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Kinematical Theory of Mössbauer Diffraction by Magnetically Ordered Crystals

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The kinematical theory of Mössbauer diffraction by magnetically ordered crystals is developed. The case of completely resolved Zeeman splitting of a Mössbauer line is examined in detail. The expressions for coherent scattering amplitudes and scattering cross sections of γ-rays at magnetic and crystalline diffraction maxima are derived for the main types of magnetic ordering (ferromagnetic, antiferromagnetic, weak ferromagnetic and helicoidal structures) in the case of the dipole Mössbauer transition. A direct connexion between the polarization of the scattered quanta and the magnetic and crystalline structure is revealed in the expressions obtained for polarization vector and the polarization density matrix (in the cases of polarized and unpolarized incident beams respectively). The explicit form of the polarization density matrix at magnetic reflexions for an antiferromagnet is given. The applications of the present results to experimental and theoretical investigations are discussed.

In a number of theoretical (Afanas'ev & Kagan, 1965, 1973; Kagan, Afanas'ev & Perstnev, 1968; Zhdanov & Kuz'min, 1968; Hannon & Trammel, 1969; Afanas'ev & Perstnev, 1969; Belyakov & Ajvazian, 1968, 1970; Chukhovskii & Perstnev, 1972) and experimental (Voitovetskii, Korsunskii, Novikov & Pazhin, 1968; Smirnov, Sklyarevskii, Voscanyan & Artem'ev, 1969; Parak, Mössbauer, Biebl, Formanek & Hoppe, 1971; Artem'ev, Sklyarevskii, Smirnov & Stepanov, 1972; Artem'ev, Perstnev, Sklyarevskii, Smirnov & Stepanov, 1973; Mirzababaev, Smirnov, Sklyarevskii, Artem'ev, Izrailenko & Babkov, 1971) papers interesting features and possible applications of Mössbauer diffraction were revealed. In particular, the experiments on Mössbauer diffraction by magnetically ordered crystals (Smirnov *et al.*, 1969; Artem'ev *et al.*, 1972, 1973) and crystals having complicated structures of electric field gradient (EFG) (Mirzababaev *et al.*, 1971) have shown the practical feasibility of magnetic and EFG structure investigations of crystals by means of Mössbauer γ-ray diffraction. Application of Mössbauer diffraction to magnetic and crystalline structure investigations looks a promising and useful supplement to X-ray, neutron, electron diffraction methods because the Mössbauer diffraction method (Mössbauerography) has some additional advantages over conventional methods (Zhdanov & Kuz'min, 1968; Parak *et al.*, 1971; Ajvazian & Belyakov, 1969*a*,*b*; Belyakov & Ajvazian, 1969; O'Connor & Spicer, 1969; Batterman, Maracci, Merlini & Pace, 1973). Other promising fields of Mössbauer diffraction investigation are the study of the γ-ray collective interaction with nuclei, the influence of the crystal lattice on nuclear processes and related topics in nuclear physics (Afanas'ev & Kagan, 1967).

The theory of Mössbauer diffraction was developed mostly for crystals without magnetic field and EFG in the sites occupied by Mössbauer nuclei. In connexion with the above-mentioned experiments there is a need for a theory applicable to the cases of magnetically ordered crystals and crystals in which Mössbauer nuclei are situated in the sites with non-zero EFG. In the papers published on this topic the simplest cases of magnetic ordering and EFG were examined in the kinematical approximation (Belyakov & Ajvazian,

1968, 1970; Ajvazian & Belyakov, 1969*a*,*b*; Andreeva & Kuz'min, 1969; Pham Zui Khien, 1970; Belyakov & Bokun, 1972*a*) and a general analysis of equations of the dynamical theory for magnetically ordered crystals was carried out (Hannon & Trammel, 1969; Afanas'ev & Kagan, 1973; Belyakov, 1971). In the present paper general kinematical formulae for Mössbauer diffraction are presented and their explicit form is given for all main types of crystals with magnetic ordering in the practically important limiting case of completely resolved Zeeman splitting of the Mössbauer spectrum.

