Investigation of diffraction of Mössbauer radiation by a Fe_3BO_6 single crystal. Interference of nuclear transitions

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The energy spectra of Bragg reflection of Mössbauer gamma radiation from a weakly ferromagnetic single crystal $^{57}Fe_3BO_6$ are studied. It is found that the interference of transitions in iron nuclei at nonequivalent positions strongly affects the shape of the spectra. The results of the measurements are compared with theoretical calculations.

The first experimental studies of diffraction of Mössbauer gamma radiation by magnetically ordered crystals demonstrated the possibility of using the Mössbauer diffraction for studying crystals, in particular, for studying their magnetic structure.[1,2] Compounds with simple crystalline and magnetic structures — Fe, α-Fe_2O_3, $FeBO_3$ crystals—were generally used in these experiments. The Mössbauer diffraction was later used to investigate compounds having a more complicated magnetic structure (see, for example, Ref. 3).

In this study we have analyzed the characteristics of diffraction of Mössbauer radiation by a weakly ferromagnetic crystal Fe_3BO_6. In this compound the effective magnetic fields of the Mössbauer nuclei are distinguished not only by their orientation but also by their magnitude, which accounts for a number of interesting, primarily interference-type effects in the Mössbauer scattering.

The Fe_3BO_6 crystal belongs to the space group $D_{2h}^{16}(P_{nma})$, information about its crystalline and magnetic structures is presented in Refs. 4 and 5. The experimental arrangement is shown in Fig. 1. A beam of 14.4-keV gamma rays from a Mössbauer source ^{57}CO with a divergence of 0.8 was diffracted by a $^{57}Fe_3BO_6$ single crystal, enriched by the resonant isotope up to 95%, and recorded by a semiconductor detection unit D. The (100) plane emerged onto the surface of the crystal, the antiferromagnetic axis was situated in the scattering plane ($\mathbf{k}_1\mathbf{k}_2$), and the ferromagnetic moment $\mathbf{m}$ was oriented perpendicular to the (100) plane. The measurements were performed at room temperature.

In this experiment we studied the Bragg scattering of resonant gamma rays in the nuclear magnetic peaks (11,0,0) and (19,0,0). The results of the measurements and of the theoretical calculations are shown in Fig. 1.

The iron ions in the Fe_3BO_6 crystal are located in two nonequivalent $4c$ and $8d$ positions.[4] The effective magnetic moments of the iron nuclei in the c and d positions differ in magnitude by approximately 6%. This difference, as well as the different

