

Journal of Alloys and Compounds 288 (1999) 25-31

Journal of ALLOYS AND COMPOUNDS

Site distribution and hyperfine parameters of tin impurities in α manganese

G. Grosse^{a,*}, F.E. Wagner^a, V.E. Antonov^b, T.E. Antonova^b

^aPhysik-Department E15, Technische Universität München, D-85747 Garching, Germany ^bInstitute of Solid State Physics, Russian Academy of Sciences, 142432 Chernogolovka, Moscow district, Russia

Received 5 February 1999

Abstract

Dilute alloys of 0.1–0.5 at.% of enriched ¹¹⁹Sn in α manganese were transformed to hydrides with hcp, fcc and β -Mn structures by exposure to pressures of molecular hydrogen up to 3 GPa at elevated temperatures and subsequent quenching to room temperature. The samples were then transformed back to α -Mn(Sn) by hot extraction of the hydrogen at temperatures up to 400°C. ¹¹⁹Sn Mössbauer spectra taken after hydrogen extraction differed considerably from those taken before the hydrogen treatment. This observation is interpreted by a strongly different distribution of Sn atoms over the four crystallographically inequivalent sites in the α -Mn structure before and after the treatment. A quantitative evaluation of the Mössbauer spectra yields the hyperfine parameters of ¹¹⁹Sn on all Mn sites and shows that the preferred tin site is the Mn-I position in the α -Mn structure. © 1999 Elsevier Science S.A. All rights reserved.

Keywords: Mössbauer spectroscopy; a Manganese; Hydrogen treatment; High pressure

1. Introduction

 α -Mn is the allotropic modification of manganese that is stable at ambient temperature. It has a complex structure with 58 atoms in the cubic unit cell and four crystallographically inequivalent sites [1]. Below its Néel temperature of 95 K, α -Mn is ordered antiferromagnetically [2,3] with a complex, non-collinear magnetic structure with six magnetically inequivalent sites [4–6]. A structure refinement based on neutron diffraction data [6] showed that the antiferromagnetic order below 95 K is accompanied by a slight tetragonal distortion of the α -Mn structure. The details of the structure above and below the Néel temperature are summarised in Table 1.

The influence of substitutional impurities on the complex magnetic order of α -Mn is an intriguing subject. The study of tin impurities in manganese is of interest, because ¹¹⁹Sn is a convenient Mössbauer probe with a high sensitivity to transferred magnetic hyperfine fields. Despite this fact, α -Mn(Sn) solid solutions have been studied by Mössbauer spectroscopy only recently [7,8]. In [7] an unusually strong effect of Sn impurities on the Néel temperature of α -Mn has been reported. This effect could not be reproduced, however, in another study [8] of the same system, in which only a small increase of the Néel temperature with Sn concentration could be observed.

In a complex structure such as that of α -Mn, a correct interpretation of Mössbauer data from impurity probes also involves the knowledge of the lattice sites occupied by the probe atoms. From neutron diffraction data for an α -Mn(Sn) solid solution with 1 at.% Sn, Nakai [7] concluded that 70% of the Sn impurity atoms occupy the Mn-II site in α -Mn (Table 1). This result is surprising since one would expect that for the relatively large Sn atoms it would be energetically preferable to occupy the largest available site in the α -Mn structure, which is the site Mn-I. In the present work a method is introduced which allows the preparation of α -Mn(Sn) samples in which the distribution of the Sn impurities over the sites in the α -Mn structure differs strongly from that in the equilibrium state. The investigation of such samples by ¹¹⁹Sn Mössbauer spectroscopy provides an alternative means to study the site distribution of Sn in α -Mn(Sn) solid solutions.

2. Experimental

Dilute alloys of 0.1, 0.2 and 0.5 at.% tin in manganese were prepared from the elements by arc-melting in an argon atmosphere. ¹¹⁹Sn isotopically enriched to 92.5% and manganese of 99.98% purity were used as starting materials. After melting the ingots were crushed into small

*Corresponding author.