The difference between X-ray and Mössbauer diffraction by magnetically ordered crystals is mainly due to the dependence of the Mössbauer scattering amplitude on the magnitude and direction of the magnetic field at the scattering nucleus (Belyakov & Ajvazian, 1968) [a weak spin dependence of the X-ray scattering amplitude (Keating, 1969) is completely neglected here]. Therefore, unlike X-ray diffraction, Mössbauer diffraction may be used for direct determination of the structures of crystals in a fully analogous way to that used in the case of neutrons. The intensities of diffraction maxima (in particular magnetic ones, if they exist for the examined structure) and the polarization of the scattered quanta depend on the magnetic structure of the crystals. Strictly speaking, Mössbauer diffraction permits one to determine the ordering of the magnetic field at Mössbauer nuclei, but since the determination of the type of magnetic-field ordering is equivalent to determination of the type of ordering of the atomic magnetic moments, we shall speak below about Mössbauer determination of magnetic structures in the common sense of these words.

Mössbauer γ-quanta are scattered both by nuclei and by electrons (Rayleigh scattering). In the typical experimental situation the Rayleigh scattering amplitude is bigger than or of the same order of magnitude as the nuclear amplitude. Therefore the intensity and polarization of the radiation at crystalline diffraction maxima are essentially dependent on interference between the Rayleigh scattering and the nuclear scattering. In magnetic diffraction maxima, which are absent in the Rayleigh scattering, the same quantities are determined by the nuclear scattering only.

Expressions for the coherent amplitude and the differential scattering cross section are given below for a magnetically ordered crystal with an arbitrary value of Zeeman splitting in the Mössbauer spectrum. For dipole Mössbauer transitions explicit forms of these expressions for all main types of magnetic ordering are presented in the case of well resolved nuclear Zeeman splitting.

I. General description of diffraction by magnetically ordered crystals

Let us examine in the kinematical approximation a coherent scattering of γ-quanta by a magnetically ordered crystal containing Mössbauer isotopes. Taking into account the expression for Rayleigh (James, 1950) and nuclear (Trammel, 1962) scattering amplitudes one readily obtains the amplitude of coherent scattering of a Mössbauer quantum by the unit cell in the form:

$$F=F_R(\hat{\mathbf{n}},\hat{\mathbf{n}}')+F_N(E;\hat{\mathbf{n}},\hat{\mathbf{n}}')=r_e(\hat{\mathbf{n}}\hat{\mathbf{n}}'^*)F^{(R)}+\sum_t P_t(E;\hat{\mathbf{n}},\hat{\mathbf{n}}')F_t^{(N)},$$

$$P_t(E_i\hat{\mathbf{n}},\hat{\mathbf{n}}')=\frac{1}{2k}C(\mathbf{k},\mathbf{k}')\,\frac{\Gamma_R}{E-E_t+i\Gamma/2}\times(w_tw_t')^{1/2}(\hat{\mathbf{n}}\hat{\mathbf{n}}_t^*)\,(\hat{\mathbf{n}}_t'\hat{\mathbf{n}}'^*),$$

$$F_t^{(N)}=\sum_{\mathbf{r}_t}\exp[i(\mathbf{k}-\mathbf{k}')\mathbf{r}_t]. \qquad (1)$$

Here $F_R(\hat{\mathbf{n}},\hat{\mathbf{n}}')$ and $F_N(E;\hat{\mathbf{n}},\hat{\mathbf{n}}')$ are Rayleigh and nuclear coherent amplitudes respectively, $r_e=e^2/mc^2$ is the classical electron radius, E is the energy and $\hat{\mathbf{n}}$ is the polarization vector of the incident γ-quantum, $\hat{\mathbf{n}}'$ is the vector of the detected polarization of the scattered quantum, $F^{(R)}$ is the Rayleigh (X-ray) structure amplitude including a Debye–Waller factor $\exp[-\frac{1}{2}Z(\mathbf{k}-\mathbf{k}')]$, Γ_R and Γ are the radiation and full widths of the Mössbauer transition,

$$C(\mathbf{k},\mathbf{k}')=\eta\,\frac{2j_2+1}{2j_1+1}\exp[-\tfrac{1}{2}Z(\mathbf{k})-\tfrac{1}{2}Z(\mathbf{k}')],$$

