FeBO_3$ CRYSTAL

$FeBO_3$ crystals are the most promising ones for measuring the diffraction of Mössbauer γ radiation (see, e.g., Ref. 24). They have a rhombohedral unit cell of edge length $a=5.520$ Å. The angles φ between the nearest edges are 49.54°. The unit cell volume V_0 is 89.52 Å^3, and the density ρ is 4.27 g/cm^3. (These data are taken from Ref. 25.) The unit cell has two Fe atoms, two B atoms and six O atoms. The reciprocal lattice is also rhombohedral, with edge length $b=0.259$ Å^{-1}. The angle φ_{rh} between the edges is 113.18° ($\cos C=-0.3936$).

In this case, the expression (30) for the amplitude of electron scattering of γ rays can be transformed into a sum over different atomic species, and for each species a structure factor can be introduced:

$$S_{bh}=\frac{1}{N_b}\sum_{a=b}\exp\{-i\mathbf{h}\mathbf{r}_a\}, \tag{46}$$

where the sum is taken only over the coordinates of type b atoms, and N_b is the number of such atoms. As a result,

$$\chi_h=\sum_b [C_r(f_b(\mathbf{h})+\Delta f_b')+iC_i\sigma_b^D]N_b e^{-W_{bh}}S_{bh}, \tag{47}$$

$$C_r=-\frac{\lambda^2 r_0}{\pi V_0 g}, \quad C_i=\frac{\lambda\cdot 10^{-3}}{2\pi V_0 g}.$$

Here we use seconds of arc as units, and $g=0.4848\cdot 10^{-5}$ rad $\cdot$ s^{-1}.

The structure factors for each atomic species in iron borate are strictly real and equal to

$$S_{\mathrm{Fe}}=\cos^2(f_{hkl}), \quad S_{\mathrm{B}}=\cos(f_{hkl}), \tag{48}$$

$$S_0=\tfrac{1}{3}\{\cos[f_{hkl}+z(h-k)]+\cos[f_{hkl}+z(k-l)]+\cos[f_{hkl}+z(l-h)]\},$$

where $f_{hkl}=0.5\pi(h+k+l)$ and $z=0.5962\pi$.

The atomic form factor $f_b(h)$ is a tabulated function of $\sin\theta_B/\lambda=h/4\pi$, and tables can be found in Ref. 26. In the isotropic approximation, the Debye–Waller factor is $\exp(-W_h)=\exp(-0.5\langle u^2\rangle h^2)$. The constant $\langle u^2\rangle$ can be found by averaging the data reported in Ref. 25; here we use $\langle u^2\rangle=0.0026$. The constants C_r and C_i in this specific case ($\lambda=0.861$ Å) are $C_r=-1.5322\cdot 10^{-2}$ and $C_i=3.157\cdot 10^{-6}$, respectively. The values of dispersion corrections can be found in Ref. 27, and the photoabsorption cross sections in Ref. 28. At the wavelength involved, the dispersion correction $\Delta f_{\mathrm{Fe}}'$ is approximately 0.4, and the corresponding values for O and B can be neglected. The dipole parts of the photoabsorption cross section are $\sigma_{\mathrm{Fe}}^D=6085$, $\sigma_{\mathrm{O}}^D=55$, and $\sigma_{\mathrm{B}}^D=9$.

The nuclear scattering occurs from iron atoms only, and the directions of the internal magnetic field at the nuclei of two atoms in the same unit cell can be approximately considered opposite. Scattering occurs via excitation of the spin $I=3/2$ state, with reradiation in the transition to the $I_0=1/2$ ground state. Accordingly, $M_g=1/2$ and $-1/2$, and $M_e=-3/2$, $-1/2$, $1/2$, and $3/2$. Here the sequence of quantum numbers corresponds to increasing energy of the levels. Selection rules allow the six transitions shown below together with the value of the quantum number M, the squares of the corresponding $3j$ symbols, and the transition energy, in the units of Γ, measured from the mean value. The sign of the quadrupole splitting constant is also given.

n	Transition	M	$(3j)^2$	$\Delta E_{0n}/\Gamma$	β_n
1	$-3/2\rightarrow-1/2$	1	3/12	−54.93	1
2	$-1/2\rightarrow-1/2$	0	2/12	−31.79	−1
3	$+1/2\rightarrow-1/2$	−1	1/12	−8.64	−1
4	$-1/2\rightarrow+1/2$	1	1/12	8.64	−1
5	$+1/2\rightarrow+1/2$	0	2/12	31.79	−1
6	$+3/2\rightarrow+1/2$	−1	3/12	54.93	1

