NEUTRON-DIFFRACTION STUDY OF THE ANTIFERROMAGNETIC TRANSFORMATION IN MANGANESE TELLURIDE

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Abstract

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NEUTRON-DIFFRACTION STUDY OF THE ANTIFERROMAGNETIC TRANSFORMATION IN MANGANESE TELLURIDE

Because manganese telluride combines semiconductor and special magnetic properties, the study of its magnetic and crystal structure at various temperatures is of great interest. As is known ([1–3]), manganese telluride belongs to the class of antiferromagnets with a Néel temperature lying in the range 307—329°K ([1–7]). In the present work, as part of a systematic study of manganese chalcogenides ([7,8]), a neutron-diffraction investigation of manganese telluride was carried out at temperatures above and below the temperature of the antiferromagnetic transformation.

The neutron diffraction patterns were recorded on the horizontal channel of the IRT reactor of the Academy of Sciences of the BSSR by means of a neutron diffractometer built on the basis of a GUR-3 X-ray diffractometer with an arm lengthened to 100 cm. A monochromatic neutron beam with wavelength $\lambda = 0.93$ Å was used in the measurements. Monochromatization was carried out with the aid of a lead crystal. The neutron detector was a counter filled with BF_3 with an enriched content of the isotope B^{10}.

In recording the neutron diffraction patterns, a cylindrical specimen 20 mm in diameter and 27 mm high, sintered from fine MnTe powder, was used. The scan was made point by point at intervals of 15—20′ outside the diffraction lines and 5—10′ in the region of the diffraction lines. At each point the pulses were counted for 5 minutes. The temperature of the specimen was monitored with a copper-constantan thermocouple. Low-temperature measurements were carried out in a specially designed cryostat, the working part of which was made of aluminum in order to reduce neutron absorption.

Figure 1 presents neutron diffraction patterns of manganese telluride taken at 120, 215, 290, and 373°K. Manganese telluride has a nickel-arsenide crystal structure of type $B8$ with lattice constants at room temperature $a = 4.143 \pm 0.002$ Å, $c = 6.711 \pm 0.003$ Å, $c/a = 1.620$ ([6]). In the neutron diffraction patterns obtained, the purely nuclear reflections (100), (002), (200), and (112) agree well with the X-ray diffraction data for the indicated values of the lattice constants.

Fig. 1. Neutron diffraction patterns of manganese telluride

Figure 1: Fig. 1. Neutron diffraction patterns of manganese telluride

Fig. 2. Temperature dependence of the magnetic moment μ (in Bohr magnetons) of the manganese ion in MnTe

Figure 2: Fig. 2. Temperature dependence of the magnetic moment μ (in Bohr magnetons) of the manganese ion in MnTe

Table 1

hkl	θ_{expt}	θ_{calc}	$\frac{I_{\text{expt}}}{I_{(100)\text{expt}}}$	$\frac{I_{\text{calc}}}{I_{(100)\text{calc}}}$
(001)	$4°10'$	$4°11'$	0.36	0.369
(100)	$7°50'$	$7°51'$	1	1
(002)	$8°25'$	$8°24'$	1.597	1.677
(101)	$8°50'$	$8°54'$	1.597	1.677
(112)	$16°10'$	$16°08'$	–	–

Along with the purely nuclear diffraction maxima, in neutron diffraction patterns taken at temperatures below the temperature of the antiferromagnetic transformation, at $\theta = 4°10'$ a diffraction maximum is clearly revealed that corresponds to a purely magnetic structure. Comparison of the intensities of the diffraction maxima determined at different temperatures indicates that the reflections (101) and (201) are mixed, caused by neutron diffraction on the crystal (nuclear) and magnetic structures.

The calculation carried out showed that the unit cell of the magnetic structure is similar to the crystallographic one, with the same constants a_M and c_M as in the crystal lattice, which agrees with the previously stated assumption ([9]). Recently an analogous model was proposed in work ([19]), although for some reason the authors believe that they are proposing a different one.

A purely magnetic reflection at $\theta = 4°10'$ is well indexed as (001), if, for example, one assumes that the magnetic structure is formed by ferromagnetic layers in the basal planes with magnetic moments perpendicular to the c axis and with antiparallel magnetic moments of neighboring basal planes.

Table 1 gives the experimental and calculated values of the angles of nuclear, magnetic, and mixed diffraction maxima obtained at room temperature, as well as the experimental and calculated ratios of the intensities of the magnetic (001) and mixed (101) reflections, together with the nuclear (002) reflections, to the intensity of the nuclear reflection (100).

Fig. 1. Neutron diffraction patterns of manganese telluride

Fig. 2. Temperature dependence of the magnetic moment μ (in Bohr magnetons) of the manganese ion in MnTe

According to the theory of neutron scattering by magnetic structures ([11]), the intensities of magnetic reflections are proportional to the square of the magnetic moment. In our case, at $\lambda = 0.99$ Å, the ratio of the intensity of the magnetic reflection $I_{(001)M}$ to the intensity of the nuclear reflection $I_{(100)N}$ is written in the form $I_{(001)M}/I_{(100)N} = 0.176\,\mu^2$. The ratio of the intensity of the mix-

···reflection $I_{(101)\mathrm{m}}$ to the intensity of the nuclear reflection

$$I_{(101)\mathrm{m}}/I_{(100)\mathrm{n}} = 0.881 + 0.0902\mu^2.$$

If the sum of the intensities of the overlapping reflections (101) and (002) is calculated, then one obtains the ratio

$$(I_{(101)\mathrm{m}} + I_{(002)\mathrm{n}})/I_{(100)\mathrm{n}} = 1.484 + 0.0902\mu^2.$$

The obtained ratios were used to calculate the magnetic moment of the manganese ions from the ratios of the intensities of the diffraction maxima obtained experimentally at different temperatures.

Figure 2 gives the curve of the temperature dependence of the magnetic moment of the manganese ions, calculated from the change in the intensity of the (101) reflection. Extrapolation of this curve to absolute zero gives a value of the magnetic moment close to that obtained from magnetic measurements ([3,5]). The value of the magnetic moment μ, calculated from the change in intensity of the (001) reflection, agrees better with the values found by Guillaud ([12]) in the compounds MnAs, MnSb, and MnBi, which, like MnTe, have a lattice of the NiAs type.

A preliminary consideration of the temperature dependence of the magnetic moment of the manganese ions indicates that the $T^{3/2}$ law ([13]), in a first approximation, satisfactorily describes the curve in Fig. 2, at least in the interval 100–300° K.

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Note: Figure translations are in progress. See original paper for figures.