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Structure of hydrogenated amorphous $Ni_{56}Dy_{44}$

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Abstract

The structure of amorphous $Ni_{56}Dy_{44}$, loaded with 32 at% and 60 at% hydrogen, was investigated by X-ray and neutron diffraction using the isotopic substitution method. The results are discussed on the basis of the pair distribution functions. The incorporation of hydrogen atoms causes a change of the Ni–Dy matrix, i.e., an increase of the atomic distances and of the coordination numbers, in particular those of the Dy–Dy correlations. The H-atoms are preferentially located in a tetrahedral Dy-coordination, but also some hydrogen–Ni coordination was found. The hydrogen–metal distances agree with the distances between tetrahedral interstitial sites and the metal atoms in the crystalline hydrides DyH_2 and $Ni_{57}H_{43}$. A distance correlation between the hydrogen atoms was found at 2.78 Å.

Keywords: Amorphous $Ni_{56}Dy_{44}$; Hydrogen; Structure; X-ray diffraction; Neutron diffraction

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1. Introduction

The structure of the metallic glass $Ni_{56}Dy_{44}$ has been investigated by neutron diffraction in a previous study [1,2], and a computer simulation of this system, using the Reverse Monte Carlo method, has been performed in [3]. In the present work we present results of a diffraction study on this alloy after absorption of hydrogen. We employed the isotopic substitution method using ^{nat}Ni (1.03), ^{60}Ni (0.28), ^{62}Ni (−0.84), a zero-scattering mixture $^{\circ}Ni$, H (−0.37), D (0.67) and a zero-scattering H,D mixture $^{\circ}$(H,D) (the figures in parentheses are the coherent scattering lengths in units of 10^{-12} cm). A detailed description of the definitions and the evaluation of structure factors and correlation functions of amorphous systems may be found in the review [4].

2. Experimental

For a detailed description of the experiment and the data evaluation we refer to [1]. Amorphous melt-spun ribbons were loaded with 32 at% and 60 at% H or D from the gaseous phase. From X-ray diffraction and neutron diffraction the total pair correlation functions $G(R)$ were determined according to the Ashcroft–Langreth normalization (see, e.g., [4]).

3. Results and discussion

The pair correlation functions from X-ray diffraction $G_x(R)$ and from neutron diffraction $G_n(R)$ are plotted in Figs. 1 and 2. These total $G(R)$ are composed of the six partial $G_{ij}(R)$ according to the weighting factors which are listed in Table 1 for 60 at% H,D. Contrast variation by the isotopic substitution method allows the identification of the individual pair correlations, which appear as separate peaks or as shoulders in the total $G(R)$ as marked in the plots. The partial coordination numbers Z_{ij} were determined by gaussian fitting to the individual peaks in the total $G(R)$ or to appropriate difference curves. The results are listed in Table 2. The Ni–Ni correlation could not be determined due to its small weighting factor.

Fig. 1a shows the $G_x(R)$ of as-quenched (as-q) $Ni_{56}Dy_{44}$ and after absorption of 59 at% H, and Fig. 1b the $G_n(R)$ of as-q $Ni_{56}Dy_{44}$ and with 32 at% $^{\circ}$(H,D) and 60 at% $^{\circ}$(H,D), respectively. As the partial $G_{ij}(R)$ involving hydrogen are not visible in these $G(R)$ functions, they reflect the Ni–Dy matrix only. Obviously the hydrogen atoms do not simply occupy the available empty sites, but play an active role by changing the structure of the host matrix. An expansion of the system is observed, which affects mainly the Dy–Dy distances, and the peaks become

