Theory of Magnetic Mössbauer Diffraction Measurement

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The theory of Mössbauer γ-ray diffraction by magnetically ordered crystals containing Mössbauer nuclei is developed in the Born approximation. It is shown that for crystals whose magnetic structure induces an ordering of magnetic fields at Mössbauer nuclei, the diffraction patterns exhibit magnetic Bragg maxima. The positions of these maxima do not coincide generally with the positions of Rayleigh maxima. The polarization of radiation scattered at Bragg angles contains information about the orientation of the magnetic fields at the Mössbauer nuclei relative to the crystallographic directions. The expressions for the polarization and coherent scattering cross section are given in the case of large nuclear Zeeman splitting for a purely nuclear scattering. Diffraction by antiferromagnetic crystals is examined in detail. The possibility of studying magnetic ordering in crystals by means of Mössbauer diffraction is discussed.

INTRODUCTION

SEVERAL groups extensively investigated Mössbauer γ-ray diffraction, and in particular diffraction by magnetically ordered crystals, both theoretically and experimentally because of the discovery of some interesting physical effects and possible applications[1–6] (additional literature is cited in these references). In a short paper, the present authors reported on the possibility of investigating magnetic ordering in crystals by means of Mössbauer diffraction. In the present paper, the theory of Mössbauer γ-ray diffraction by magnetically ordered crystals is developed in the Born approximation for a more general case than in Ref. 6. In addition, the derivations of some expressions of Ref. 6 are presented.

It is well known that the Mössbauer effect is widely used for the investigation of magnetic structures. In published work the analysis of magnetic structures was based on the study of the Mössbauer absorption spectra and their dependence on the direction of the magnetic field applied to the single-crystal absorber. This method permits one to make certain conclusions on the character of the magnetic ordering in the crystal (see, e.g., Ref. 7). This kind of information however is, in principle, insufficient for the complete determination of the magnetic structure. For example, the period of the magnetic ordering cannot be obtained by this method. As has been shown in Ref. 6, Mössbauer γ-ray diffraction gives more detailed information on the magnetic structure than Mössbauer absorption experiments. For magnetically ordered crystals Mössbauer scattering exhibits magnetic Bragg maxima and gives information on magnetic ordering analogous to that obtained by neutron diffraction. But whereas neutron diffraction determines the ordering of atomic magnetic moments, Mössbauer diffraction determines the ordering of the magnetic fields at the Mössbauer nuclei. In Mössbauer diffraction the intensity and polarization of the γ rays at Bragg maxima depend on the orientation of the magnetic fields at the nuclei relative to the crystaloghaphic axes. Since the ordering of the magnetic fields at the nuclei is a consequence of the atomic-moment ordering, Mössbauer diffraction permits one to make conclusions about the character of the atomic-moment ordering. The physical reason for the possibility of investigating magnetic structures by means of Mössbauer diffraction is caused by the dependence of the Mössbauer scattering amplitude on the magnitude and direction of the magnetic field at the scattering nucleus.

In the theory presented Rayleigh scattering and its interference with the nuclear scattering is neglected. Since we are primarily concerned with the magnetic diffraction maxima this simplification is insignificant indeed due to the fact that Rayleigh scattering does not contribute to these maxima.

MÖSSBAUER SCATTERING AMPLITUDE

We consider the scattering of Mössbauer γ rays from a crystal which has an ordering of the magnetic fields at the Mössbauer nuclei. The Mössbauer nuclei in the crystal are assumed to be located at the sites having p different values of the magnetic field $\mathbf{H}_l$. It is supposed that all p values are large enough to produce nuclear Zeeman splitting which is much greater than the width of the Mössbauer level and the linewidth of incident γ ray is less than Zeeman splitting of nuclear levels. It is also supposed that the relaxation time of nuclear spins in the crystal is much longer then the lifetime of the Mössbauer level.