E-mail address: ggrosse@ph.tum.de (G. Grosse)

Space group I43m (at 305 K)					Space group	Space group I42m (at 15 K)					
Atom	Site ^a		x	у	z	Atom	Site		x	у	z
Mn-I	2a	4 3m	0	0	0	Mn-I	2a	4 2m	0	0	0
Mn-II	8c	3m	.318	.318	.318	Mn-II	8i	m	.319	.319	.317
Mn-III	24g	m	.358	.358	.035	Mn-IIIa	8i	m	.362	.362	.041
	-					Mn-IIIb	16j	1	.353	.033	.356
Mn-IV	24g	m	.091	.091	.283	Mn-IVa	8i	m	.092	.092	.279
						Mn-IVb	16j	1	.090	.285	.089

Crystal structure of α -Mn above and below the Néel temperature [6]

^a Wykoff notation with multiplicity and site symmetry.

pieces and annealed at 600°C in evacuated quartz tubes. The annealing time varied between 10 and 30 h. The annealed samples were then ground to a powder and characterised by X-ray diffraction using FeK α radiation. The diffraction patterns showed that the samples had the α -Mn structure. In the case of the 0.5 at.% Sn alloy, a small amount of a β -Mn(Sn) phase was observed, while in the other alloys no impurity phases were detectable.

The samples were then transformed to hydrides by exposing them to molecular hydrogen at pressures up to 3 GPa and temperatures up to 800°C, using a high-pressure technique described elsewhere [9,10]. The preparation conditions were chosen so as to synthesize β , γ and ε manganese hydrides [10], which have metal lattices with β -Mn, fcc, and hcp structures, respectively. These hydrides are metastable under ambient conditions. The hydrides and their conditions of preparation are listed in Table 2.

The hydrogen was then extracted from the prepared hydrides by heating the samples in vacuum to temperatures up to 400°C. The hot extraction took about 20–30 min and was stopped when no further release of hydrogen gas was detectable. The hydrogen release typically started about 5-10 min after the start of the heating.

Before hydrogen loading and after the hot extraction, Mössbauer spectra were taken using a source of 119m Sn in CaSnO₃. Spectra at 4.2 K were measured in a He bath cryostat with both source and absorber at 4.2 K, and

Table 2							
Conditions	of	preparation	of	the	studied	hydride	samples

Name ^a	Sn-conc. ^b	P^{c}	T^{d}	Type ^e	x^{f}
β-0.2	0.2	0.6	800	β-MnH	0.11
β-0.5	0.5	0.6	800	β-MnH	0.10
γ-0.2	0.2	2.0	800	γ -MnH	0.41
<i>ɛ</i> -0.1	0.1	2.9	325	<i>ε</i> -MnH	0.85
<i>ɛ</i> -0.2	0.2	2.8	325	ε -MnH	0.89
<i>ɛ</i> -0.5	0.5	2.9	325	<i>ε</i> -MnH	0.86

^a Symbolic name by which the sample is referred to in the text.

^b Tin concentration (at.%).

^c Hydrogen pressure (GPa) during the hydrogenation.

 $^{\rm d}$ Temperature (°C) during the hydrogenation.

^e Structure type of the produced hydride.

 $^{\rm f}$ Hydrogen content (hydrogen-to-metal ratio) of the produced hydride $Mn_{1-y}Sn_{y}H_{x}$.

spectra in the range 10–300 K were measured in a gas flow cryostat with the source at room temperature. The 23.9 keV γ -rays were detected by a scintillation counter, and a Pd foil of 35- μ m thickness was used to attenuate the SnK α X-rays from the Mössbauer source. The spectra were evaluated by fitting transmission integrals of Voigt profiles to the measured data. Details of the fitting procedure will be described later. The ratio of resonant quanta to all detected events was determined by separate measurement of a β -Sn reference absorber of known thickness and *f* factor [11].

3. Results and discussion

3.1. Mössbauer spectra

Representative Mössbauer spectra of ¹¹⁹Sn in α -Mn after annealing at 600°C but before the hydrogen treatment are shown in Fig. 1. At room temperature the spectrum of α -Mn(Sn) is a slightly broadened single line with an isomer shift of 1.45 mm/s (Fig. 1, top). The saturation corrected absorber linewidth of 0.38 mm/s is only slightly larger than the natural linewidth of 0.32 mm/s. At 4.2 K the spectrum of α -Mn(Sn) splits magnetically (Fig. 1, bottom). While it is possible to fit the spectrum with a single, slightly broadened sextet pattern with a hyperfine field of 3.6 Tesla and an isomer shift of 1.44 mm/s, better fits are obtained by allowing for two or three sextets. The fit shown in Fig. 1 is based on a model described below that takes into account all the possible sites that Sn can occupy in the α -Mn structure.