η is the abundance of the Mössbauer isotope, $\mathbf{k}(\mathbf{k}')$ is the wave vector of the incident (scattered) γ-quantum, $j_1(j_2)$ is the spin of the ground (excited) nuclear state. The index t marks the different Zeeman transitions *via* which the scattering proceeds. The Zeeman transitions are regarded as different ones if their energies E_t are different or if (when the energies coincide) there are different directions of magnetic field $\mathbf{H}_t$. $\hat{\mathbf{n}}_t(\hat{\mathbf{n}}_t')$ is the polarization vector of the γ-quantum emitted in the direction $\mathbf{k}(\mathbf{k}')$ in the transition with index t, $w_t\equiv w_t(\mathbf{k})$ is a normalized angular distribution of γ-quanta in the same transition, $w_t'\equiv w_t(\mathbf{k}')$, unit vectors are marked by a caret ∧, $\mathbf{r}_t$ is the radius vector of the site with magnetic field $\mathbf{H}_t$. The quantities $\hat{\mathbf{n}}_t$ and w_t depend on the multipolarity of Mössbauer transition and the orientation of the magnetic field on the nuclei (Belyakov & Ajvazian, 1968, 1970).

For dipole transitions $\hat{\mathbf{n}}_t$ and w_t are determined by the formulae

$$\hat{\mathbf{n}}_t=(\cos\alpha_t\hat{\boldsymbol{\chi}}_{2t}+i\sin\alpha_t\hat{\boldsymbol{\chi}}_{1t})\exp(iM_t\varphi_t),$$
$$\tan\alpha_t=e_{1t}/e_{2t},\quad \hat{\boldsymbol{\chi}}_{1t}=\mathbf{k}\times\mathbf{H}_t/|\mathbf{k}\times\mathbf{H}_t|,\quad \hat{\boldsymbol{\chi}}_{2t}=\hat{\mathbf{k}}\times\hat{\boldsymbol{\chi}}_{1t}, \qquad (2)$$

$$w_t=\varepsilon_t(e_{1t}^2+e_{2t}^2),\quad \varepsilon_t=\frac{8\pi^2}{\sqrt{1+M_t^2}}\times\left|\begin{pmatrix} j_2 & 1 & j_1\\ M_t-m_1 & M_t & m_1\end{pmatrix}\right|^2,$$

$$e_{1t}=(1-l)\sin(\theta_t-M_t\pi/2)-lM_t^2,$$
$$e_{2t}=(1-l)M_t^2-l\sin(\theta_t-M_t\pi/2)$$

where l is equal to zero for an electric $E1$ and to one for a magnetic $M1$ transition, m_1 and m_2 are projections of the spins j_1 and j_2 on the directions of $\mathbf{H}_t$ and $M_t = m_2 - m_1$, θ is the angle between $\mathbf{k}$ and $\mathbf{H}_t$, φ_t is the azimuthal angle of $\mathbf{k}$ (the polar axis is directed along $\mathbf{H}_t$). The quantities $\hat{\mathbf{n}}'_t$ and w'_t are also determined by the equations (2) if $\mathbf{k}$ is substituted by $\mathbf{k}'$.

The differential cross section of coherent scattering by a magnetically ordered crystal related to one magnetic unit cell is equal to

$$\frac{d\sigma_E(\mathbf{k},\hat{\mathbf{n}};\mathbf{k}',\hat{\mathbf{n}}')}{d\Omega_{\mathbf{k}'}} = \frac{(2\pi)^3}{V}\sum_{\tau}|F|^2\delta(\mathbf{k}-\mathbf{k}'-2\pi\tau)$$
$$= \frac{(2\pi)^3}{V}\sum_{\tau}[\sigma^{(R)}(\hat{\mathbf{n}},\hat{\mathbf{n}}')+\sigma^{(N)}(E;\hat{\mathbf{n}},\hat{\mathbf{n}}')$$
$$+\sigma^{(RN)}(E;\hat{\mathbf{n}},\hat{\mathbf{n}}')]\,.\,\delta(\mathbf{k}-\mathbf{k}'-2\pi\tau) \qquad (3)$$

where $d\Omega_{\mathbf{k}'}$ is an element of solid angle in the $\mathbf{k}'$ direction, τ is the reciprocal magnetic-lattice vector, V is the volume of the magnetic unit cell, $\sigma^{(R)}(\hat{\mathbf{n}},\hat{\mathbf{n}}')$, $\sigma^{(N)}(E;\hat{\mathbf{n}},\hat{\mathbf{n}}')$ and $\sigma^{(RN)}(E;\hat{\mathbf{n}},\hat{\mathbf{n}}')$ are Rayleigh, nuclear and interference terms in the cross section respectively.