First we express the amplitude of the Mössbauer scattering by an individual nucleus. There are two stages in the resonant scattering process: (1) absorption

[1] Yu. Kagan, A. M. Afanas'ev, and I. P. Perstnev, Zh. Eksperim. i Teor. Fiz. **54**, 1530 (1968) [English transl.: Sov. Phys.—JETP **27**, 819 (1968)].
[2] J. P. Hannon and G. T. Trammel, Phys. Rev. **169**, 315 (1968).
[3] V. A. Belyakov and Yz. Ajvazian, Phys. Letters **27B**, 352 (1968); Izv. Akad. Nauk. USSR, Ser. Fiz. **33**, 690 (1969).
[4] V. K. Voitovetskii, I. L. Korsunskii., A. I. Novikov., and Yu. F. Pazin, Zh. Eksperim. i Teor. Fiz. **54**, 1361 (1968) [English transl.: Sov. Phys.—JETP **27**, 729 (1968)].
[5] V. V. Sklyarevskii, G. V. Smirnov, A. N. Artem'ev, B. Shestak, and S. Kadechkov, JETP Letters **8**, 295 (1968).
[6] V. A. Belyakov and Yu. M. Ajvazian, JETP Letters **7**, 477 (1968); Usp. Fiz. Nauk **97**, 743 (1969).
[7] N. Blum, A. J. Freeman, J. W. Shaner, and L. Grogzins, J. Appl. Phys. **36**, 1169 (1965).

of the incident γ quantum accompanied by transition of the nucleus to the exited state and (2) emission of the γ quantum by the excited nucleus. The above assumed relations between the width of the Mössbauer level, the linewidth of the incident γ rays, the nuclear Zeeman splitting and the nuclear spin relaxation time permit one to assume that, if the resonant scattering conditions for the nucleus are met, the scattering proceeds via definite Zeeman levels of the initial and intermediate nuclear states. Therefore the scattering amplitude may be written in the form[8,9]

$$f(\mathbf{k},\mathbf{n};\mathbf{k}',\mathbf{n}')_{m_1m_2m_3} = C(\mathbf{n}^*\cdot\mathbf{n}_{m_2m_2})(\mathbf{n}'\cdot\mathbf{n}_{m_3m_2}{}'^*)[I(\mathbf{k})_{m_2m_1}I(\mathbf{k}')_{m_2m_3}]^{1/2}, \quad (1)$$

where $\mathbf{k},\mathbf{k}'$ are wave vectors of the incident and scattered γ quanta, respectively, $\mathbf{n}$ is the polarization vector of the initial γ quantum, $\mathbf{n}'$ is the polarization vector corresponding to polarization of the scattered γ quanta which is of interest to us, $\mathbf{n}_{m_im_f}$ ($\mathbf{n}_{m_im_f}{}'$) is the polarization vector of the γ quantum emitted in the Zeeman transition $m_i \to m_f$ in the k (k') direction, $I(\mathbf{k})_{m_im_f}(I(\mathbf{k}')_{m_im_f})$ is the intensity of emission in the same transition and in the same direction, and C is a factor whose explicit form[10] is unimportant here. Taking into account the assumption made above and the dependence of C on the incident γ-quantum energy we shall assume, that C differs from zero only when the incident γ-quantum energy is equal to the energy of $m_2 \to m_1$ transition. The scattering amplitude is characterized by three indices m_1, m_2, m_3, denoting the nuclear moment projections on the magnetic-field direction in the initial, intermediate, and final states of the scattering nucleus.

