HYPERFINE STRUCTURE OF THE MOSSBAUER SPECTRUM OF $FeMn_2Al$

A. S. Ilyushin

Vestnik Moskovskogo Universiteta. Fizika,
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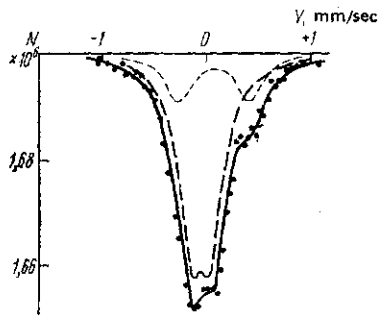
The hypertine structure of the Mossbauer spectrum of $FeMn_2Al$ has been calculated, and it is shown that the ion atoms in this structure of β-Mn type are in different electronic states. The ordering of the iron atoms in the β-Mn structure has been determined by experiment.

The compound $FeMn_2Al$ is isostructural with β-Mn (space group $P4_13$) at 650° [1], and the Mossbauer spectrum has a hyperfine structure, but no detailed interpretation of this was given in [1].

Here we interpret the hyperfine structure in the Mossbauer spectrum of $FeMn_2Al$ from data on the crystal structure.

The method of synthesizing such intermetallides has been described [1-2]. The Mossbauer spectra were recorded at room temperature on powder specimens of $FeMn_2Al$ in an El'ron spectrometer with a $^{57}Co(Pd)$ source. The spectrometer was calibrated by means of a standard specimen of carbonyl α-Fe.

The figure shows a typical Mossbauer spectrum for $FeMn_2Al$; this has a hyperfine structure and consists of at least three lines differing in intensity. Intermetallides isostructural with β-Mn are paramagnetic [2], which shows that the hyperfine structure for $FeMn_2Al$ should be considered only on the basis of the quadrupole interaction and the type of crystal structure.



Mossbauer absorption spectrum of $FeMn_2Al$ (the zero velocity position corresponds to the center of the Mossbauer spectrum of α-Fe at room temperature).

Previous studies [3-5] have shown that β-Mn has a complex crystal structure with 20 atoms in the cubic unit cell, which lie in two structurally nonequivalent positions I and II. The type I positions accomodate eight atoms, while II accomodates twelve, and in both cases the atoms do not have a spherically symmetrical environment. As a consequence, one expects hyperfine structure in the Mossbauer spectrum on account of quadrupole interaction. Quadrupole interaction in a paramagnetic gives a symmetrical doublet in the Mossbauer spectrum if there is no crystalline anisotropy [6].

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The observed spectra for $FeMn_2Al$ were interpreted on the assumption that the iron atoms lie in type I and type II positions. Each position has its own Mossbauer spectrum and its own isomeric chemical shift δ_I or δ_{II}. It was also assumed that quadrupole splitting occurs in both positions. The theoretical spectra were constructed by varying δ_I and δ_{II}, the quadrupole splittings ΔE_I and ΔE_{II}, and the relative intensity of the spectral doublets I_I/I_{II}. The best agreement between theory and experiment was obtained with the parameters given in the table.

The dashed line in the figure shows the doublets corresponding to the positions I and II in the β-Mn structure, while the solid line shows the theoretical Mossbauer spectrum for this model. This agrees well with experiment.

The data in the table on the isomeric chemical shift for $FeMn_2Al$ indicate that the electronic states of the iron atoms in positions I and II differ from one another and also from the electronic state of iron in standard body-centered cubic α-Fe. The quadrupole splittings for the I and II doublets are also different, and ΔE_I is larger than the splitting for position II. This is in good agreement with the crystal structure of β-Mn, because the type I positions have the atomic environment differing more substantially from spherically symmetrical than is the case for II.

Position	δ, mm/sec	ΔE, mm/sec	Integral intensities of doublets, rel. units
I	+0,053	0,69	300
II	−0,069	0,12	1000

If the iron atoms are randomly distributed over the I and II positions in $FeMn_2Al$, the ratio of the integral intensities for the I and II doublets would be proportional to the ratio of the number of type I positions to the number of type II positions in the β-Mn structure, which is 8/12 = 0.667. The observed ratio is 0.3, which shows that the iron atoms in $FeMn_2Al$ are preferentially located in type II positions, i.e., there is ordering of the iron atoms in the β-Mn structure. This interpretation of the hyperfine structure for $FeMn_2Al$ provides a means of examining the ordering of the iron compounds and alloys isostructural with β-Mn.

REFERENCES

1. W. E. Wallace, A. S. Ilyushin, and D. Lopez, Proceedings of the International Conference on Mossbauer Spectroscopy (Poland), vol. 2, p. 99, 1975.
2. A. S. Ilyushin and W. E. Wallace, J. Sol. Stat. Chem., vol. 17, p. 385, 1976.
3. G. D. Preston, Phil. Mag., vol. 5, p. 1207, 1928.
4. P. I. Kripyakevich, Kristallografiya, vol. 5, p. 273, 1960.
5. C. W. Kimball, J. K. Tison, and M. V. Nevitt, J. Appl. Phys., vol. 38, p. 1153, 1967.
6. V. I. Gol'danskii (editor), Chemical Applications of Mossbauer Spectroscopy [in Russian], Moscow, 1970.

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