The cross section (3) depends on the detected polarization vector $\hat{\mathbf{n}}'$. The vector $\hat{\mathbf{n}}'=\hat{\mathbf{n}}'_0$ which maximizes the cross section is a polarization vector of the scattered γ-quantum. The corresponding cross section $d\sigma_E(\mathbf{k},\hat{\mathbf{n}};\mathbf{k}',\hat{\mathbf{n}}') \equiv d\sigma_E(\mathbf{k},\hat{\mathbf{n}};\mathbf{k}')$ is a differential cross section of the incident γ-quantum with polarization vector $\hat{\mathbf{n}}$. From equations (1) and (3) it follows that $\hat{\mathbf{n}}'_0$ depends on the initial polarization and the magnetic structure of the crystal and is determined by the expression:

$$\hat{\mathbf{n}}'_0 = \mathbf{N}/|\mathbf{N}|,\ \mathbf{N} = r_e F^{(R)}\mathbf{k}'\times(\hat{\mathbf{n}}\times\mathbf{k}')$$
$$+\frac{1}{2k}C(\mathbf{k},\mathbf{k}')\sum_t F_t^{(N)}\frac{\Gamma_R}{E-E_t+i\Gamma/2}(w_t w'_t)^{1/2}(\hat{\mathbf{n}}\hat{\mathbf{n}}_t^*)\hat{\mathbf{n}}'_t\,. \qquad (4)$$

The cross section $d\sigma_E(\mathbf{k},\hat{\mathbf{n}};\mathbf{k}')$ can be derived from equation (3) by summation on vectors $\hat{\mathbf{n}}'$ of final polarization. The scattering cross section of unpolarized radiation $d\sigma_E(\mathbf{k},\mathbf{k}')$ one gets by averaging $d\sigma_E(\mathbf{k},\hat{\mathbf{n}};\mathbf{k}')$ over the initial polarization. For magnetic reflexions the Rayleigh amplitude $F_R(\hat{\mathbf{n}},\hat{\mathbf{n}}')\equiv 0$ and the cross section (3) reduces to the nuclear term $\sigma^{(N)}$ only.

For an unpolarized incident beam the scattered radiation is partially polarized. The corresponding polarization density matrix is

$$\varrho_{un} = \frac{\sum_{j=1,2} d\sigma_E(\mathbf{k},\hat{\mathbf{n}}_j;\mathbf{k}')\varrho(\hat{\mathbf{n}}'_{0j})}{\sum_{j=1,2} d\sigma_E(\mathbf{k},\hat{\mathbf{n}}_j;\mathbf{k}')} \qquad (5)$$

where $\hat{\mathbf{n}}_1,\hat{\mathbf{n}}_2$ are orthogonal unit vectors of the initial polarization, $\hat{\mathbf{n}}'_{0j}$ is the polarization vector of the scattered quantum determined by equation (4) with $\hat{\mathbf{n}}=\hat{\mathbf{n}}_j$, and $\varrho(\hat{\mathbf{n}}'_{0j})$ is the polarization density matrix corresponding to the polarization vector $\hat{\mathbf{n}}'_{0j}$.

From equations (4), (5) it follows that the polarization of quanta scattered at crystalline reflexions contains information on both the magnetic and crystalline structures. The polarization density matrix for magnetic reflexions depends not only on the nuclear parameters but on the magnetic structure and the location in the unit cell of Mössbauer atoms.

II. The case of completely resolved Zeeman splitting

The formulae given above determine the intensity and polarization of the coherently scattered radiation for arbitrary relations between Zeeman spliting and the width of the Mössbauer line. In the experimentally important case of completely resolved Zeeman splitting the expressions for amplitudes and cross sections become essentially simpler. In this case Mössbauer scattering proceeds *via* definite Zeeman levels of the ground and excited nuclear states and therefore only one term with E_t equal to the energy E_0 of the corresponding Zeeman transition is essential in the sum of equation (1).

Diffraction for all the main types of magnetic ordering in crystals is examined below for dipole Mössbauer transitions in the case of completely resolved Zeeman splitting, which is the same for all Mössbauer nuclei in the unit cell (the magnetic fields $\mathbf{H}_t$ may be different in orientation only). The explicit forms of the coherent amplitude and the nuclear $\sigma^{(N)}$ and interference $\sigma^{(RN)}$ terms of the $d\sigma_E(\mathbf{k},\mathbf{k}')$ scattering cross section for unpolarized quanta are given.