The spectra of alloys with 0.1 and 0.5 at.% Sn look like those of Fig. 1, except for a β -Mn(Sn) impurity in the 0.5 at.% alloy, which at room temperature shows as a quadrupole doublet with a splitting of about 0.8 mm/s and an isomer shift of about 1.65 mm/s [12,13]. The presence of this impurity can be explained by assuming that after the arc-melting the Sn concentration was not quite homogeneous and locally reached values above the solubility limit of about 1 at.% of Sn in α -Mn at the annealing temperature of 600°C [14]. This would lead to local precipitations of a

Table 1





Fig. 1. Mössbauer spectra of an α -Mn(Sn) sample with 0.2 at.% ¹¹⁹Sn before any hydrogen treatment. The sample had been annealed at 600°C for several hours.

β-Mn(Sn) phase with a Sn concentration of about 2 at.%, the lower solubility limit of Sn in β-Mn at 600°C [14]. From the intensity of the β-Mn(Sn) component in the Mössbauer spectrum and its assumed Sn content the impurity phase concentration can be estimated to be 5 at.%. Below about 25 K the Mössbauer spectrum of a β-Mn(Sn) phase with 2 at.% Sn splits magnetically with a broad distribution of hyperfine fields [15] and is not easily separated from the spectrum of α-Mn(Sn).

The 4.2 K Mössbauer spectra obtained after hydrogen extraction are shown in Fig. 2. They differ drastically from those measured before the hydrogen treatment. The spectra of outgassed β-Mn hydrides clearly show a paramagnetic β -Mn(Sn) component, which means that upon hydrogen extraction the transformation back to α -Mn was incomplete. In the case of the β -0.5 sample the paramagnetic quadrupole doublet has a broad shoulder which indicates that the β -Mn(Sn) phase is on the verge of splitting magnetically. The fact that the β -Mn(Sn) component is still at least partly paramagnetic at 4.2 K shows that its Sn content is significantly below 1 at.% [15] and thus suggests a rather homogeneous distribution of the Sn atoms. The spectra of all other samples are of considerable complexity, but are all quite similar and show no paramagnetic component that could correspond to a β -Mn(Sn) phase. The most probable reason for the complexity of the spectra is a different distribution of the Sn atoms over the crystallographically and magnetically inequivalent sites of the α -Mn structure in the hydrogen treated samples.

3.2. Fitting procedure

A correct interpretation of the Mössbauer spectra of ^{119}Sn in $\alpha\text{-Mn}(\text{Sn})$ after hydrogen extraction must therefore take into account all possible sites the Sn atoms can occupy in the α -Mn structure. In this structure there are four crystallographically inequivalent sites, conveniently designated Mn-I through Mn-IV (Table 1). At the Néel temperature of 95 K, two of these, Mn-III and Mn-IV, split into two magnetically inequivalent sites each [4,6]. This symmetry breaking is accompanied by a tetragonal distortion of the cubic unit cell, which renders the magnetically inequivalent sites also crystallographically slightly different [6]. While this distortion can hardly be expected to have a measurable effect on the isomer shift or the quadrupole splitting of the Mössbauer spectra, the magnetic inequivalence of the sites has certainly to be taken into account. One can therefore expect up to six distinct components in the Mössbauer spectra of dilute ¹¹⁹Sn in α-Mn below its Néel temperature.

Without any additional information it would be difficult to identify these six components in a single 4.2 K spectrum of α -Mn(Sn) with any certainty. One can assume, however, that these six components are present in all spectra of ¹¹⁹Sn in α -Mn, both before and after the hydrogen treatment and have equal hyperfine parameters but different intensities. Furthermore, the crystallographic and magnetic symmetry places certain constraints on the hyperfine parameters of the different sites. One is that the electric field gradient and thus the quadrupole splitting on site Mn-I must vanish due to its cubic symmetry. To assess the magnitude of possible quadrupole splittings on the other sites, a point charge model for the electric field gradient was applied using the next neighbour atom coordinates listed in [16]. This yielded a ratio of quadrupole splittings of 0.14:1.00:0.89 for the sites Mn-II through Mn-IV, which indicates that the quadrupole splitting on site II is small. In the fitting model it was therefore assumed to be zero.

