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Electronic Structure Of MnSi1.7 According to Mössbauer Spectroscopy Data

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ABSTRACT: In the present work, a Mössbauer study of the MnSi1.7 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 57Fe and 119Sn.

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 ° 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 MnSi1.7 and below the temperature of the polymorphic transformation of FeSi2. The concentration of iron in Mn1-xFexSi1.7 alloys varied from 0 to 30 at%. The tin concentration in the Mn1-xFexSi1.7 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 ° K. Sources were 57Co in chrome and BaSn119mO3. A typical spectrumis shown in Fig. 1.

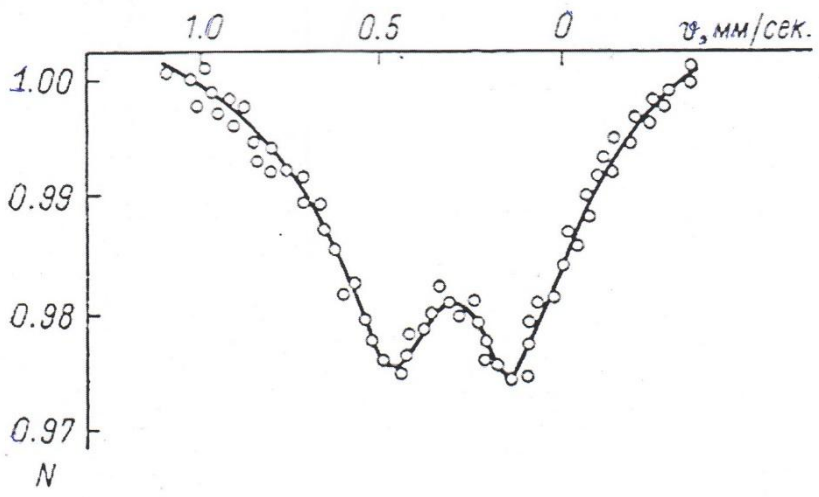

figure.1

The parameters of the Mössbauer spectra of 57Fe in MnSi1.7 correspond to iron atoms with the 3d5 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 57Fe 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.

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III.RESULT AND DISCUSSION

Based on the fact that in the Mn1-xFexSi1.7 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 57Fe 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 3d5 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 MnSi1.7. The semiconductor compound MnSi1.7 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 · 1020 cm-3. On the other hand, depending on the level of doping with impurities, the FeSi2 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 Mn1-xFexSi1.7 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 · 1020 to 2.6 · 1020 cm-3. Using Mössbauer spectroscopy data, we can explain the donor effect of iron upon its substitution for manganese - the introduction of iron in MnSi1.7 is accompanied by the introduction of an equivalent number of electrons into the conduction band.

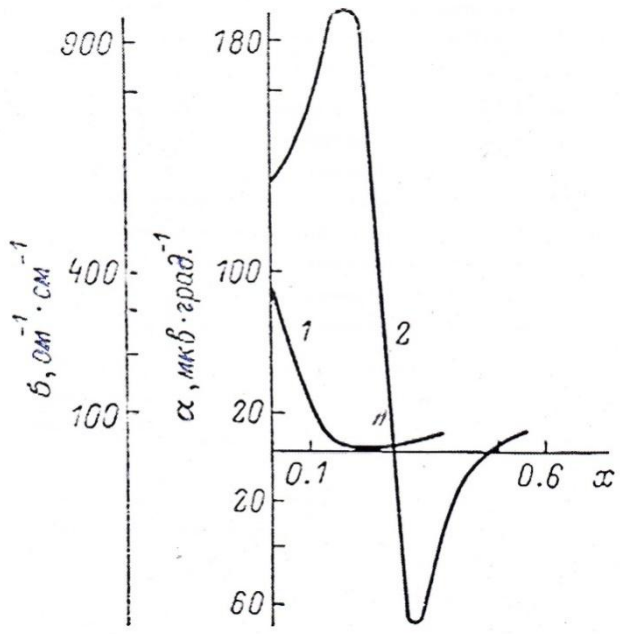

Figure2

IV. CONCLUSION

The parameters of the Mössbauer spectra of 119Sn and MnSi1.7 correspond to tin atoms with the electronic configuration sp3 in a tetrahedral environment. According to [4], tin isomorphically replaces silicon in the MnSi1.7 structure, and therefore the sp3 - electronic configuration of tin atoms can be realized only if it is realized in silicon. In other words, Si atoms in MnSi1.7 have a tetrahedral chemical bond system.

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