1. *Ferromagnet*

There is one and only one value of magnetic field $\mathbf{H}_t \equiv \mathbf{H}$. One can readily find the coherent amplitude from equations (1) and (2). The nuclear and interference terms in the cross section are

$$\sigma_f^{(N)} = \frac{1}{k^2}C^2(\mathbf{k},\mathbf{k}')|F^{(N)}|^2\frac{\gamma_M^2}{(E-E_0)^2+\Gamma^2/4}\cdot$$
$$\times\tfrac{1}{2}(\sin^2\theta+2|M|\cos^2\theta)$$
$$\times(\sin^2\theta'+2|M|\cos^2\theta')\,,$$

$$\sigma_f^{(NR)} = \frac{r_e}{k}C(\mathbf{k},\mathbf{k}')|F^{(R)}F^{(N)}|\frac{\gamma_M^2}{(E-E_0)^2+\Gamma^2/4}$$
$$\times\{[A(M)\cos\delta_{NR}+B(M)\sin\delta_{NR}](E-E_0)$$
$$+\frac{\Gamma}{2}[A(M)\sin\delta_{NR}-B(M)\cos\delta_{NR}]\}\,,$$

$$A(M) = \cos M\Delta\varphi\{\sin\left[(1-l)\theta+(-M)^{1+l}\frac{\pi}{2}\right] \qquad (6)$$
$$\times\sin\left[(1-l)\theta'+(-M)^{1+l}\frac{\pi}{2}\right]$$
$$\times(\sin\theta\sin\theta'+\cos\theta\cos\theta'\cos\Delta\varphi)$$
$$+\sin\left[l\theta+(-M)^{2-l}\frac{\pi}{2}\right]$$

$$\times \sin\left[l\theta' + (-M)^{2-l}\frac{\pi}{2}\right]\cos\Delta\varphi\}$$
$$+\sin^2 M\Delta\varphi[(1-l)(\cos^2\theta+\cos^2\theta')$$
$$+2l\cos\theta\cos\theta'],$$

$$B(M)=\tan M\Delta\varphi\{A(M)-[(1-l)(\cos^2+\theta\cos^2\theta')$$
$$+2l\cos\theta\cos\theta']\},$$

where $\gamma_M=\Gamma_R\varepsilon_t$ is a partial radiation width for the Zeeman transition, $\theta(\theta')$ is the angle between $\mathbf{k}(\mathbf{k}')$ and $\mathbf{H}$, $\Delta\varphi=\varphi-\varphi'$ is the difference between the azimuth angles of $\mathbf{k}$ and $\mathbf{k}'$ (see Fig. 1), δ_{NR} is the phase of $F^{(N)}F^{(R)*}$ and the meaning of l is the same as in equation (2).

2. *Antiferromagnet*

The magnetic field $\mathbf{H}_t$ takes two values, $\mathbf{H}$ and $-\mathbf{H}$. The nuclear coherent amplitude has the form:

$$F_{\text{Naf.}}(E;\hat{\mathbf{n}},\hat{\mathbf{n}}')=\frac{1}{2k}C(\mathbf{k},\mathbf{k}')\frac{\Gamma_R}{E-E_0+i\Gamma/2} \quad (7)$$
$$\times(ww')^{1/2}[(\hat{\mathbf{n}}\hat{\mathbf{n}}_H^*)(\hat{\mathbf{n}}_H'\hat{\mathbf{n}}'^*)$$
$$+(\hat{\mathbf{n}}\hat{\mathbf{n}}_H)(\hat{\mathbf{n}}_H'^*\hat{\mathbf{n}}'^*)F_{-H}^{(N)}],$$

where the subscript $t=1,2$ is replaced by H, $-H$ and all other quantities are defined above.