The expressions for $\mathbf{n}_{m_2m_1}$, $I(\mathbf{k})_{m_2m_1}$ in the case of a 2^L-pole Mössbauer transition are:

$$\mathbf{n}_{m_2m_1} = \left[(\cos\alpha)\frac{\mathbf{k}\times[\mathbf{k}\times\hat{h}]}{|\mathbf{k}\times[\mathbf{k}\times\hat{h}]|} + i(\sin\alpha)\frac{\mathbf{k}\times\hat{h}}{|\mathbf{k}\times\hat{h}|}\right]e^{iM\varphi}, \quad \tan\alpha = \frac{e_2}{e_1}, \quad (2)$$

$$e_1 = (2L+1)^{1/2}\left\{\left[\begin{pmatrix} l & 1 & L \\ M+1 & -1 & -M\end{pmatrix}Y_l{}^{-M-1}(\theta,0) - \begin{pmatrix} l & 1 & L \\ M-1 & 1 & -M\end{pmatrix}Y_l{}^{1-M}(\theta,0)\right]\cos\theta + \sqrt{2}\sin\theta\begin{pmatrix} l & 1 & L \\ M & 0 & -M\end{pmatrix}Y_l{}^{-M}(\theta,0)\right\}, \quad (3)$$

$$e_2 = (2L+1)^{1/2}\left[\begin{pmatrix} l & 1 & L \\ M+1 & -1 & -M\end{pmatrix}Y_l{}^{-M-1}(\theta,0) + \begin{pmatrix} l & 1 & L \\ M-1 & 1 & -M\end{pmatrix}Y_l{}^{1-M}(\theta,0)\right], \quad (4)$$

$$I(\mathbf{k})_{m_2m_1} = a\begin{pmatrix} j_1 & L & j_2 \\ m_1 & M & -m_2\end{pmatrix}(e_1{}^2+e_2{}^2). \quad (5)$$

Here $M = m_2 - m_1$; j_1, j_2 are moments of the ground and excited nuclear states respectively, $\hat{h}$ is a unit vector in the direction of the magnetic field at scattering nucleus, θ is the angle between $\hat{h}$ and $\hat{k} = \mathbf{k}/|\mathbf{k}|$, and φ is an azimuthal angle of $\mathbf{k}$ in a coordinate system the z axis of which coincides with the direction of the magnetic field. The quantity l in Eqs. (3) and (4) is equal to L for magnetic and $L-1$ for electric nuclear transitions. The factor a is proportional to the square of the reduced nuclear matrix element eight and is not essential here. $\mathbf{n}_{m_2m_1}{}'$ and $I(\mathbf{k}')_{m_2m_3}$ are given by the Eqs. (2)–(5), replacing $\mathbf{k}$ by $\mathbf{k}'$, θ by θ', φ by φ' and m_1 by m_3.

The dependence of the scattering amplitude on the vectors $\hat{h},\mathbf{k},\mathbf{k}'$ is expressed via the angles θ, θ', φ, φ'. As follows from Eqs. (1) and (2) the dependence on φ,φ' appears in a phase factor only. For a coherent scattering amplitude ($m_1 = m_3$) which is used below, this phase factor is equal to $e^{-iM(\varphi'-\varphi)}$.

CROSS SECTION OF COHERENT SCATTERING BY CRYSTAL AND POLARIZATION OF SCATTERED QUANTA

We express the cross section for coherent Mössbauer γ-ray scattering using Eq. (1). The kinematical theory of diffraction[11] in Born approximation for an infinite crystal leads one to the following expression for the differential cross section for scattering an incident $\mathbf{n}$, $\mathbf{k}$, γ quantum into the direction $\mathbf{k}'$ with the polarization vector $\mathbf{n}'$

$$d\sigma(\mathbf{k},\mathbf{n};\mathbf{k}',\mathbf{n}') = \frac{A\eta^2}{(2j_1+1)^2}\Big|\sum_{l=1}^{P} f_l(\mathbf{k},\mathbf{n};\mathbf{k}',\mathbf{n}')e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}_l}\Big|^2 \times\sum_{\tau}\delta(\mathbf{k}-\mathbf{k}'-\tau)d\Omega_{\mathbf{k}'}$$

$$= \Big|\sum_{l=1}^{P}(\mathbf{n}^*\cdot\mathbf{n}_{tl})(\mathbf{n}'\cdot\mathbf{n}_{tl}{}'^*)F_l\Big|^2\sum_{\tau}\delta(\mathbf{k}-\mathbf{k}'-\tau)d\Omega_{\mathbf{k}'}, \quad (6)$$

$$F_l = Ce^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}_l}[I(\mathbf{k})I(\mathbf{k}')]^{1/2}.$$

[8] V. A. Belyakov, Zh. Eksperim. i Teor. Fiz. **54**, 1162 (1968) [English transl.: Sov. Phys.—JETP **27**, 622 (1968)]; V. A. Belyakov and V. P. Orlov, *ibid.* **56**, 1366 (1969).

