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The Local Atomic Structure Study of Ordered Fe₃Si and Disordered by Grinding Fe₇₅Si₂₅ Alloys with EXAFS and Mössbauer Techniques

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Abstract. The ordered Fe₃Si and disordered Fe₇₅Si₂₅ alloys are studied by X-ray diffraction, Mössbauer spectroscopy and EXAFS -analysis. The X-ray diffraction pattern and Mössbauer spectrum of the Fe₇₅Si₂₅ alloy in comparison with those of the ordered sample give evidence for the set of local atomic configurations of Fe atom and are characteristic for the disordered *bcc* samples of the Fe-Si system. The comparison of $\chi(k)$ in these alloys shows noticeable differences, especially in 3.5-5 Å⁻¹ region. Combining all the data obtained with the model $\chi(k)$ one can draw the conclusion that the changes in the Fe atom local structure of the Fe₇₅Si₂₅ alloy are connected with breaking a long-range order but do not correspond to a chaotic distribution of atoms.

1. Introduction

The local atomic structure study of nonordered system "transition metal-metalloid" is of a considerable interest for understanding its influence on physical properties. While a great deal of experimental data on the local atomic structure obtained by numerous structure-sensitive techniques has been accumulated, for microcrystalline and nanocrystalline metastable disordered binary systems of Fe - sp-element there is a lack of information from direct structural methods. It is known that mechanical grinding allows to obtain microcrystalline Fe alloys with Al, Si in a monophasic disordered state over a wide concentration range (up to 60 - 70 at.% sp-element). The manners of the description of the concentration behaviour of their magnetic characteristics are based on various hypotheses on the local atomic structure: a chemical short-range order [1], the change of the effective coordination number in the nearest surrounding [2], the distribution of grains in sizes within a nanometric scale [3]. That is why in this work we combine both common methods yielding data on macrostructure (X-ray diffraction) and indirect data on local structure (Mössbauer spectroscopy) with EXAFS measurements. One of the alloys studied is a characteristic for equilibrium crystalline compounds (Fe₃Si) while the other one - for metastable disordered systems (Fe₇₅Si₂₅). This pair is a good model sample to trace order-disorder changes.

2. Experimental

The Fe alloys with 25 at.% Si were melt from Fe and Si of high purity in an Ar induction furnace. Then the Fe₇₅Si₂₅ alloy was ground in a ball mill for 30 h in an argon atmosphere. The Fe₃Si alloy was obtained from the ground alloy by annealing for 1h at 800 °C and then for 10h at 400 °C. Both samples were tested by X-ray diffraction and Mössbauer spectroscopy. X-ray diffraction analysis was performed using filtered Fe- K_α radiation. The Mössbauer spectra on ⁵⁷Fe nuclei were taken with a ⁵⁷Co-source in a chromium matrix at the temperatures 300 and 80 K. The monophasic state of the samples was also checked in the measurement of temperature dependence of magnetic susceptibility. The EXAFS-experiment was performed with a laboratory spectrometer RAS-1 at T = 300 K using a Mo-tube and bent (1340) SiO₂ crystal-monochromator.

3. Results and discussion

X-ray diffraction patterns for the Fe₃Si (a) and Fe₇₅Si₂₅ (b) samples given in Fig.1 show that both of them are monophasic. In the Fe₃Si pattern besides *bcc* phase peaks there are DO₃ superlattice (111) and (200) peaks of equal intensity (marked "I") proving that the chemical long-range order parameters are close to the maximum for this superlattice in stoichiometric alloy. For the Fe₇₅Si₂₅ alloy there are only broadened peaks of *bcc* structure. The lattice parameters calculated for them are close and equal to 1/2 $\bar{a}$ (Fe₃Si) = 2.82545 Å and $\bar{a}$ (Fe₇₅Si₂₅) = 2.8368 Å, respectively. The Mössbauer spectra and restored from them hyperfine magnetic field distribution functions P(H) are shown in Fig.2. For the Fe₃Si compound (a) they consist of only 2 sextets and 2 peaks in P(H), corresponding to 2 nonequivalent configurations of the Fe atom: 1- with 8 Fe atoms and 2 - with 4 Fe and 4 Si atoms nearest neighbours. The Mössbauer spectrum and P(H) of Fe₇₅Si₂₅ are characteristic of a disordered state with a set of nonequivalent surroundings of the Fe atom. Preceding mathematical processing of the spectrum also showed that the probabilities of Fe atom nearest surroundings differed from the chaotic distribution of the Fe and Si

atoms in a *bcc* lattice with coordination number of the nearest atoms $Z=8$. Mössbauer study of the *bcc* Fe-Si alloys [1] allowed to conclude that the considerable changes of the local atomic structure in the two nearest spheres took place on increasing the Si concentration. The same thing is testified by the comparison of the normalized oscillating parts $\chi(k)$ of the disordered *bcc* alloys $\text{Fe}_{85}\text{Si}_{15}$ and $\text{Fe}_{67}\text{Si}_{33}$ (Fig.3,d,e) with that of the $\text{Fe}_{75}\text{Si}_{25}$ alloy (Fig.3,c). What kind of the changes appear can be seen from EXAFS measurements of the ordered Fe_3Si and disordered $\text{Fe}_{75}\text{Si}_{25}$ alloys shown in Fig.3.

Figure 1: X-ray diffraction patterns Fe_3Si and $\text{Fe}_{75}\text{Si}_{25}$ alloys.

Figure 2: Mössbauer spectra and $P(H)$ of Fe_3Si , $\text{Fe}_{75}\text{Si}_{25}$ alloys.

Figure 3: Model $\chi(k)$ (a), and experimental $\chi(k)$ for Fe_3Si (b), for $\text{Fe}_{75}\text{Si}_{25}$ (c), for $\text{Fe}_{85}\text{Si}_{15}$ (d) and for $\text{Fe}_{67}\text{Si}_{33}$ (e).

Figure 4: The Fourier transform of EXAFS for Fe_3Si (a) and for $\text{Fe}_{75}\text{Si}_{25}$ (b).

Comparing $\chi(k)$ (b) and (c) it is seen that the main differences take place in the $3.5\text{--}5\text{ \AA}^{-1}$ region, where the backscattering amplitude values of the Si atom is higher than those of the Fe atom. The model $\chi(k)$ the Fe_3Si compound calculated with model partial radial distribution functions (RDF) of ideal DO_3 superlattice (Fig.3,a) is seen to be in a good agreement with the experimental one. Some trivial models of RDF for the disordered alloy $\text{Fe}_{75}\text{Si}_{25}$ corresponding to chaotic atoms distribution do not explain the differences observed in $\chi(k)$. Fourier transform analysis results for both alloys (Fig.4) reflect the fact that there are some changes in the first two spheres and the noticeable changes in the next spheres confirm breaking the chemical long-range order. All of that allows to make only a qualitative evaluation of the change of the local chemical arrangement. To obtain correct detailed information on partial RDF some more structure experiments will be essential.

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