

ELECTRONIC STRUCTURE OF $MnSi_{1.7}$ ACCORDING TO MESSBAUER SPECTROSCOPY DATA

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ABSTRACT: In the present work, a Mössbauer study of the $MnSi_{1.7}$ compound on impurity atoms of iron and tin was undertaken. These atoms isomorphically replace manganese and silicon, respectively, and therefore it is possible to determine the electronic structure of Mn and Si atoms from the parameters of the Mössbauer spectra of ^{57}Fe and ^{119}Sn .

KEY WORDS: Mössbauer spectra, local atomic symmetry, electronic configuration of atoms, X-ray phases, single- phase.

I. INTRODUCTION. The samples were synthesized in sealed quartz ampoules, followed by homogenizing annealing at $600^{\circ}C$ for 500 hours. The use of such a long annealing was caused by the need for heat treatment at a temperature below the peritectic transformation temperature of $MnSi_{1.7}$ and below the temperature of the polymorphic transformation of $FeSi_2$. The concentration of iron in $Mn_{1-x}Fe_xSi_{1.7}$ alloys varied from 0 to 30 at%. The tin concentration in the $Mn_{1-x}Fe_xSi_{1.7}$ alloys varied from 0.1 to 0.7 at%. The single-phase nature of the samples was determined by x-ray phase analysis.

II. MATERIALS AND METHODS. Mössbauer spectra were recorded on an electrodynamic type spectrometer at $295^{\circ}K$. Sources were ^{57}Co in chrome and $BaSn^{119}mO_3$. A typical spectrum is shown in Fig. 1.

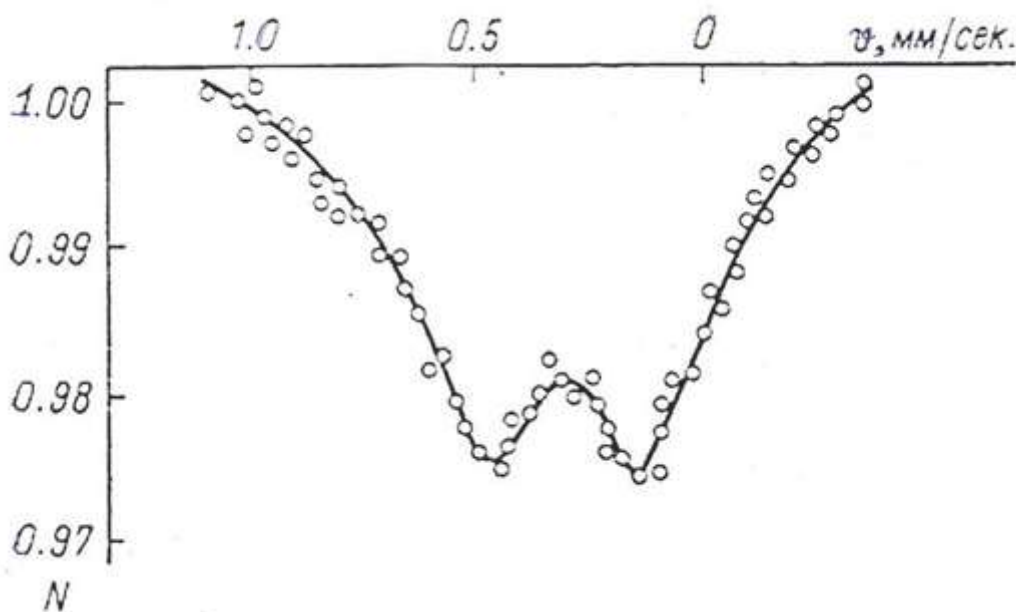




Figure No.1

The parameters of the Mössbauer spectra of ^{57}Fe in $\text{MnSi}_{1.7}$ correspond to iron atoms with the $3d^5$ electronic configuration located in a distorted cubic environment. Given the symmetry of the $6S$ electronic state, a small quadrupole splitting of the Mössbauer spectra indicates significant gradients of electric fields on ^{57}Fe nuclei. This, obviously, can only be the case of significant deviations of the local symmetry of Fe atoms from cubic. The X-ray structural data of the authors of [1] confirm this assumption.