[9] Yu. M. Aivazian and V. A. Belyakov, Zh. Eksperim. i Teor. Fiz. **56**, 316 (1969).

[10] G. T. Trammell, Phys. Rev. **126**, 1045 (1962).

[11] R. W. James, *The Optical Principles of the Diffusion of X-Rays* (London, 1950), Chap. 1.

Here $\boldsymbol{\tau}$ is the reciprocal lattice vector of the crystal magnetic structure, $\mathbf{r}$ determines the position of the scattering nucleus, l specifies quantities corresponding to lth value of magnetic field, η is the Mössbauer isotope concentration, and A is a factor which is inessential for us and is omitted below. In Eq. (6) the amplitude is defined by Eq. (1) for $m_3=m_1$. The summation in Eq. (6) runs over the Mössbauer nuclei within the unit cell. The polarization vector of the radiation scattered at the Bragg angle $\mathbf{n}_0'$ is determined by

$$\mathbf{n}_0'=\frac{\mathbf{N}}{|\mathbf{N}|},\quad \mathbf{N}=\sum_{l=1}^{P}\mathbf{n}_{tl}'(\mathbf{n}\cdot\mathbf{n}_{tl}^*)F_l^*. \tag{7}$$

The total differential scattering cross section in the direction $\mathbf{k}'$, $d\sigma(\mathbf{k},\mathbf{n};\mathbf{k}')$ is equal to

$$d\sigma(\mathbf{k},\mathbf{n};\mathbf{k}')\equiv d\sigma(\mathbf{k},\mathbf{n};\mathbf{k}',\mathbf{n}_0')$$
$$=\Big|\sum_{l=1}^{P}(\mathbf{n}^*\cdot\mathbf{n}_{tl})\mathbf{n}_{tl}'F_l\Big|^2\sum_{\tau}\delta(\mathbf{k}-\mathbf{k}'-\boldsymbol{\tau})d\Omega_{\mathbf{k}'}. \tag{8}$$

The expression for the differential scattering cross section for scattering of unpolarized incident radiation into the direction $\mathbf{k}'$ with polarization vector $\mathbf{n}'$, $d\sigma(\mathbf{k};\mathbf{k}',\mathbf{n}')$ can be obtained using Eq. (7) in the form

$$d\sigma(\mathbf{k};\mathbf{k}',\mathbf{n}')$$
$$=\tfrac{1}{2}\Big|\sum_{l=1}^{P}\mathbf{n}_{tl}(\mathbf{n}_{tl}'^*\cdot\mathbf{n}')F_l\Big|^2\sum_{\tau}\delta(\mathbf{k}-\mathbf{k}'-\boldsymbol{\tau})d\Omega_{\mathbf{k}'}. \tag{9}$$

The total differential scattering cross section of unpolarized radiation in direction $\mathbf{k}'$, $d\sigma(\mathbf{k};\mathbf{k}')$, can be obtained from Eq. (9) by summation over the final polarization and is equal to

$$d\sigma(k;k')=\tfrac{1}{2}\sum_{ll'}(\mathbf{n}_{tl}\cdot\mathbf{n}_{tl'}^*)(n_{tl}'^*\cdot\mathbf{n}_{tl'}')F_lF_{l'}^*$$
$$\times\sum_{\tau}\delta(\mathbf{k}-\mathbf{k}'-\boldsymbol{\tau})d\Omega_{\mathbf{k}'}. \tag{10}$$

