Journal of Alloys and Compounds 477 (2009) 4–7

Contents lists available at ScienceDirect

Journal of Alloys and Compounds

journal homepage: www.elsevier.com/locate/jallcom

Spin- and charge density around Rh impurity in α-Fe studied by ^{57}Fe Mössbauer spectroscopy

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ARTICLE INFO

Article history:
Received 22 September 2008
Accepted 7 October 2008
Available online 2 December 2008

PACS:
75.50.Bb
75.30.Fv
71.45.Lr
76.80.+y

Keywords:
Spin and charge density
Mössbauer spectroscopy
Impurities in metals

ABSTRACT

Random solution of rhodium in ferromagnetic α-Fe of the BCC structure has been investigated by means of the 14.4-keV Mössbauer transition in ^{57}Fe at room temperature. Rhodium atoms have been randomly substituted on the iron sites with the concentration up to 15 at.%. Contributions to the hyperfine field and isomer shift on the iron nuclei have been determined as the function of the distance between iron nucleus and rhodium impurity up to the third co-ordination shell. Rhodium atom as the nearest iron neighbor changes iron hyperfine field by +0.73 T, as the second neighbor makes change by +0.70 T and finally as the third neighbor changes the field by +0.43 T. Corresponding changes in the isomer shift are as follows: −0.015 mm/s, −0.005 mm/s and +0.039 mm/s. The average hyperfine field and the isomer shift increase linearly versus rhodium concentration at rates 0.156 T/at.% and 4.42×10^{-3} mm/(s at.%), respectively. Hence, addition of rhodium lowers the electron density ρ on the iron nucleus at the rate $\partial\rho/\partial c = -1.52 \times 10^{-2}$ electron a.u.$^{-3}$ (at.%)$^{-1}$.

1. Introduction

Mössbauer spectroscopy is sensitive to the local environment of the resonant atom. In particular one can investigate influence of the adjacent impurity on the hyperfine field and isomer shift experienced by the resonant nucleus [1,2]. Perturbations to the spin- and charge density on the iron nucleus due to the impurity located on the regular lattice site of the BCC iron could be seen to the second or sometimes to the third co-ordination shell [3,4]. Rhodium dissolves randomly in the BCC α-Fe up to about 11 at.% at low temperature equilibrium [5]. However, the α-phase is stable at low temperature up to about 55 at.% of rhodium. For the rhodium concentration range 11–55 at.% one can observe a tendency for ordering into the B2 structure. No ordering occurs for rapidly quenched samples with the rhodium concentration less than 19 at.% [5]. Chemically disordered α-phase is ordered ferromagnetically at room temperature. The Curie temperature decreases with the rhodium addition, but it is still quite above the room temperature even for the most rhodium abundant disordered BCC phase. The iron–rhodium system has been investigated by the Mössbauer spectroscopy in the past [6–9], but usually for the high rhodium concentrations or for the rhodium concentrations leading to the ordered B2 phase. We have investigated random solutions of rhodium in the α-Fe for the rhodium concentration up to 15 at.% by means of the room temperature Mössbauer spectroscopy.

2. Experimental

Samples were prepared by arc melting of the appropriate amounts of the constituent elements under protective argon atmosphere. Natural iron of the 99.97+ at.% purity and rhodium of 99.9 at.% purity were used to make samples. Samples of about 1.5 g were prepared by melting constituents three times to assure ingot homogeneity. Rapid cooling of the samples from the melt assured random distribution of the rhodium impurity. No weight losses were observed during sample preparation, and therefore the starting composition could be treated as the resulting sample composition. Mössbauer absorbers were prepared as powders embedded in the epoxy disks with about 30 mg Fe/cm^2. A commercial ^{57}Co(Rh) source was used. Transmission geometry with the source and absorbers kept at room temperature has been applied. Raw spectra were collected in 4096 channels in the round-corner triangular mode with the help of the MsAa-3 spectrometer [10,11]. All spectral shifts are reported versus room temperature total shift in α-Fe.

3. Data evaluation

Folded spectra were evaluated within the model described previously [4,12]. A transmission integral approximation was used. The model depends on the following assumptions. It is assumed

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doi:10.1016/j.jallcom.2008.10.013

Table 1

Essential results obtained within models with $\sigma = 2$ and $\sigma = 3$. The last row for each model shows respective averages, where appropriate. The averages have been calculated for the rhodium concentration c ranging from 2 to 12 at.%. Symbols $<B>_\sigma$ and $<S>_\sigma$ stand for the average field and shift, respectively. Symbols $B_0^{(\sigma)}$ and $S_0^{(\sigma)}$ denote contributions to the field and shift due to the atoms beyond the σ-th co-ordination shell. Symbols ΔB_1, ΔB_2 and ΔB_3 stand for contributions to the field caused by the rhodium atom located as the first, second and third neighbor, respectively. Symbols ΔS_1, ΔS_2 and ΔS_3 denote corresponding contributions to the shift.