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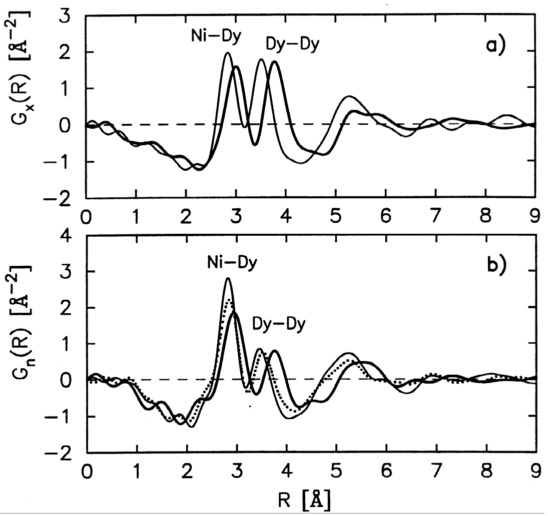

Fig. 1. Total pair correlation functions of amorphous $Ni_{56}Dy_{44}$. (a) $G_x(R)$ from X-ray diffraction; thin line, as quenched; thick line, with 59 at% H. (b) $G_n(R)$ from neutron diffraction, thin line, as-quenched; ···, with 32 at% ^{0}(H,D); thick line, with 61 at% ^{0}(H,D).

broader. At the same time Z_{NiDy} increases slightly, whereas Z_{DyDy} shows a substantial increase (Table 2). This indicates that the hydrogen atoms occupy preferentially those empty sites in the amorphous structure which are built by Dy-neighbours.

The $G_n(R)$ functions in Fig. 2a–d display the strong contrast variation effects, such as the reversal of the metal–hydrogen peaks upon H–D substitution (Fig. 2a–c), the reversal of the Ni–D and Ni–Dy peaks upon ^{nat}Ni–^{62}Ni substitution (Fig. 2d) and the absence of Ni–(Dy,H,D) peaks when a zero-scattering Ni–isotopic mixture ^{0}Ni was employed (Fig. 2c). In Fig. 2c a distance correlation between the hydrogen atoms at $R_{\mathrm{HH}}=2.78$ Å is indicated. For the number of Ni-atoms around hydrogen values close to $Z_{\mathrm{H(D)Ni}}=2$ were found and for the number of Dy-atoms values in the range $3.5<Z_{\mathrm{H(D)Dy}}<4$. This means that the hydrogen atoms occupy tetrahedral Dy_4-sites, however, due to their high content in the alloy, also sites with Ni-neighbours.