In this case the radiation scattered at the Bragg angle is polarized partially. The radiation is completely polarized only for ferromagnetic ordering of the magnetic fields at Mössbauer nuclei. The polarization density matrix of the scattered radiation for an unpolarized incident beam is given by

$$\rho_{un}=\frac{\sum_{i=1,2}d\sigma(\mathbf{k},\mathbf{n}_i;\mathbf{k}')\rho(\mathbf{n}_{0i}')}{\sum_{i=1,2}d\sigma(\mathbf{k},\mathbf{n}_i;\mathbf{k}')}, \tag{11}$$

where n_1,n_2 are two orthogonal unit vectors of the initial polarization, $\mathbf{n}_{0i}'$ is the polarization vector of scattered radiation corresponding to the initial polarization vector $\mathbf{n}_i$, and $\rho(\mathbf{n})$ is the polarization density matrix of a γ quantum with polarization vector $\mathbf{n}$.[12]

[12] A. I. Akhiezer and V. B. Berestetskii, Kvantovaya Electrodinamika, Fizmatgiz, 1959 (unpublished).

For the case of the scattering of a partially polarized beam one obtains the scattering cross section $d\sigma_P(\mathbf{k};\mathbf{k}',\mathbf{n}')$ in the form

$$d\sigma_P(\mathbf{k};\mathbf{k}',\mathbf{n}')=[1-P(\mathbf{n})]d\sigma(\mathbf{k};\mathbf{k}',\mathbf{n}')$$
$$+P(\mathbf{n})d\sigma(\mathbf{k},\mathbf{n};\mathbf{k}',\mathbf{n}'). \tag{12}$$

Here $P(\mathbf{n})$ is the degree of polarization of the incident radiation, $\mathbf{n}$ describes polarization which is present partially in the incident beam. In this case the polarization density matrix of scattered radiation may be represented as follows:

$$\rho_P=\frac{[1-P(\mathbf{n})]d\sigma(\mathbf{k};\mathbf{k}')\rho_{un}+P(\mathbf{n})d\sigma(\mathbf{k},\mathbf{n};\mathbf{k},'\mathbf{n}')\rho(\mathbf{n}_0')}{[1-P(\mathbf{n})]d\sigma(\mathbf{k};\mathbf{k}')+P(\mathbf{n})d\sigma(\mathbf{k},\mathbf{n};\mathbf{k}',\mathbf{n}_0')}, \tag{13}$$

where the quantities $\mathbf{n}_0'$ and ρ_{un} are defined by Eqs. (7) and (11), respectively.

Equations (6)–(13) impose no restrictions on $\mathbf{H}_l$, values of the magnetic fields at Mössbauer nuclei, except the requirement that these magnetic fields should be strong enough to produce large splittings of the nuclear levels. Particularly, $|\mathbf{H}_l|$ may be different. In this case the conditions of resonance scattering are different for different $|\mathbf{H}_l|$. Therefore in Eqs. (6)–(13) only those amplitudes are not equal to zero for which the conditions of resonance scattering are satisfied.

We now examine diffraction by a crystal for which the magnetic period or symmetry of the magnetic elementary cell is different from that of the crystalline unit cell. In this case the diffraction maxima given by Eqs. (6) and (8)–(10) can be subdivided into two types: (i) crystalline maxima, i.e., those existing in Rayleigh scattering, and (ii) magnetic maxima, i.e., those absent in Rayleigh scattering. Neglect of the Rayleigh scattering is fully justified for the magnetic maxima.

To conclude this section we note that for crystals which have a magnetic period different from the crystalline one there are atoms in the lattice which are crystallographically equivalent but magnetically nonequivalent. The situation in which the magnetic nonequivalence of the atoms is connected only with the different orientation of their magnetic moments looks like the most natural one. Therefore, we assume that the magnetic fields at the crystallographically equivalent but magnetically nonequivalent sites differ by their direction only. This means that in the magnetic unit cell there are at least two sites l and l' for which $|\mathbf{H}_l|=|\mathbf{H}_{l'}|$ and the resonance scattering conditions are the same for corresponding Mössbauer nuclei.