(49)

The Lamb–Mössbauer factor in the isotropic approximation is

$$f_{am}=f_{LM}=\exp(-\langle u^2\rangle K^2)=0.8707$$

irrespective of the index m. Moreover, in specific calculations the values $\eta=0.95$ and $\alpha=8.21$ have been used. The total transition energy is

$$\frac{E_n}{\Gamma}=\frac{E_{0n}}{\Gamma}h+\frac{\Delta}{2}\beta_n+C, \tag{50}$$

where $h=1+\varepsilon$, $\varepsilon\ll 1$ is the correction due to the effective field at the nucleus, $\Delta=1.95$ is the quadrupole splitting constant, and $C=3$ is the chemical shift.

The nuclear scattering matrix can thus be written in the form

$$\hat{p}=g_0[(\tfrac{3}{4}f_1+\tfrac{1}{4}f_4)\hat{P}_{+1}+(f_2+f_5)\hat{P}_0+(\tfrac{1}{4}f_3+\tfrac{3}{4}f_6)\hat{P}_{-1}], \tag{51}$$

where $f_n=[2\hbar(\omega-\omega_n)/\Gamma+i]^{-1}$ are resonance factors for the six indicated transitions,

$$g_0=-\frac{2\pi\eta f_{LM}}{g(1+\alpha)V_0K^3}\frac{(2I+1)}{(2I_0+1)}=-6.692, \tag{52}$$

$$\hat{P}_{-1}=\hat{P}_A-\hat{P}_0+i\hat{P}_B, \quad \hat{P}_{+1}=\hat{P}_A-\hat{P}_0-i\hat{P}_B, \tag{53}$$

$$\hat{P}_0=\tfrac{1}{2}[1+(-1)^{h+k+l}](\mathbf{m}_{ms}\mathbf{n}_0)(\mathbf{m}_{m's'}\mathbf{n}_0),$$

$$\hat{P}_A=\tfrac{1}{2}[1+(-1)^{h+k+l}](\mathbf{m}_{ms}\mathbf{m}_{m's'}),$$

$$\hat{P}_B=\tfrac{1}{2}[1-(-1)^{h+k+l}]([\mathbf{m}_{ms}\mathbf{m}_{m's'}]\mathbf{n}_0). \tag{54}$$

Here h, k, and l are the indices of the reciprocal lattice vector $\mathbf{h}_{mm'}'$.

In Eqs. (53) and (54), the vector $\mathbf{n}_0$ determines the orientation of the magnetic field at the iron atom with coordinates (0,0,0). This vector is strictly orthogonal to the (1,1,1) direction of the reciprocal lattice, i.e., it is in the plane of the crystal surface. However, it can have an arbitrary direction in the plane itself. We introduce an angle φ_H and define the direction of the vector $\mathbf{n}_0$ in the following way:

$$\mathbf{n}_0=\mathbf{a}\sin\varphi_H+\mathbf{b}\cos\varphi_H, \tag{55}$$

$$\mathbf{a}=\mathbf{A}/A, \quad \mathbf{A}=[\mathbf{Z}\mathbf{s}_0], \quad \mathbf{b}=[\mathbf{a}\mathbf{Z}]. \tag{56}$$

Here, as before, $\mathbf{Z}$ is the unit vector of the inward normal at the crystal surface.

5. DIFFRACTION GEOMETRY: POLARIZATION

To calculate the full kinematic scattering matrix, it is necessary to find expressions for the three vectors $\mathbf{e}_{m\pi}$, $\mathbf{e}_{m\sigma}$, and $\mathbf{s}_m$ in each beam, with $m=0$, h, and g. The problem is solved in the simplest way if the formulas from Pinsker's book[3] are used. The reciprocal lattice vectors $\mathbf{h}$ and $\mathbf{g}$ define a circle of radius R. For a vector $\mathbf{R}$ from the center to a point O we have

$$\mathbf{R}=a\mathbf{h}+b\mathbf{g}, \quad (\mathbf{R}+\mathbf{h})^2=R^2, \quad (\mathbf{R}+\mathbf{g})^2=R^2. \tag{57}$$

The coefficients a and b are then easily found:

$$a=-\frac{g^2(h^2-\mathbf{hg})}{2[h^2g^2-(\mathbf{hg})^2]}, \quad b=-\frac{h^2(g^2-\mathbf{hg})}{2[h^2g^2-(\mathbf{hg})^2]}. \tag{58}$$

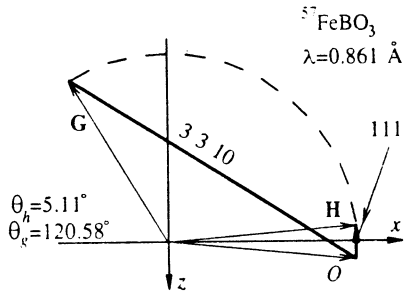

FIG. 2. Geometry of coplanar three-beam diffraction.