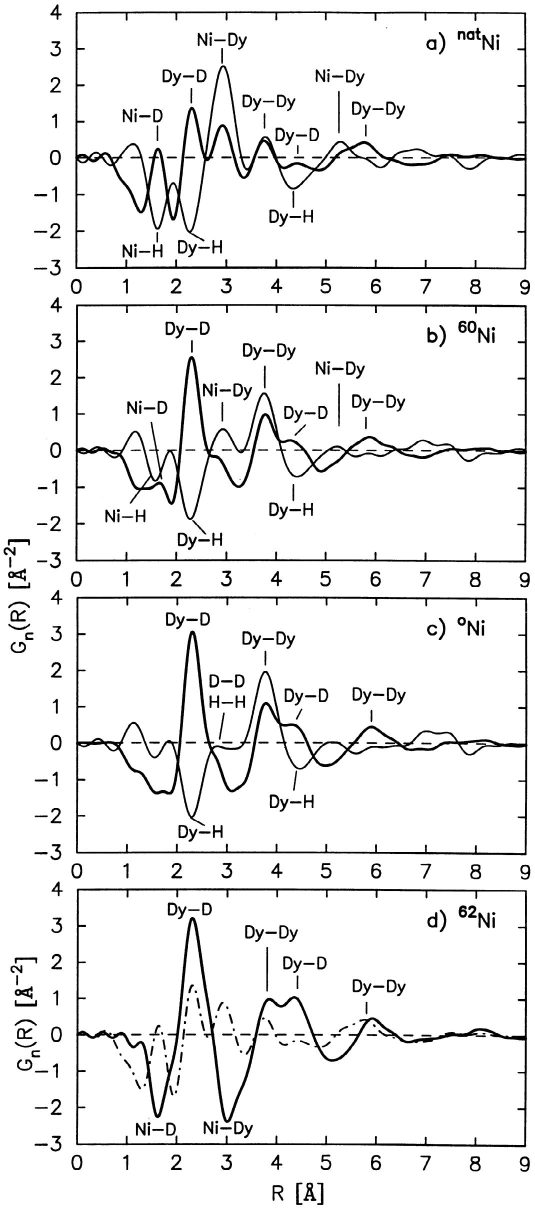

Fig. 2. Total pair correlation functions $G_n(R)$ of amorphous $Ni_{56}Dy_{44}$ +60 at% H,D from neutron diffraction. Thin lines, with H; thick lines, with D. (a) ^{nat}Ni, (b) ^{60}Ni, (c) ^{0}Ni, (d) ^{62}Ni; –·–·, same curve as thick line in (a).

Table 1
Weighting factors W_{ij} of the contributions of the partial correlation functions $G_{ij}(R)$ to the total $G_n(R)$ of amorphous $Ni_{56}Dy_{44}$ +60 at% H,D in Figs. 1 and 2

Used isotopes	Ni–Ni	Dy–Dy	Ni–Dy	H–Ni, D–Ni	H–Dy, D–Dy	H–H, D–D
X-rays	0.04	0.15	0.16	0	0	0
^{nat}Ni, ^{0}(H,D)	0.07	0.12	0.18	0	0	0
^{nat}Ni, H	0.07	0.11	0.17	−0.12	−0.16	0.06
^{nat}Ni, D	0.05	0.09	0.14	0.18	0.24	0.16
^{60}Ni, H	0.01	0.16	0.07	−0.05	−0.21	0.07
^{60}Ni, D	0.01	0.12	0.05	0.06	0.30	0.19
^{0}Ni, H	0	0.16	0	0	−0.23	0.08
^{0}Ni, D	0	0.12	0	0	0.31	0.19
^{62}Ni, D	0.04	0.10	−0.13	−0.16	0.25	0.16

Table 2
Atomic distances R_{ij}(Å), widths of bond lengths (HWFM) σ_{ij}(Å) and coordination numbers Z_{ij} (j-atoms around i-atoms)

Alloy	R_{NiNi}, σ_{NiNi}, Z_{NiNi}	R_{NiDy}, σ_{NiDy}, Z_{NiDy}	R_{DyDy}, σ_{DyDy}, Z_{DyDy}	R_{HNi}, σ_{HNi}, Z_{HDy}	R_{HDy}, σ_{HDy}, Z_{HDy}
$Ni_{56}D_{44}$	2.48	2.84	3.50		
as-quenched [2]	0.41	0.45	0.50		
	3.1	5.2	6.9		
$Ni_{56}Dy_{44}$		2.84	3.52		
+32 at% H		0.53	0.58		
		5.1	8.3		
$Ni_{56}Dy_{44}$		2.91	3.77	1.62	2.29
+60 at% H		0.62	0.63	0.40	0.49
		5.8	9.4	2.0	3.5–4

A comparison of the hydrogen–metal distances in amorphous $(Ni_{56}Dy_{44})_{40}H_{60}$ with the distances in the crystalline hydrides DyH_2 and $Ni_{57}H_{43}$ is interesting. $R_{HDy}=2.29$ Å agrees with the distance between H-atoms on tetrahedral interstitial sites in crystalline DyH_2 and the Dy-atoms (2.25 Å), whereas the H–Dy distance from octahedral H-sites in DyH_2 is larger (2.60 Å). Also the H–Ni distance $R_{HNi}=1.62$ Å agrees with the distance between tetrahedral sites and Ni-atoms (1.62 Å) in the $Ni_{57}H_{43}$ hydride and is smaller than the distance from octahedral sites (1.87 Å).

4. Conclusions

X-ray and neutron diffraction experiments show that loading the metallic glass $Ni_{56}Dy_{44}$ with hydrogen causes structural changes, i.e., an increase of the atomic distances and also of the coordination numbers, in particular those of the Dy–Dy correlations. At 60 at% hydrogen, the hydrogen atoms occupy preferentially tetrahedral Dy_4-sites, but also Ni–hydrogen correlation is found.

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