DIFFRACTION BY AN ANTIFERROMAGNETIC CRYSTAL

The coherent Mössbauer γ-ray scattering by an antiferromagnetic single crystal having one Mössbauer nucleus in the crystalline unit cell is described by the

formulas of the previous section for $p=2$. Following the remarks in the previous section we assume $\mathbf{H}_1=-\mathbf{H}_2$.

From Eqs. (6) and (7) for the differential cross section $d\sigma(\mathbf{k},\mathbf{n};\mathbf{k}',\mathbf{n}')$ and polarization vector one obtains

$$d\sigma(\mathbf{k},\mathbf{n};\mathbf{k}',\mathbf{n}') = \frac{\eta^2C^2}{(2j_1+1)^2} I(\mathbf{k})I(\mathbf{k}')\,|(\mathbf{n}^*\cdot\mathbf{n}_t)(\mathbf{n}'\cdot\mathbf{n}_t'^*) \pm(\mathbf{n}^*\cdot\mathbf{n}_t^*)(\mathbf{n}'\cdot\mathbf{n}_t')\,|^2 \sum_\tau \delta(\mathbf{k}-\mathbf{k}'-\boldsymbol{\tau})\,d\Omega_{\mathbf{k}'} \quad (14)$$

and

$$\mathbf{n}_0'=\mathbf{N}_1/|\mathbf{N}_1|, \quad \mathbf{N}_1=\mathbf{n}_t'(\mathbf{n}\cdot\mathbf{n}_t^*)\pm\mathbf{n}_t'^*(\mathbf{n}\cdot\mathbf{n}_t). \quad (15)$$

In deriving Eqs. (14) and (15) with the help of Eq. (1) one must take into account that, when the direction of the magnetic field at the emitting nucleus is reversed, the probability for emission of a γ quantum in a certain direction remains unchanged and the polarization vector transforms into the complex conjugated quantity, i.e., $I(\mathbf{H},\mathbf{k})=I(-\mathbf{H},\mathbf{k})$ and $\mathbf{n}_{t2}=\mathbf{n}_{t1}^*\equiv\mathbf{n}_t^*$. In Eqs. (14) and (15) the lower sign must be used for the magnetic maxima and the upper sign for the crystalline maxima.

In the same way, one obtains from Eq. (10) the following expression for $d\sigma(\mathbf{k};\mathbf{k}')$:

$$d\sigma(\mathbf{k};\mathbf{k}') = \frac{\eta^2C^2}{(2j_1+1)^2} I(\mathbf{k})I(\mathbf{k}')(1\pm\cos2\alpha\,\cos2\alpha'\,\cos2\delta) \times\sum_\tau \delta(\mathbf{k}-\mathbf{k}'-\boldsymbol{\tau})\,d\Omega_{\mathbf{k}'}, \quad (16)$$

where for the direction $\mathbf{k}(\mathbf{k}')$ the quantity $\alpha(\alpha')$ is defined by Eqs. (2)–(4) and $\delta=M(\varphi'-\varphi)$.

The cross sections $d\sigma(\mathbf{k},\mathbf{n};\mathbf{k}')$ and $d\sigma(\mathbf{k};\mathbf{k}'\mathbf{n}')$ may be easily obtained from Eqs. (8)–(10) by the same method or by means of the relevant averaging and summation of Eq. (14). The polarization properties of the scattered radiation are described by the formulas of the previous section if the corresponding cross section and Eq. (15) for $\mathbf{n}_0'$ are used. In particular, for the purely magnetic maxima it follows from Eq. (15), that if $\mathbf{H}_1$ and $\mathbf{H}_2$ are perpendicular to the scattering planes, right (left) circular polarization of the incident radiation transforms to left (right) polarization of the scattered radiation. In the case of arbitrary orientation of $\mathbf{H}_1$, $\mathbf{H}_2$ relative to the crystal scattering planes, circular polarization of the incident radiation transforms to elliptical polarization of the scattered radiation.