For the sites Mn-III and Mn-IV, noticeable quadrupole splittings can be expected and were allowed in the fits. Below the Néel temperature these two sites each split into a pair of two magnetically inequivalent sites with a multiplicity ratio of 1:2 (Table 1). Any measurable redistribution of Sn atoms can certainly occur only at temperatures far above the antiferromagnetic transition at 95 K, where the sites within a pair are equivalent. Thus the occupation probability within a pair must be given by the multiplicity ratio and the relative Mössbauer areas within each pair should show the same ratio. Since below the Néel temperature the sites within a pair are crystallographically still almost equivalent, they are expected to show the same isomer shift in the 4.2 K Mössbauer spectra. The quadrupole splittings, however, may differ, as it is the projection of the electric field gradient on the direction of the hyperfine field that determines the effective quadrupole splitting observed in the spectra.



Fig. 2. 4.2 K Mössbauer spectra of α-Mn(Sn) samples after hydrogen loading and hot extraction. The sample codes are given in Table 2.

The fitting model thus allows for two components with zero quadrupole splitting and two pairs of components with non-vanishing quadrupole splitting. Within each pair both components are constrained to have an intensity ratio of 1:2 and the same isomer shift. The effective quadrupole splittings are allowed to be different within each pair. The first two components correspond to the sites Mn-I and Mn-II, and the two pairs of components correspond to the site pairs Mn-IIIa and Mn-IIIb, and Mn-IVa and Mn-IVb, respectively.

Each individual component was described by a sextet pattern of Gaussian broadened Lorentzian lines (Voigtprofiles). The Gaussian broadening arises from distributions of the hyperfine field, quadrupole splitting and isomer shift. The latter two contributions cannot be separated as they affect the linewidths of the six lines in the same way. This leaves two distinguishable contributions to the Gaussian width, of which the width of the hyperfine field distribution was allowed differ for the individual components, whereas the width due to isomer shift and quadrupole splitting distributions was somewhat arbitrarily assumed to be the same for all components in one spectrum. This was done to limit the number of free parameters in the fits. For the Lorentzian width a fixed value close to the natural linewidth was used.

In applying this fitting model to the 4.2 K spectra of the studied α -Mn(Sn) samples before and after the hydrogen treatment, the hyperfine parameters, including the widths of the hyperfine field distributions, of the described components were constrained to be the same for all spectra. Only the relative intensities of the components and the line broadening due to distributions of the isomer shift and quadrupole splitting were allowed to differ between the different spectra, taking into account the differing tin occupation of the corresponding sites and varying degrees of strain and lattice imperfection in the different samples. These constraints restricted the number of free parameters for the individual spectra to six: four intensities, one linewidth and the background level. In addition to that there are 20 parameters common to all spectra: four isomer

shifts, four quadrupole splittings, six hyperfine fields and six field distribution widths.

3.3. Fit results and site assignments

By the described method all 4.2 K spectra of samples with the α -Mn structure can be fitted remarkably well (Figs. 1 and 2). The spectrum of the β -0.2 sample could be included into the fit after allowing for a quadrupole doublet corresponding to a β -Mn(Sn) phase that did not transform back to α -Mn(Sn) during the hydrogen extraction. The α -Mn(Sn) fraction in the spectrum of sample β -0.5, however, was too small for a meaningful analysis.

The hyperfine parameters of the different components obtained in this way are summarised in Table 3. Since the fitting model can distinguish neither between the sites Mn-I and Mn-II nor between the sites Mn-III and Mn-IV, the assignment given in the table has to be based on physical arguments, the basic idea being that after the hydrogen extraction the distribution of the tin over the individual sites is much closer to random than in the well annealed samples, where most of the tin occupies one preferred site.

The sites Mn-I and Mn-II can be distinguished by their different multiplicity as follows: In the spectra of well annealed α -Mn(Sn) samples, before any hydrogen treatment, the component with an isomer shift S = 1.45 mm/sand a hyperfine field of 3.6 T is by far the strongest (Fig. 1). The corresponding site - either Mn-I or Mn-II according to the fit results - is thus the one preferably occupied by Sn. After the hydrogen treatment, the site distribution of the Sn atoms is strongly different. This is most probably so because the phase transformation from the fcc and hcp hydride phases, in which all metal sites are equivalent, to the α -Mn phase is too fast for the Sn atoms to reach their preferred lattice positions by diffusion processes, which will still be rather slow at the extraction temperature. The expected site distribution of the Sn atoms after the hydrogen extraction is thus expected to be a random distribution with a possible bias towards the sites preferred by Sn. The relative areas of the components in the Mössbauer spectra should therefore be proportional to the