For crystals with a symmetry centre $|F_{-H}^{(N)}|=|F_H^{(N)}|$, the nuclear term in the cross section has the form:

$$\sigma_{\text{af.}}^{(N)}=\frac{1}{k^2}C^2(\mathbf{k},\mathbf{k}')|F_H^{(N)}|^2\frac{\gamma_M^2}{(E-E_0)^2+\Gamma^2/4}$$
$$\times[(\sin^2\theta+2|M|\cos^2\theta)(\sin^2\theta'+2|M|\cos^2\theta')$$
$$+\cos(2M\Delta\varphi-\delta)\sin^2\theta\sin^2\theta'] \quad (8)$$

where δ is the phase of $F_H^{(N)}F_{-H}^{(N)*}$ (for magnetic reflexions $\delta=\pi$). The interference term $\sigma_{\text{af.}}^{(RN)}$ is determined by equation (6) for a ferromagnet if the factor in the curly bracets is replaced by

$$[A(M)\cos\delta_H+A(-M)\cos\delta_H+B(M)\sin\delta_H$$
$$+B(-M)\sin\delta_{-H}]\cdot(E-E_0)$$
$$+\frac{\Gamma}{2}[A(M)\sin\delta_H+A(-M)\sin\delta_{-H}$$
$$-B(M)\cos\delta_H-B(-M)\cos\delta_{-H}]$$

where $\delta_H(\delta_{-H})$ is the phase of $F_H^{(N)}F^{(R)*}(F_{-H}^{(N)}F^{(R)*})$. At magnetic reflexions only the nuclear term in equation (8) is not equal to zero and equation (8) holds for crystals with a symmetry centre as well as for crystals without one. It follows from equation (8) that for Mössbauer transitions with $M=0$ magnetic reflexions are absent. Note that the angular dependence of the magnetic reflexion intensity determined by equation (8) turns out to be correct for an arbitrary value of Zeeman splitting of the Mössbauer spectrum.

3. *Weak ferromagnet*

The magnetic field $\mathbf{H}_t$ takes two values, $\mathbf{H}$ and $\mathbf{H}_\zeta$. The angle between $\mathbf{H}$ and $\mathbf{H}_\zeta$ is $\pi-\zeta$ where ζ is a small quantity. The scattering cross section at magnetic reflexions for transitions with $M=0$ is equal to

$$\sigma_{\text{wf.}}^{(N)}(M=0)=\frac{1}{k^2}C^2(\mathbf{k},\mathbf{k}')|F_H^{(N)}|^2\cdot 2\sin^2\zeta/2$$
$$\times[\sin^2\theta+\sin^2\theta'-\cos^2\psi-\cos^2\psi'$$
$$+(\cos\theta\cos\psi+\cos\theta'\cos\psi'$$
$$-2\cos\psi\cos\psi'\sin\zeta/2)^2$$
$$+2\sin\zeta/2(\cos\theta\cos\psi+\cos\theta'\cos\psi'$$
$$-\sin\zeta/2)]. \quad (9)$$

The angles ζ, $\theta(\theta')$, $\psi(\psi')$ are defined in Fig. 1, where $\mathbf{H}_F=\mathbf{H}+\mathbf{H}_\zeta$.

For transitions with $M=\pm 1$ the expressions for the coherent amplitudes and cross sections differ from the case of the antiferromagnet (with antiferromagnetic axis A–A; see Fig. 1) by small terms proportional to ζ and therefore are not given here.

4. *Helicoidal structure*

Let us examine the FS spiral. This structure is completely determined by an angle β and a vector $\mathbf{k}_0$. The direction of $\mathbf{k}_0$ determines the orientation of the helicoidal axis, $2\pi/k_0$ is the magnetic period and β is the angle between magnetic field and the axis. In equation (3) $\tau=\tau_{cr}+s\mathbf{k}_0$ correspond to magnetic reflexions (satellites) where τ_{cr} is the reciprocal-lattice vector and the integer $s\neq 0$. Because the direction of the atomic magnetic moments (for constant β) is determined by the azimuthal angle α (counted around the helicoidal axis) the scattering amplitude by an individual atom f will depend on α. For this reason the coherent am-

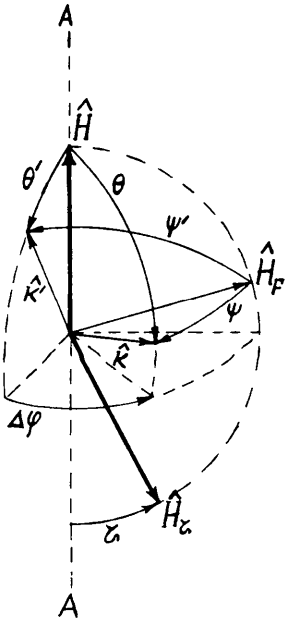

Fig. 1. The geometry of the Mössbauer effect with a magnetic field.

plitude F depends on s and is equal to Fourier transform of the amplitude $f(\alpha)$:

$$F_s=\frac{1}{2\pi}\int_0^{2\pi} f(\alpha)\exp(is\alpha)\mathrm{d}\alpha\,. \tag{10}$$

The number of satellites depends on the multipolarity of the transition and in the case of the FS spiral is equal to $4L$; for the CS spiral it is equal to $(4L)^2$. The explicit form of the coherent amplitude for dipole transitions is given by Belyakov & Bokun (1972*b*).