In the general case $Ks_0=\mathbf{R}+c\mathbf{p}$, where $\mathbf{p}=\mathbf{P}/P$ is a unit vector in the $\mathbf{P}=[\mathbf{hg}]$ direction. Obviously, $c=\pm\sqrt{K^2-R^2}$, and the sign is found from the condition $s_{0z}>0$. In the coplanar case $c=0$. The vectors in question are

$$\mathbf{s}_m=\mathbf{s}_0+\mathbf{h}_m/K,\quad \mathbf{e}_{m\pi}=\mathbf{E}/E,\quad \mathbf{E}=[\mathbf{ps}_m],$$
$$\mathbf{e}_{m\sigma}=[\mathbf{s}_m\mathbf{e}_{m\pi}],\quad \gamma_m=s_{mz}. \tag{59}$$

Thus, all geometric quantities necessary for the calculation of polarization matrices can be found automatically. It is only necessary to give the indices of two reflections, h,k,l and h',k',l', and the coordinates of the inward normal to the surface hit by the beam in the reciprocal lattice basis Z_h, Z_k, and Z_l. The latter are almost always -1, -1, and -1. The choice of the polarization vectors in the form (59) is convenient in that in the coplanar case all vectors $\mathbf{e}_m=\mathbf{p}$ coincide with those for two-beam diffraction. The magnetic field polarization vectors are $\mathbf{m}_{m\pi}=\mathbf{e}_{m\sigma}$ and $\mathbf{m}_{m\sigma}=-\mathbf{e}_{m\pi}$.

6. SPECIFIC EXAMPLE

The theory developed above makes it possible to study, with the help of numerical simulation, any multibeam configuration. A detailed analysis of all pertinent effects is beyond the scope of this paper. Here, as an application of the theory, we consider one case of coplanar three-beam diffraction from the 1,1,1 and 3,3,10 planes[13] of the 14.4-KeV Mössbauer line ($\lambda=0.861$ Å) in a $FeBO_3$ crystal. The geometric parameters are shown in Fig. 2. This case is of interest in that the 1,1,1(H) reflection is structurally forbidden—i.e., the electronic scattering amplitude is zero and nuclear scattering occurs with a change in polarization state, and only for the four extreme lines of the hyperfine structure. The 3,3,10 (G) reflection is structurally allowed. In this case, along with electronic scattering, nuclear scattering occurs without a change in the polarization state.

Such a qualitatively different character of scattering by two sets of planes is impossible in the case of x rays, and