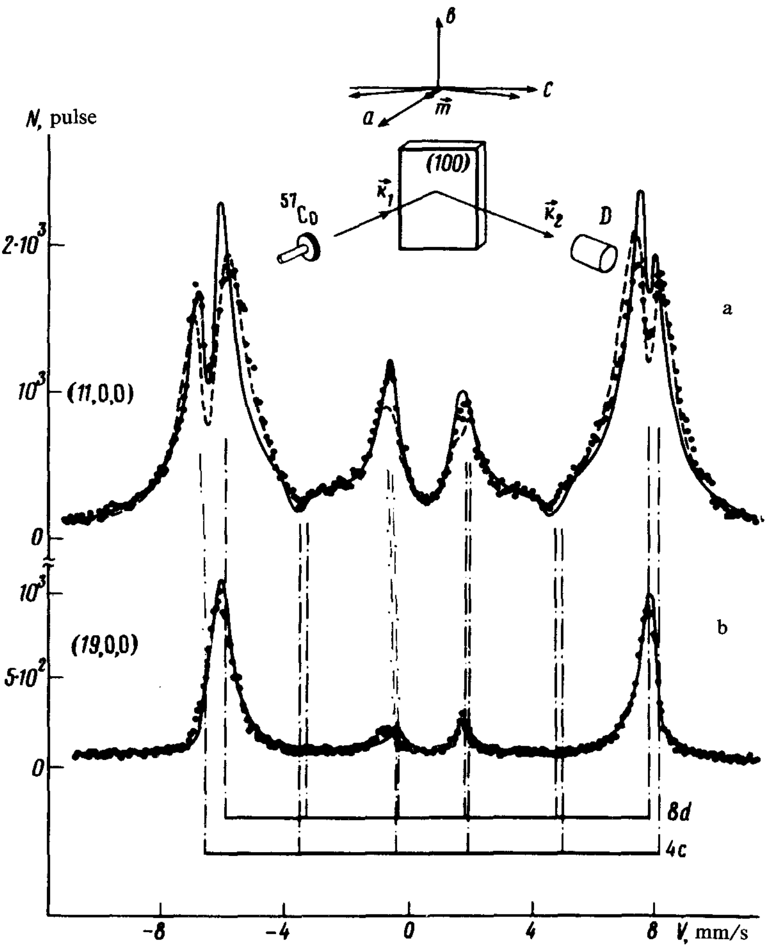

FIG. 1. Energy dependence of the intensity of the diffracted gamma radiation for reflections (11,0,0) (a) and (19,0,0) (b) from a $^{57}Fe_3BO_6$ crystal. The solid and dashed curves show the results of theoretical calculations for the perfect and mosaic crystals, respectively.[6,7] The vertical dashed lines show the positions of the resonances for iron nuclei located in the 4*c* and 8*d* positions. The inset shows the experimental arrangement.

magnitudes of the isomeric shift and the difference in the structure of the gradients of the electric fields at nonequivalent sites[8] leads to the fact that the position of the resonance lines for iron nuclei in *c* and *d* positions (the *c* and *d* lines) generally do not coincide. The contribution of iron nuclei in the *c* and *d* positions to the Bragg scattering interfere with each other; in contrast to Ref. 9, the interference term is appreciable, since the energy separation between the *c* and *d* lines corresponding to the same Mössbauer transition is small. Thus the difference in the position of the *c* and *d* lines at room temperature is within the range of $\sim 0.5\,\Gamma$ (for the third line in the spectrum) to $\sim 6\,\Gamma$ (for the first line in the spectrum), where Γ is the natural width of the Mössbauer line.

The interference of c and d lines has a large effect on the shape of the spectrum of the diffracted radiation. With a constructive interference, when the structural factors for the iron atoms in the c and d positions have an identical sign [reflection (11,0,0)], the contributions of the c and d lines add at the edges and subtract between the lines. In this case, the resulting resonant line is broadened and a depression may appear at the center of the line. The depressions in the energy dependence are clearly seen in Fig. 1a at the edges of the lines in the spectrum corresponding to the nuclear transitions $-3/2$–$-1/2$ and 3/2–1/2. For the central lines corresponding to the transitions 1/2–1/2 and $-1/2$–1/2, the depressions are essentially missing, since the distance between the c and d lines in this case is small ($\lesssim 1.2\,\Gamma$). In addition, the width of the line of the source in our experiment was $\sim 2\,\Gamma$, which led to a "smearing" of the fine details of the spectrum. Interference nevertheless leads to the fact that the intensity of the third line is much higher than that of the fourth line.

In the case of destructive interference the contributions of the c and d lines to the scattering cancel each other, giving rise to a narrowing of the resultant resonance line. We observed experimentally the narrowing of the line due to diffraction scattering of resonant gamma rays in the (19,0,0) reflection, for which the measurement results are shown in Fig. 1b. For this reflection the narrowing of the line is small and for the sixth line in the spectrum it is $\sim 12\%$ of the width of the single line. The relatively small effect is explained by the fact that the structural factors for iron atoms in the c and d positions for the (19,0,0) reflection differ approximately by a factor of 3, which does not permit interference to be manifested to the maximum extent. We note that of the two central lines in the spectrum of the reflection (19,0,0), the fourth line is the most intense line, rather than the third, as in the case of the (11,0,0) reflection, which is also attributable to destructive interference.

Comparison of the experimental spectra with the theoretical spectra reveals a good agreement between theory and experiment. The spectrum of the (19,0,0) reflection is described well by the theoretical curves both for the ideal and for the mosaic crystals, which coincide in the figure within the limits of the lines. In the case of the (11,0,0) reflection the central lines in the spectrum are described better in the model of the perfect crystal and the outermost lines are described better in the model of the mosaic crystal, which can be explained by the different degree of perfection of this crystal in the bulk.

A knowledge of the different odd orders of reflection (h 00) in the Fe_3BO_6 crystal permits changing the magnitude and sign of the contribution from the c and d lines to the purely nuclear scattering of the resonant gamma rays, while tuning to a particular transition makes it possible to change the distance between the interfering lines. Thus the diffraction of Mössbauer gamma radiation by a Fe_3BO_6 crystal permits a thorough study of the interference of nuclear transitions and its effect on the energy dependence of the intensity of the scattered radiation.

In addition, the interference of c and d lines, which is sensitive to the type of magnetic ordering in the crystal, can be used to study the magnetic structure of the specimen. Our experiments show that the magnetic structure of Fe_3BO_6 is the same as the structure determined previously by neutron diffraction.[5]

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