c (at.%) ±0.1	$<B>_\sigma$ (T) ±0.02	$B_0^{(\sigma)}$ (T) ±0.02	ΔB_1 (T) ±0.03	ΔB_2 (T) ±0.02	ΔB_3 (T) ±0.03	$<S>_\sigma$ (mm/s) ±0.002	$S_0^{(\sigma)}$ (mm/s) ±0.002	ΔS_1 (mm/s) ±0.003	ΔS_2 (mm/s) ±0.002	ΔS_3 (mm/s) ±0.002
0	32.95					0				
$\sigma = 2$										
2	33.30	33.05	0.89	0.89		0.009	0.008	−0.002	0.014	
4	33.61	33.14	0.85	0.83		0.019	0.015	−0.002	0.018	
6	33.92	33.23	0.85	0.79		0.028	0.021	−0.010	0.034	
8	34.24	33.33	0.85	0.76		0.036	0.027	−0.016	0.041	
10	34.54	33.39	0.84	0.79		0.045	0.033	−0.015	0.040	
12	34.81	33.43	0.86	0.77		0.051	0.037	−0.015	0.040	
15	35.22	33.43	0.88	0.81		0.063	0.046	−0.016	0.040	
			+0.86	**+0.81**				**−0.011**	**+0.032**	
$\sigma = 3$										
2	33.29	32.99	0.75	0.70	0.40	0.009	0.002	−0.015	−0.004	0.040
4	33.60	32.98	0.70	0.62	0.52	0.019	0.010	−0.015	−0.010	0.034
6	33.90	32.98	0.72	0.69	0.45	0.027	0.010	−0.016	−0.003	0.036
8	34.22	33.05	0.71	0.69	0.40	0.036	0.010	−0.015	−0.004	0.039
10	34.51	32.99	0.73	0.76	0.40	0.044	0.010	−0.015	−0.004	0.040
12	34.79	32.94	0.75	0.73	0.42	0.052	0.010	−0.013	−0.007	0.041
15	35.20	32.90	0.76	0.74	0.40	0.063	0.010	−0.013	−0.004	0.040
			+0.73	**+0.70**	**+0.43**			**−0.015**	**−0.005**	**+0.039**

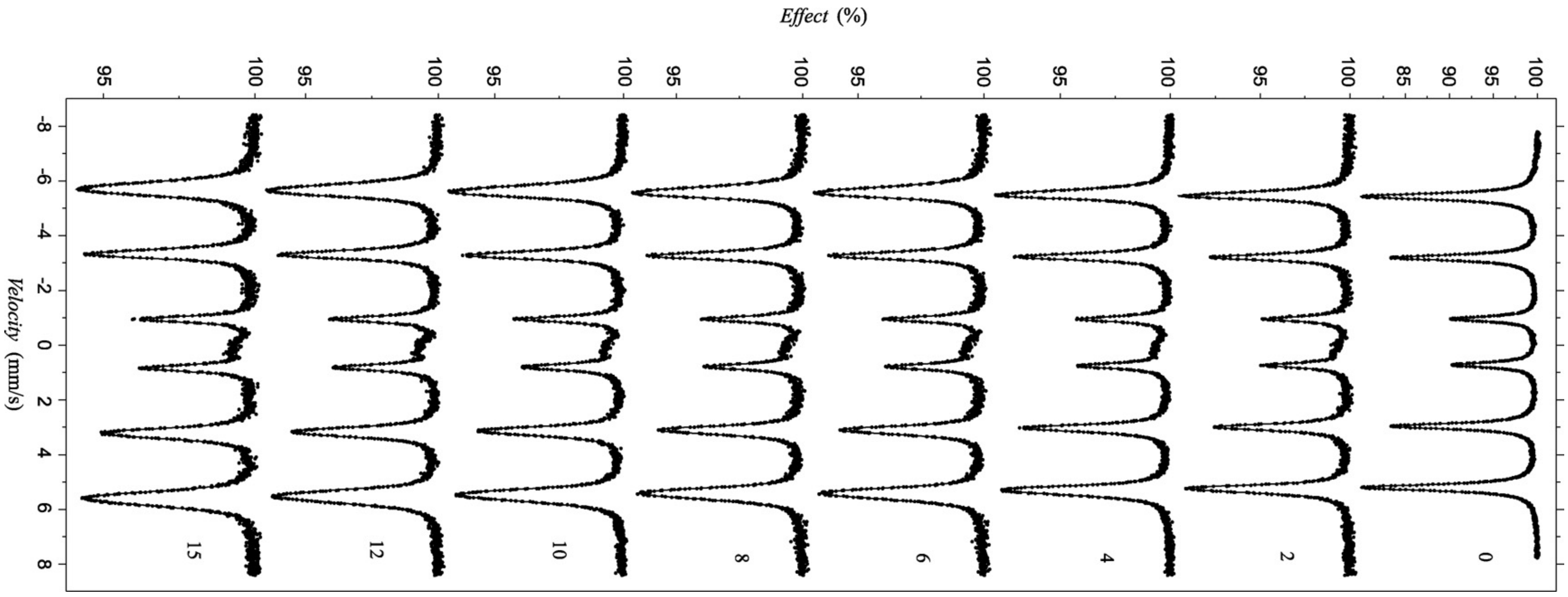

Fig. 1. Mössbauer transmission spectra are shown for various rhodium concentrations.