To obtain the explicit form of the angular dependence of the examined quantities one must know the multipolarity of the Mössbauer transition. The angular dependences of some quantities for dipole transitions are given below. The most widely known 14.4-keV Mössbauer transition in ^{57}Fe is an $M1$ dipole transition.

TABLE I. $\tan\alpha$ for electric ($E1$) and magnetic ($M1$) dipole transitions.

m_2-m_1	$E1$	$M1$
0	0	∞
±1	$\mp1/\cos\theta$	$\mp\cos\theta$

The formulas for $\tan\alpha$, which determine the polarization vector [Eqs. (2) and (3)] are given in Table I.

For the scattering cross section $d\sigma(\mathbf{k};\mathbf{k}')$ one obtains using Eq. (15), the table, and Eqs. (4) and (5) or e_i tabulated in Ref. 8

$$d\sigma_0(\mathbf{k};\mathbf{k}') = \frac{2a^2\eta^2C^2}{(2j_1+1)^2}\begin{pmatrix} j_1 & 1 & j_2 \\ m_1 & 0 & -m_2 \end{pmatrix}^4 \times\begin{Bmatrix} \sin^2\theta\,\sin^2\theta' \\ 0 \end{Bmatrix}, \quad (17)$$

$$d\sigma_{\pm1}(\mathbf{k};\mathbf{k}') = \frac{2a^2\eta^2C^2}{(2j_1+1)^2}\begin{pmatrix} j_1 & 1 & j_2 \\ m_1 & \pm1 & -m_2 \end{pmatrix} \times\begin{Bmatrix} \cos^2\theta+\cos^2\theta'+\sin^2\theta\,\sin^2\theta'\,\cos^2\phi \\ \cos^2\theta+\cos^2\theta'+\sin^2\theta\,\sin^2\theta'\,\sin^2\phi \end{Bmatrix}, \quad (18)$$

where M, the subscript of $d\sigma$, is equal to m_2-m_1 and $\phi=\varphi'-\varphi$. The lower lines at the right-hand sides of Eqs. (17) and (18) relate to magnetic maxima; the upper lines relate to crystalline ones.

It follows from Eq. (17) that magnetic maxima are absent for scattering proceeding via a transition with $M=0$. This result relates not only to dipole transitions. It holds for transitions of any multipolarity. Absence of magnetic maxima is explained by the identity of the Mössbauer scattering amplitude for both directions of magnetic field $\mathbf{H}$ and $-\mathbf{H}$ for $M=0$. Note that Eqs. (16) and (17) do not take into account in direct form the angular dependence connected with possible Mössbauer factor anisotropy. This dependence is included in the factor C and, if it is necessary, must be taken into account separately.

The formulas of this section taken with lower sign describe magnetic diffraction maxima for the antiferromagnetic crystals with an arbitrary number of Mössbauer nuclei in an unit cell. But in this case the expressions for cross sections must be multiplied by

$$|\textstyle\sum_l e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}_l}|^2,$$

where the summation is limited to the unit cell and runs over Mössbauer nuclei located at the sites with one of the two values of magnetic field $\mathbf{H}_1$ or $\mathbf{H}_2$. The relevant formula for the crystalline maxima can be derived from the general expressions of the previous section.

For numerical illustration of the case of an antiferromagnet we give values of the first Bragg angles for

Mössbauer scattering by a single crystal of $\alpha-Fe_2O_3$ (14.4-keV Mössbauer transition in ^{57}Fe). The first two magnetic maxima, where Rayleigh scattering is absent, are approximately at 5° and 6°, and correspond to the scattering by the crystal planes {111} and {100}, respectively. The first two crystalline maxima corresponding to the scattering by the planes {110} and {211} are at 7.5° and 9°.

