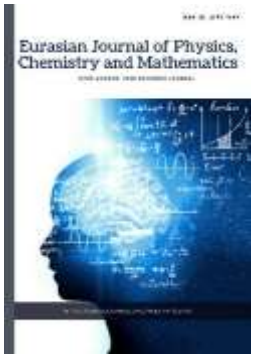

Electronic Structure of MnSi1,7 Po Dannim Mossbauer Spectroscopy

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ABSTRACT

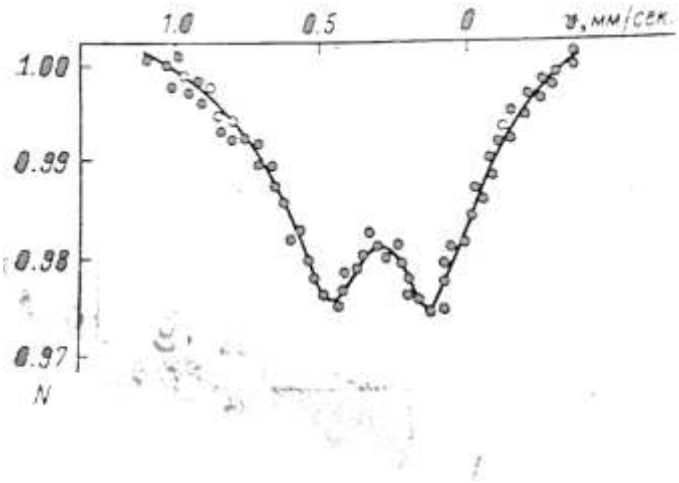
In the present work, a Messbauer study of the $MnSi_{1.7}$ compound on impurity iron and tin atoms was undertaken. These atoms isomorphically substitute for manganese and silicon, respectively, and therefore it is possible to determine the electronic structure of Mn and Si atoms from the parameters of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

Keywords: Magnesium, silicon, spectrum, glands, electron, structure, concentration, megastructure, atom

Introduction

The samples were synthesized in sealed quartz ampoules followed by homogenizing annealing at 6000C for 500 hours. The use of such a long annealing was caused by the need to conduct heat treatment at a temperature below the temperature of the peritectic transformation of MnSi1.7 and below the temperature of the polymorphic transformation of FeSi2. The iron concentration in the Mn1-xFex Si1.7 alloys varied from 0 to 30 at.%. The concentration of tin in Mn1-xFex Si1.7 alloys varied from 0.1 to 0.7 at.%. The single-phase nature of the samples was determined by X-ray phase analysis.

Mössbauer spectra were taken on an electrodynamic type spectrometer at 2950K. The sources were 57Co in chromium and BaSn 119mO3. A typical spectrum is shown in Fig. 1



Pic. 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. Taking into account the symmetry of the electronic state of 6S, a slight quadrupole splitting of the Mössbauer spectra indicates significant gradients of electric fields on the 57Fe nuclei. This can obviously be true in the case of significant deviations of the local symmetry of Fe atoms from the cubic one. The X-ray diffraction data of the authors confirm this assumption [1].

Based on the fact that substitutional solid solutions exist in the Mn1-xFexSi1,7 system up to 30 at% [2], and also taking into account the independence of the parameters of the Mössbauer spectra of 57Fe found by us from composition in this concentration range, we can conclude that Mn atoms and Fe are electronic, that is, they have an electronic configuration of 3d5, although their charge states are different (+2y manganese and +3y iron). It is interesting to compare the obtained Mössbauer data with data on the influence of the electrical properties of MnSi1.7. The semiconductor compound MnSi1.7 occurs exclusively with p-type conductivity [3].

Doping it with various electroactive additives does not lead to a change in the type of conductivity. The hole concentration at room temperature, measured at room temperature, is not lower than 4 1020 cm-3. However, when these semiconductors are mutually dissolved, a solid solution with stable n-type conductivity is always formed.

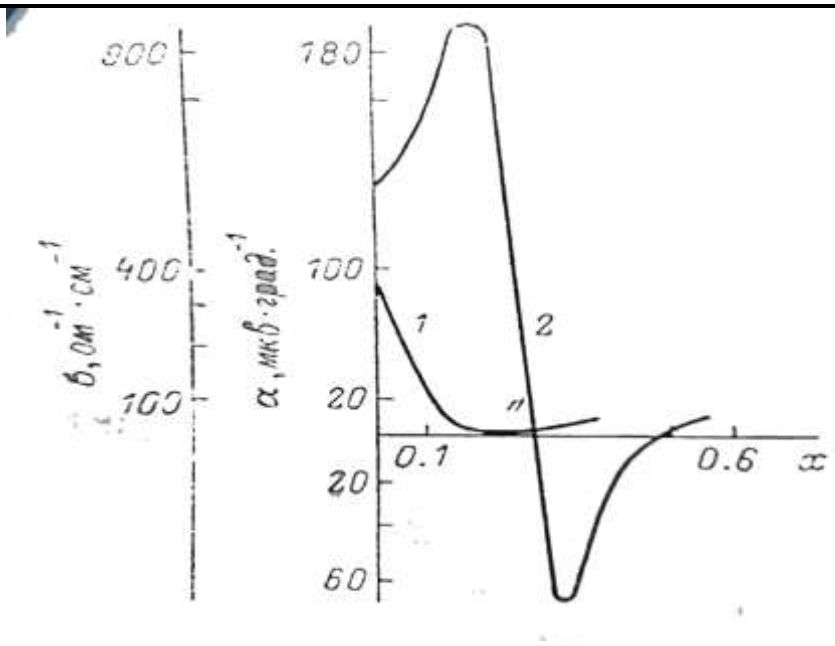


Fig .2.

Figure 2 shows the change in electrical conductivity and thermal power of the Mn1-xFex Si1.7 solid solution. The obtained dependence has the form characteristic for the conditions of compensation of holes by electrons of mixed conductivity.

When replacing manganese with iron in an amount of up to 17 at. % thermoelectric power increases, apparently due to the compensation of holes by electrons. It follows from measurements of the Hall effect that in this interval there is a decrease in the electron concentration from 4·1020 to 2.6·1020 cm-3. . Using the data of Mössbauer spectroscopy, one can explain the donor effect of iron when it replaces manganese - the introduction of iron into MnSi1.7 is accompanied by the introduction of an equivalent number of electrons into the conduction band.

The parameters of the Mössbauer spectra of , 119Sn in MnSi1.7 correspond to tin atoms from the electronic spectra of sp3. located in a tetrahedral environment [4]. According to , tin isomorphically displaces 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, the Si atoms in MnSi1.7 have a tetrahedral system of chemical bonds.

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