III. RESULT AND DISCUSSION. Based on the fact that in the $\text{Mn}_{1-x}\text{Fe}_x\text{Si}_{1.7}$ system, solid substitution solutions exist up to 30 at. % [2], and also taking into account the independence of the parameters of the Mössbauer spectra of ^{57}Fe that we found on the composition in this concentration range, we can conclude that the Mn and Fe atoms are isoelectronic, i.e. have the $3d^5$ electronic configuration, although their charge states differ (+2 y manganese and +3 y iron).

It is interesting to compare the obtained Mössbauer data with data on the effect of iron on the electrical properties of $\text{MnSi}_{1.7}$. The semiconductor compound $\text{MnSi}_{1.7}$ is found exclusively with p-type conductivity [3].

Doping it with various electro active additives does not lead to a change in the type of conductivity. The concentration of holes at room temperature, measured at room temperature, is not lower than $4 \cdot 10^{20} \text{ cm}^{-3}$. On the other hand, depending on the level of doping with impurities, the FeSi_2 semiconductor compound can have both n- and p-type conductivity. However, upon the mutual dissolution of these semiconductors, a solid solution with stable n-type conductivity is always formed.

Figure 2 shows the change in electrical conductivity and thermo power in a $\text{Mn}_{1-x}\text{Fe}_x\text{Si}_{1.7}$ solid solution. The obtained dependence has the form characteristic of the conditions for compensating holes by electrons of mixed conductivity. When manganese is replaced by iron in an amount of up to 17 at.%, The thermo power increases, apparently, due to the compensation of holes by electrons. From the measurements of the Hall effect, it follows that in this interval there is a decrease in the electron concentration from $4 \cdot 10^{20}$ to $2.6 \cdot 10^{20} \text{ cm}^{-3}$. Using Mössbauer spectroscopy data, we can explain the donor effect of iron upon its substitution for manganese - the introduction of iron in $\text{MnSi}_{1.7}$ is accompanied by the introduction of an equivalent number of electrons into the conduction band.



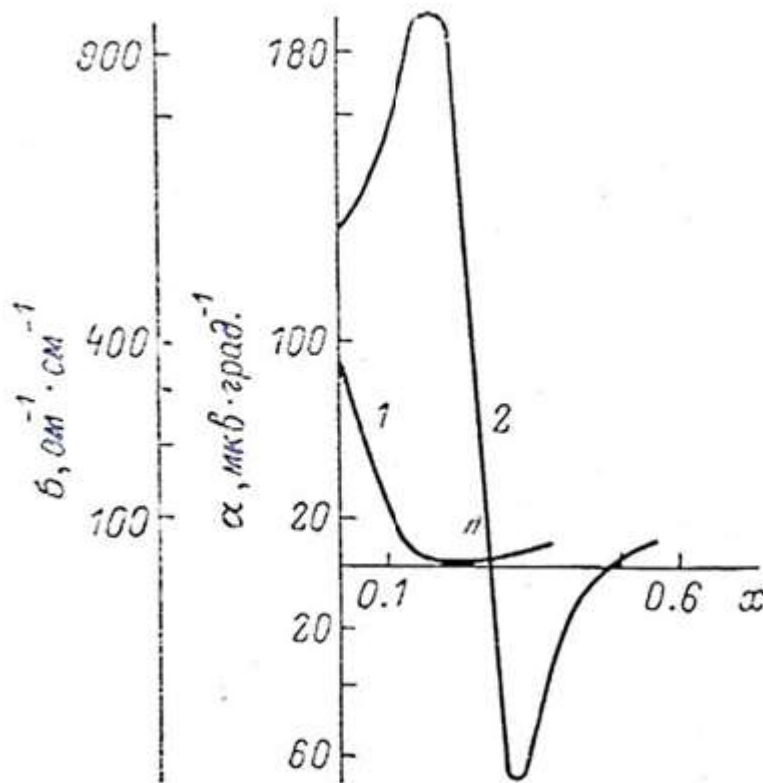


Figure No.1

IV. CONCLUSION. The parameters of the Mössbauer spectra of ^{119}Sn and $\text{MnSi}_{1.7}$ correspond to tin atoms with the electronic configuration sp^3 in a tetrahedral environment. According to [4], tin isomorphically replaces silicon in the $\text{MnSi}_{1.7}$ structure, and therefore the sp^3 - electronic configuration of tin atoms can be realized only if it is realized in silicon. In other words, Si atoms in $\text{MnSi}_{1.7}$ have a tetrahedral chemical bond system.

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