Table 3

Hyperfine parameters of ^{119}Sn on the six magnetically inequivalent sites of the $\alpha\text{-Mn}$ structure

Site	S^{a}	\varDelta^{b}	$B_{ m hf}^{\ \ m c}$	$\sigma^{ ext{d}}$	
Mn-I	1.45	0	3.6	0.4	
Mn-II	1.61	0	2.8	1.0	
Mn-IIIa	1.62	+0.55	7.8	0.8	
Mn-IIIb	1.62	-0.23	7.2	0.8	
Mn-IVa	≈1.9	≈ 0	20.8	4.3	
Mn-IVb	≈1.9	≈ 0	10.8	4.3	

 $^{\rm a}$ Isomer shift (mm/s) relative to ${\rm CaSnO_3}$ at the same temperature.

^b Quadrupole splitting $eQV_{zz}/2 \cdot (3 \cos^2 \theta - 1)/2$ (mm).

^c Mean hyperfine field in Tesla.

^d Width of the Gaussian hyperfine field distribution in Tesla.

50 β-0.2 45 0 γ-0.2 Occupation probability [%] ε-0.1 40 × 0 + Δ ε-0.2 Δ 35 × ε-0.5 Δ 30 0 25 -0 20 -15 -10 - $\Delta +$ 5 0 Mn-II Mn-III Mn-IV Mn-I

Fig. 3. Relative intensities of the components attributed to the sites Mn-I through Mn-IV in the 4.2 K Mössbauer spectra of hydrogen treated α -Mn(Sn) samples after hydrogen extraction. The horizontal lines represent the relative multiplicities of the sites in the α -Mn structure.

multiplicities of the corresponding sites, again with a possible bias towards the preferred sites.

Fig. 3 shows the observed fractional Mössbauer areas in the spectra obtained after hydrogen treatment together with the crystallographic site multiplicities. For a random distribution of tin over the different sites, the fractional Mössbauer areas and the site multiplicities should be the same. With the site assignment used in Fig. 3 and Table 3, the observed areas are consistent with the site multiplicities. The reverse assignment of the sites Mn-I and Mn-II, however, would imply that the preferred site for tin occupation would be Mn-II and that this site is occupied below its statistical weight in the hydrogen treated samples. A physical mechanism that would lead to such an occupation inversion during the hydrogen extraction is hardly conceivable. The component with isomer shift S =1.45 mm/s and a hyperfine field of 3.6 T has thus to be assigned to the site Mn-I, which also implies that it is site Mn-I which is preferably occupied by tin in α -Mn(Sn) samples annealed at 600°C.

It is worthwhile to note that this conclusion is independent of details of the applied fitting model. It is merely based on the observation that the strongest component of the Mössbauer spectra of annealed α -Mn(Sn) samples is by far the weakest in the spectra obtained after hydrogen treatment and should therefore arise from the site with lowest multiplicity. While the observation that the site Mn-I is the preferred site for Sn occupation is in disagreement with the results of Nakai [7], it is supported by the fact that with a nearest neighbour distance of 2.713 Å [16] the Mn-I site is the largest in the α -Mn structure. The nearest neighbour distance from the Mn-II site, 2.485 Å, is already considerably smaller. These values have to be compared, for example, with the nearest neighbour distance in β -Sn, 3.02 Å [16]. Possible reasons for the differing results of [7] are difficult to analyse as the author neither shows the neutron data his conclusions are based on nor gives details on their evaluation.

The assignment of the remaining two pairs of components to the sites Mn-III and Mn-IV is less conclusive than that for the sites Mn-I and Mn-II. One can assume that the occupation of the smallest site Mn-IV with a nearest neighbour distance of 2.239 Å leads to considerably stronger strains and thus to a broader distribution of hyperfine fields than the occupation of the site Mn-III with a nearest neighbour distance of 2.448 Å. Based on this argument, the component with the highest hyperfine field and the broadest field distribution has tentatively been assigned to the site Mn-IV. This assignment is in line with the observation that the occupation of the smaller site Mn-IV in the samples after hydrogen extraction is generally somewhat smaller than that of site Mn-III (Fig. 3), although the multiplicities of the two sites are equal.