For a crystal with one Mössbauer nucleus in the unit cell the nuclear term in the scattering cross section is determined by the following expression:

$$\sigma_{\mathrm{hel.}}^{(N)}(s=0,\pm1,\pm2)=\frac{1}{k^2}\,C^2(\mathbf{k},\mathbf{k}')\,\frac{(\gamma_M/16)^2}{(E-E_0)^2+\Gamma^2/4}$$

$$\times\begin{cases}\frac{1}{2}\sin^4\beta(1+\cos^2\theta)\,(1+\cos^2\theta')\to(s=\pm2)\,,\\ 2\sin^4\beta(\cos^2\beta)^{1-|M|}[(1-M\cos\beta)^{2|M|}\\ \quad\times(1+\cos^2\theta)\sin^2\theta'+(1+M\cos\beta)^{2|M|}\\ \quad\times\sin^2\theta(1+\cos^2\theta')+(-\frac{1}{2}\sin^2\beta)^{|M|}\\ \quad\times\sin2\theta\sin2\theta'\cos\Delta\varphi\to(s=\pm1)\,,\\ (\sin^4\beta+8|M|\cos^2\beta)\,(1+\cos^2\theta)\,(1+\cos^2\theta')\\ \quad+8(\cos^4\beta-|M|\cos2\beta)\sin^2\theta\sin^2\theta'\\ \quad+\frac{1}{2}(8+8\cos^2\beta)^{|M|}\,.\,\sin^2(2-|M|)\beta\\ \quad\times\sin2\theta\sin2\theta'\cos\Delta\varphi\\ \quad+\sin^4\beta\sin^2\theta\sin^2\theta'\cos2\Delta\varphi\to(s=0)\end{cases} \tag{11}$$

where $\theta(\theta')$ is the angle between the helicoidal axis and $\mathbf{k}(\mathbf{k}')$, $\varphi(\varphi')$ is the azimuthal angle of $\mathbf{k}(\mathbf{k}')$ (counted around the helicoidal axis), $\Delta\varphi=\varphi-\varphi'$. The interference term $\sigma_{\mathrm{hel.}}^{(RN)}$ differs from zero for $s=0$ only and is determined by equation (6) if for $A(M),B(M)$ we use the following expressions:

$$\begin{aligned}A(M)=&(|M|\cos^2\beta+2^{-|M|}\sin^2\beta)\\ &\times[(1+\cos\theta\cos\theta')\cos\Delta\varphi+(2l-1)\\ &\times(\cos\theta-\cos\theta')\sin\Delta\varphi]\\ &+2^{-|M|}[1+(-1)^M\cos2\beta]\sin\theta\sin\theta',\\ B(M)=&M(2l-1)\cos\beta[(2l-1)\\ &\times(1+\cos\theta\cos\theta')\sin\Delta\varphi-(\cos\theta-\cos\theta')\\ &\times\cos\Delta\varphi]\,.\end{aligned} \tag{12}$$

The polarization characteristics of quanta scattered at the satellites are examined by Belyakov & Bokun (1972*b*).

Note that results of diffraction measurements are described as a rule not by equations (6), (8), (9), (11) directly but by the expressions derived from these by integration over the energy with some weight function included. The form of this function and the results of the corresponding integration are determined by the shape of the Mössbauer line of the source (and the detector if a resonant detector is used) and are well known (Pham Zui Khien, 1970; O'Connor & Black, 1964).

