JOURNAL OF THE PHYSICAL SOCIETY OF JAPAN VOL. 17, SUPPLEMENT B-III, 1962
PROCEEDINGS OF INTERNATIONAL CONFERENCE ON MAGNETISM AND CRYSTALLOGRAPHY, 1961, VOL. III

Neutron Diffraction Study of Antiferromagnetism in $FeSn_2$*

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The intermetallic compound $FeSn_2$ has been studied by neutron diffraction. The magnetic structure of the iron atoms in the unit cell is established. The first neighbours are ferromagnetic, the second and third neighbhours are antiferromagnetic. The Néel temperature is found to be 384°K in agreement with susceptibility measurements.

The magnetic properties of intermetallic compounds in the binary system, consisting of iron group transition metals and IVb group elements in the periodic table have been studied by various workers[1-5),7)]. Of these $MnSn_2$, $FeGe_2$ and $FeSn_2$ have the C16 type of structure. These compounds have been shown to be antiferromagnetic at low temperatures by magnetic susceptibiiity measurements. In this paper we report a neutron diffraction investigation of $FeSn_2$ which makes it possible to decide on the magnetic structure of iron atoms in the crystal lattice.

Tin granules and electrolytic iron were mixed in stoichiometric proportion and melted in an alumina crucible in an argon atmosphere at a temperature of 1250°C for complete dissolution of iron. The melt was allowed to cool, crushed and powdered. The powder was sealed in quartz tubes in vacuum and soaked for three days at 460°C until the peretectic reaction was complete. The sample was analysed by X-ray diffraction for absence of FeSn and Sn lines and found to be so. The powder pattern revealed the C16 type of lattice corresponding to $FeSn_2$. However, the neutron diffraction pattern of the bulk sample showed a slight contamination of β-Sn.

The neutron diffraction patterns of the sample were taken with the crystal spectrometer at the Apsara reactor. Monochromatic neutrons of wavelength 1.22 Å obtained by reflection from (111) planes of lead single crystal were used. The powder sample was contained in a flat aluminium casette inside a vacuum chamber with provision for heating the sample. The measured transmission of the sample was 0.85. Neutron diffraction patterns obtained at 300°K and 400°K are shown in Fig. 1.

The neutron diffraction pattern at room temperature shows the magnetic peaks (100) and (210) which are absent in the high temperature run at 400°K. The peaks are indexed as per the chemical unit cell which is body centred tetragonal with $a=6.502$ Å and $c=5.315$Å. The positions of iron and tin atoms in the chemical unit cell are shown in Fig. 2. The structure factor for (100) and (210) reflec-

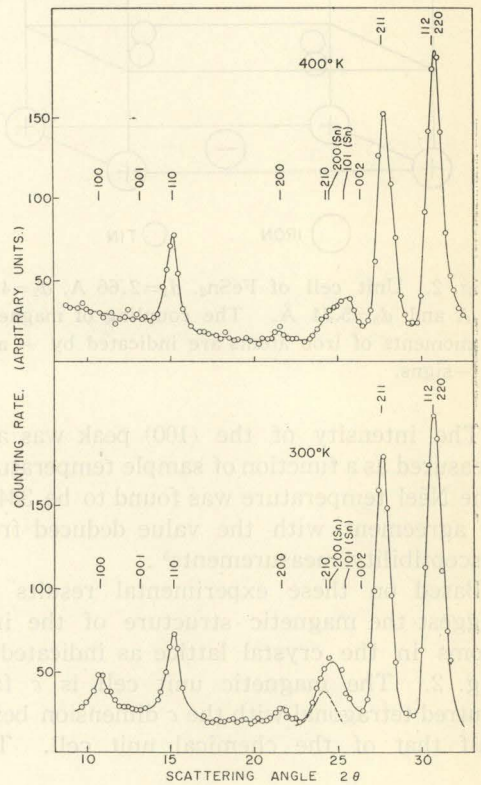

Fig. 1. Neutron diffraction pattern of $FeSn_2$ at 300°K and 400°K. The peaks are indexed as per the chemical unit cell. (100) and (210) are magnetic peaks.

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tions due to nuclear scattering are identically zero. Hence these peaks are due purely to magnetic scattering from the iron atoms. The (210) magnetic peak at room temperature is not resolved in the diffraction pattern and is contaminated by the adjacent peaks of β-Sn. However, from the change in the shape of the composite peak at higher temperature, it is obvious that the (210) peak disappears at higher temperature. The high temperature run also shows the paramagnetic diffuse scattering.

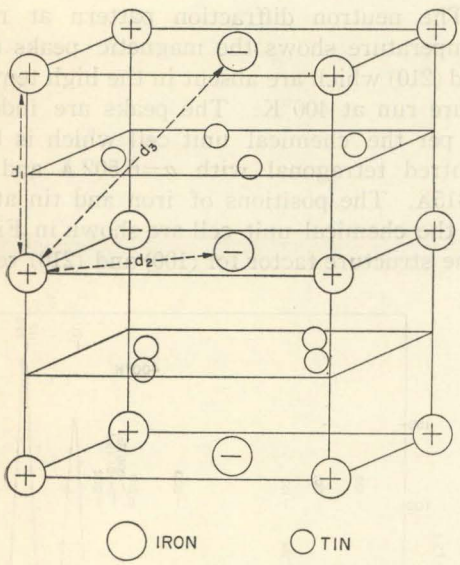

Fig. 2. Unit cell of $FeSn_2$. d_1=2.66 A, d_2=4.62 A and d_3=5.34 Å. The coupling of magnetic moments of iron atoms are indicated by + and −signs.

The intensity of the (100) peak was also measured as a function of sample temperature. The Néel temperature was found to be 384°K in agreement with the value deduced from susceptibility measurements[3].

Based on these experimental results we suggest the magnetic structure of the iron atoms in the crystal lattice as indicated in Fig. 2. The magnetic unit cell is *c* face centred tetragonal with the *c* dimension being half that of the chemical unit cell. The antiferromagnetic arrangement of the magnetic moments in the cell are indicated by + and − signs. The nearest neighbours are coupled ferromagnetically. The second and the third nearest neighbour iron atoms are coupled antiparallel. The nearest neighbour distance is 2.66Å, and from the (*J-r*) (Exchange integral verses interatomic distance) curve for iron these should be coupled parallel. The second and third neighbours are coupled antiparallel due to super-exchange interaction via the intervening Sn atoms. The angle Fe-Sn-Fe in the two cases are 113° and 148° respectively.

The magnetic structure of $FeGe_2$ and $MnSn_2$ have been inferred by Yasukochi *et al*[4,5] from general arguments based on Guillaud's[6] (*J-r*) curve. It is seen that our results for $FeSn_2$ are not in agreement with their predictions. According to them the first and second neighbours are antiparallel and the third neighbours parallel. Considering that $FeGe_2$ and $MnSn_2$ are isomorphous with $FeSn_2$ both in their structural and magnetic behaviours, it can be inferred that their magnetic structure also should be the same as that of $FeSn_2$. However neutron diffraction measurements are required to verify this.

We are thankful to Dr. R. Ramanna for his keen interest in our work. Our thanks are also due to Mr. M.R.L.N. Murthy for technical assistance. We are obliged to the staff of the Metallurgy Division for preparing the sample and for X-ray analysis.

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