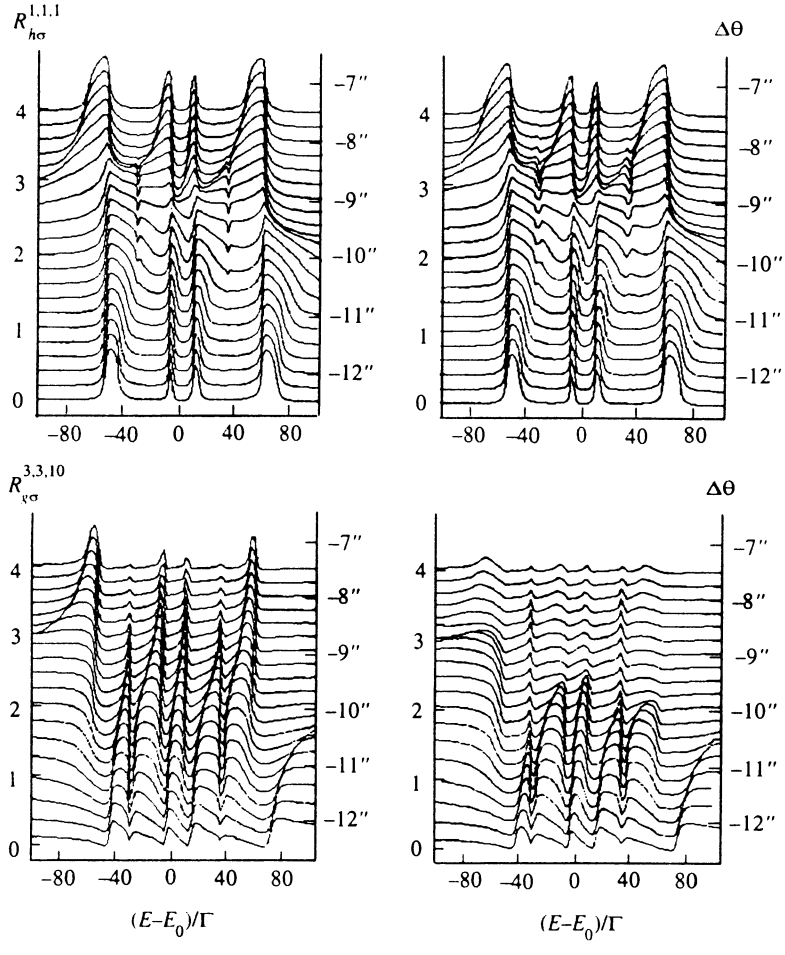

FIG. 3. Energy and angular dependence of the 1,1,1 and 3,3,10 reflection coefficients for the sigma-polarized plane wave in the two- (left) and three-beam (right) cases.

has never been considered. Furthermore, the character of the interaction for various hyperfine components strongly depends on the orientation of the magnetic field at the nucleus. Another new feature is that the coefficient in front of the resonance factor in the amplitude of scattering with polarization variation is purely imaginary, while in the case of scattering without polarization variation it is strictly real. This should obviously markedly weaken multiple interaction. Moreover, while the H-reflection is symmetric, i.e., the incident and diffracted beams form the same angles with the surface, the G-reflection is, on the contrary, markedly asymmetric ($\beta_g=-0.1034$). As follows from (22), this results in the G-wave amplitude being ten times smaller than that of the H-wave, and, consequently, the influence of the G-wave on the H-wave is much weaker than that of the H-wave on the G-wave.

The features noted above, which can be found by a preliminary analysis, are fully confirmed by the results of a straightforward numerical calculation of the reflection indices as functions of the energy position between resonances (energy spectra) for various deviations from the Bragg angle. I have calculated two-dimensional energy–angle arrays for different values of the incident beam polarization (pi or sigma) and magnetic field orientation at the nucleus. The strongest interaction arises for the sigma-polarized incident beam and the magnetic field in the scattering plane ($\varphi_H=0$). Figure 3 shows the calculated results for this case. The reflection coefficients

$$R_{ms}=\sum_{s'} J(ms',0s), \tag{60}$$

where $m=h,g$ and $s=\pi,\sigma$ have been calculated for polarized radiation. To give a graphic example of multiple interaction, the two- and three-beam curves are shown in two plots of the same row. It is worth noting that for the indicated deviations from the Bragg angle, the two-beam case is impossible. It can be realized experimentally by varying the frequency of the incident radiation or some crystal lattice parameter (e.g., the temperature) at other angles. The curves are purely illustrative, and have been obtained by setting the matrix elements corresponding to the second reflection to zero.

As follows from the calculations, over the range of angles corresponding to three-beam diffraction, the H-beam intensity varies only slightly, while the G-beam intensity decreases markedly. The decrease in reflection for Bragg diffraction, when we go from the two-beam to the three-beam case, is a standard effect in the case of x rays,[1,3] and is usually accounted for by energy conservation (a 100% reflection becomes a 50% one, but in two beams). In this case the reflection coefficients are not so large, and the phenomenon is a phase effect, i.e., the amplitudes of the waves scattered from the O- and H-beams into the G-beam have different phases, which leads to their attenuation. It is necessary to note that the decrease occurs only at angles large in comparison with the dynamic Bragg angle, which corresponds to $\Delta\theta\approx-10''$. For small angles, on the contrary, the reflection increases slightly.

The main feature of multiple diffraction in general and of the present case in particular is the possibility of studying simultaneously a variety of diffractive reflections both in isolation and conjointly. The large number of parameters describing the interaction and diffraction geometry turn the study of each specific case into an independent investigation, and the amount of experimental data is much greater than in the two-beam case. The main result of this paper is a general formulation of the problem and a procedure for the analysis of specific physical situations.

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