III. Polarization properties

Let us examine the polarization of Mössbauer quanta at diffraction maxima. In the general case the polarization density matrix of the scattered quanta $\varrho(E)$ depends on the energy E and the degree of polarization of the incident beam [see equations (4) and (5)]. The dependence of $\varrho(E)$ on the energy leads to a dependence of the results of polarization measurements on the energy line shape of the incident beam and on the energy resolution of the detector. The polarization characteristics are given below for the case when ϱ does not depend on energy, namely for magnetic reflexions for an antiferromagnet. The density matrix (5) of the polarization unit vectors $\hat{\boldsymbol{\chi}}_1'=\mathbf{k}'\times\mathbf{H}/|\mathbf{k}'\times\mathbf{H}|$, $\hat{\boldsymbol{\chi}}_2'=\hat{\mathbf{k}}'\times\hat{\boldsymbol{\chi}}_1'$ has the following Stokes parameters for the $M1$ transition:

$$\begin{aligned}\zeta_1&=\frac{\sin^2\theta\cos\theta'\sin2\Delta\varphi}{\cos^2\theta+\cos^2\theta'+\sin^2\theta\sin^2\theta'\sin^2\Delta\varphi}\,,\\ \zeta_2&=0\,,\\ \zeta_3&=\frac{\cos^2\theta'-\cos^2\theta-\sin^2\theta\,(1+\cos^2\theta')\sin^2\Delta\varphi}{\cos^2\theta+\cos^2\theta'+\sin^2\theta\sin^2\theta'\sin^2\Delta\varphi}\,.\end{aligned} \tag{13}$$

To obtain corresponding expressions for the $E1$ transition it is enough to make the following substitution in equation (13): $\zeta_1\to-\zeta_1$ and $\zeta_3\to-\zeta_3$.

The density matrix (13) is real ($\zeta_2=0$). This means that the scattered radiation is partially linearly polarized. The corresponding vector of linear polarization and the unit vector $\hat{\boldsymbol{\chi}}_1'$ form the angle υ which is determined by the relation $\operatorname{ctan}2\upsilon=\zeta_3/\zeta_1$. If $\zeta_1=0$ the density matrix is diagonal in the unit vectors used and the scattered radiation is partially polarized along one of them (along $\hat{\boldsymbol{\chi}}_1'$, if $\zeta_3>0$ and along $\hat{\boldsymbol{\chi}}_2'$, if $\zeta_3<0$; if $\zeta_3=\zeta_1=0$ the radiation is unpolarized). In particular the scattered quanta are polarized along one of the polarization unit vectors $\hat{\boldsymbol{\chi}}_1'$ or $\hat{\boldsymbol{\chi}}_2'$ if the antiferromagnetic axis lies in the scattering plane or is orthogonal to it. In the first case the degree of polarization $P=|\cos^2\theta-\cos^2\theta'|/(\cos^2\theta+\cos^2\theta')$; in the latter case scattered radiation is fully polarized. Note that the polarization density matrix (13) for magnetic reflexions does not depend on the location of the atoms in the unit cell. It depends on the orientations of the magnetic fields only. Therefore measurement of the polarization density matrix for magnetic reflexions determines uniquely the orientation of the antiferromagnetic axis. The polarization density matrix for crystalline reflexions depends not only on the orientation of the magnetic fields but also on the location of the atoms in the unit cell (Andreeva & Kuz'min, 1973). Therefore polarization measurements may be used to obtain information on crystal structure.

Conclusion

The results of the kinematical theory of Mössbauer diffraction given above are interesting from both

theoretical and experimental points of view. The formulae presented may be directly used for description of an experiment under the conditions which justify application of the kinematical approximation. For the strongest reflexions in the case of 100% abundance of the Mössbauer isotope the kinematical approximation is applicable at exact resonance only for a very thin crystal with the thickness $d \leq d_{\max} \sim 10^{-4}$ cm. For smaller abundance $d_{\max}$ increases inversely proportional to the abundance. If the crystal is thick enough, the kinematical approximation is not applicable at some distance from the exact resonance, where the nuclear scattering cross section is smaller. In direct analogy with X-ray diffraction, Mössbauer diffraction by mosaic crystals may be described by the formulae given if the absorption (James, 1950) and the dependence of the absorption coefficient on polarization (Perstnev & Chukhovskii, 1973) are taken into account.

The results of the kinematical theory are also useful in the dynamical theory. The expressions for the coherent amplitudes enter into the formulae of the dynamical theory. Therefore the explicit form of the amplitude given above can be used in the dynamical-theory analysis of the dependence of the reflected intensity and polarization on the magnetic structure of the crystal and the γ-quantum energy.

It is useful to keep in mind also that the dynamical theory expressions for the intensity and polarization of the scattered quanta in the limit of thin crystals reduce to the corresponding expressions of the present paper.

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