It is remarkable that in the sample β -0.2 the components with the largest magnetic hyperfine fields are missing, which means that the Sn occupation of site Mn-IV is much smaller than in the other samples after hydrogen treatment. The reason for this behaviour might lie in details of the mechanism of the β - α phase transformation during the hydrogen extraction. There are two crystallographically inequivalent sites in the β -Mn structure. It is conceivable that the site mainly occupied by Sn in β -Mn(Sn) hydrides is not transformed into the Mn-IV site during the hydrogen extraction.

3.4. Alternative explanations

While the site distribution model described above provides a consistent picture of the behaviour of Sn as a Mössbauer probe in α -Mn(Sn) solid solutions, it is necessary to consider also alternative explanations for the differing spectra obtained before and after hydrogen treatment of Mn(Sn) alloys and for the complexity of the latter. The most probable alternative explanation would be the formation of impurity phases during the hydrogen treatment. Since X-ray diffractograms showed no phases other than α -Mn(Sn) in the hydrogen treated samples, such impurity phases must either be amorphous or represent only a very small volume fraction of the sample. The latter is possible only if the Sn concentration in the impurity phases is significantly higher than the overall Sn content of the samples.

In the Mn–Sn system there are three intermetallic phases that need to be considered as potential impurity phases: Mn₃Sn, Mn₂Sn and MnSn₂ [14]. Mn₃Sn is an antiferromagnet with a Néel temperature of 400–420 K [17], Mn₂Sn is a ferrimagnet with a Curie temperature of 260–270 K [18], and MnSn₂ is again an antiferromagnet with a Néel temperature of 325 K [19]. Thus the ordering temperatures of all intermetallic phases are significantly higher than that of α -Mn(Sn), whose Néel temperature is around 100 K [8]. Fig. 4 shows Mössbauer spectra of the



Fig. 4. Mössbauer spectra of sample ε -0.2 after hydrogen treatment at various temperatures.

 ε -0.2 sample after hydrogen extraction at several temperatures. While the Néel transition at around 100 K is considerably smeared out compared to well annealed α -Mn(Sn) [8,20], the sample is clearly paramagnetic at 200 K, well below the ordering temperatures of the known Mn–Sn intermetallic phases, which thereby can be excluded as possible impurity phases.

Another possibility that needs to be considered is the formation of a tin rich mixed Mn–Sn hydride phase which is stable at the applied hydrogen extraction temperatures. The only such hydride phase known so far is Mn_3SnH_x . A Mössbauer study of this hydride [21] showed, however, that it is magnetically ordered up to above room temperature and thus cannot account for the spectra of outgassed Mn(Sn) hydrides. The only remaining alternatives, namely



Fig. 5. Site occupation probability of Sn impurities in α -Mn(Sn) (sample ε -0.1) after different treatments.

the formation of one or more yet unknown Mn–Sn intermetallic phases or hydrides thereof, or of an amorphous Mn–Sn alloy phase, seem quite improbable.

3.5. Annealing behaviour

The site distribution of the tin impurities can be influenced by further thermal treatment of the samples after hydrogen extraction. This is shown in Fig. 5 for the ε -0.1 sample. A 48 h treatment at 250°C in vacuum leads to a small but noticeable migration of Sn atoms from Mn-II sites to Mn-I sites. After 48 h at 400°C, the population of the Mn-I site has increased considerably and that of the Mn-III and M-IV sites has gone down accordingly by a factor of 2–3. The rightmost points in Fig. 5 show the site distribution in the initial α -Mn(Sn) samples before the hydrogen treatment. This distribution can be considered to represent the equilibrium state at the annealing temperature of 600°C. Almost 80% of the Sn atoms occupy the Mn-I site, about 15% occupy site Mn-II and the remainder is distributed about equally over the sites Mn-III and Mn-IV.

4. Conclusions

By high pressure loading of dilute Mn(Sn) alloys with hydrogen and subsequent hot extraction it is possible to prepare α -Mn(Sn) samples in which the distribution of the Sn impurity atoms over the four crystallographic sites in the α -Mn structure deviates strongly from the equilibrium distribution. The study of such samples by ¹¹⁹Sn Mössbauer spectroscopy allowed the determination of the hyperfine parameters of ¹¹⁹Sn on all four Mn sites and the identification of the site preferably occupied by Sn. In equilibrium at 600°C about 80% of the Sn atoms occupy the site Mn-I, which has the largest volume of all sites in the α -Mn structure.

Acknowledgements

The work was supported by the Grants No. 99-02-17299 and 96-15-96806 from the Russian Foundation for Basic Research.

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