CONCLUSION

We discuss the results obtained in connection with the simplifying assumptions made above. The assumption that in the crystal the nuclear Zeeman splitting is greater than the width of nuclear levels and relaxation time of nuclear spins is longer than lifetime of the Mössbauer level is valid for many real cases. The neglect of extinction means that the expressions in the previous sections are valid for thin crystals for which the thickness is less than or of the order of the extinction length l_{ext}, i.e., $\gtrsim 10^{-3}$ cm. This length determines also the angular width of diffraction maxima $\Delta\theta\sim\lambda/l_{ext}$, where λ is wavelength of Mössbauer radiation. This estimate gives $\Delta\theta\sim 1'$ and agrees with the experimental results of the work.[4] As was pointed out above, the neglect of Rayleigh scattering is always justified for magnetic maxima, but for crystalline maxima it can be justified only for special cases. For example, the authors of Ref. 13 observed a purely nuclear diffraction maximum by choosing the Bragg conditions for which Rayleigh scattering amplitude was reduced to zero. Thus for some conditions one may expect not only qualitative but quantitative agreement of the theory with experiment. One can get rid of some assumptions of the present paper if one follows the work[1] in which the dynamical theory of Mössbauer diffraction was considered and Rayleigh scattering was taken into account for an unsplit Mössbauer line. We have not discussed the temperature dependence of the coherent scattering cross section. In a temperature interval in which the magnetic structure does not change it is fully determined by the same dependence of the Lamb-Mössbauer factor included in C and A Eqs. (1) and (6).

[13] R. J. Black and J. R. Duerdoth, Proc. Phys. Soc. (London) **84**, 169 (1964).

We note that Mössbauer diffraction was experimentally observed for crystals having no magnetic ordering and for crystals whose magnetic ordering prohibits purely nuclear magnetic maxima, e.g., in Refs. 4 and 14. In the case of crystals whose magnetic ordering permits purely nuclear maxima, Mössbauer diffraction will not apparently demand essential experimental complications. Perhaps the corresponding experiments will be even simpler because, for these crystals, the difficulties connected with separation of Mössbauer and Rayleigh scattering are absent for some diffraction maxima. The latter crystals are also a convenient object for investigation of some dynamical effects of Mössbauer diffraction, e.g., the effect of suppression of nuclear inelastic channels.[15]

A recently published communication about the first experimental observation of magnetic maxima in Mössbauer diffraction[16] confirms these last speculations.

The consequences of the Mössbauer scattering amplitude dependence on the value of magnetic field at the scattering nucleus were examined here. Analogous consequences for diffraction, in particular the existence of purely nuclear diffraction maxima,[17] are due to the dependence of the Mössbauer scattering amplitude on the electric field gradient at a scattering nucleus.[9] The theory of Mössbauer diffraction by crystals containing Mössbauer nuclei at sites with a nonuniform electric field was developed by the authors,[9] in the same approximation as in the present paper. Note, that in the paper[9] the expressions for the explicit form of the angular dependence of the coherent scattering cross section in the case of dipole transitions are incorrect, because the dependence of the scattering amplitude on the difference of azimuthal angles of vectors $\mathbf{k}$ and $\mathbf{k}'$ was omitted.[18]

[14] R. J. Black, D. A. O'Connor, and G. Longworth, Rev. Mod. Phys. **36**, 462 (1964).

[15] A. M. Afanas'ev and Yu. M. Kagan, Zh. Eksperim. i Teor. Fiz. **48**, 327 (1965) [English transl.: Sov. Phys.—JETP **21**, 215 (1965)].

[16] G. V. Smirnov, V. V. Sklyarevskii, R. A. Voskanyan, and A. N. Artem'ev, JETP Letters **9**, 123 (1969).

[17] V. A. Belyakov and Yu. M. Ajvazian, JETP Letters **9**, 637 (1969).

[18] The author's attention was drawn to this point by Dr. J. Hannon.