Neutron Diffraction with the Metallic Glass Ni$_{31}$Dy$_{69}$ (+ 10 a/o D) Using Isotopic Substitution

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Z. Naturforsch. 40a, 191–192 (1985); received January 17, 1985

By neutron diffraction using the method of isotopic substitution with the amorphous alloy Ni$_3$Dy$_{69}$ the partial structure factors $S_{NN}$, $S_{DD}$, and $S_{ND}$ were obtained, furthermore with the same specimen containing 10 a/o deuterium a partial structure factor $S_{DD}$ resulted. For the evaluation of $S_{DD}$ it was necessary to perform the neutron diffraction experiment with an alloy whose both components were zero-scattering isotopic mixtures of Ni or Dy, respectively.

1. Introduction

With the amorphous alloys Ni$_{31}$B$_{69}$ (Ref. [1]) as well as Ni$_{60}$P$_{20}$ (Ref. [2]) pronounced correlations of Ni–Ni, B–B as well as P–P were found. The same stands for the correlations of Ni–Ni, Ni–Y and Y–Y as was reported recently for the alloy Ni$_3$Y$_{7}$ (Ref. [3]). Since convenient isotopes are available from the element dysprosium, the present paper is concerned with Ni$_{31}$Dy$_{69}$ alloys, thus continuing the study of Ni-base alloys. As will be shown, it is also possible in this case to study the distribution of the free volume, whereby deuterium can be used as a marker, since it is to be expected that deuterium atoms fit well into any empty space. Thus in principle it is possible to reveal the deuterium-deuterium correlation by neutron diffraction within a binary alloy whose components are zero-coherent-scatterers.

2. Theoretical Fundamentals

The total structure factor according to Faber Ziman for a ternary system containing the three atomic species 1, 2, and 3 can be written as

$$S_{T}(Q) = S_{11}(Q) + S_{22}(Q) + S_{33}(Q) + 2S_{12}(Q) + 2S_{13}(Q) + 2S_{23}(Q)$$

with

$$S_{ij}(Q) = \langle b_i b_j \rangle + \langle b_i \rangle \langle b_j \rangle$$

From (1) follows that the contribution $S_{11}(Q)$ from deuterium (element 3) within the amorphous alloy formed by the elements 1 and 2 can be measured directly by one scattering experiment if $b_1 = b_2 = 0$. Equations (1) and (3) then yield

$$S_{T}^{Z}(Q) = S_{11}(Q).$$

3. Experimental

Four melt spun amorphous alloys were put into V-containers and at room temperature diffusion experiments were performed at the instrument D4B at the high flux reactor ILL Grenoble, using neutrons with a wavelength of 0.7 Å. At the same time the background scattering, the crucible scattering, and the Cd-rod scattering were measured.

The isotopic composition of the four specimens was as follows:

i) natNi$_{31}$natDy$_{69}$, nat = natural isotopic abundance,

ii) natNi$_{31}$Dy$_{69}$, Dy = zero coherent scattering mixture of natDy and 162Dy,

iii) Ni$_{31}$Dy$_{69}$, Dy = zero coherent scattering mixture of 162Ni and 162Ni,

iv) Ni$_{31}$Dy$_{69}$ + 10 a/o D; the deuterium was loaded under high pressure.

The densities of the ribbons were determined by the Archimedian method using Dibrom-ethane yielding for the mean atomic density $\rho_0$ as average value finally $\rho_0 = 0.0412$ Å$^{-3}$.

4. Results and Discussion

The data were corrected according to [4]. Concerning the correction for magnetic scattering the best way to do would have been to perform a diffraction experiment with Dy$_{69}$Ni$_{31}$ containing no deuterium at all. However, this could not be done because of lack of material. Thus, for the magnetic correction of the curves obtained with the specimens, the run of the curve obtained with specimen iv after correction for absorption and background scattering was used. For the evaluation of the curve obtained with specimen iv a smooth curve was subtracted in order to separate the slightly oscillating part of the corrected intensity. This difference $\Delta S_{DD}$ is shown in Fig. 1 in magnified scale. The distance between the two deuterium atoms amounts to about 0.64 Å which would yield a maximum in $S(Q)$ at about $2 \pi / 0.64 = 9.81$ Å$^{-1}$. The $\Delta S_{DD}$ curve in Fig. 1 indeed shows a pronounced peak around 10 Å$^{-1}$. However, to correlate this with the existence of Dy$_2$-molecules within the Ni$_3$Dy$_{69}$ specimens further experiments with higher D$_2$ content will be done in near future. The total structure factors (not shown here) exhibit no premaxima. This is in contrast to the total factors reported for Ni$_3$Y$_{7}$ (Ref. [3]) though the $\Delta h$-values in the present case are much more larger.
Figure 1 shows the partial structure factors which are indeed very similar to those obtained in [3] with Ni$_{33}$Y$_{67}$. Apparently the Y atoms can be substituted by Dy without remarkable change in the structural arrangement. The same stands also for the partial radial distribution functions which are shown in Figure 2.

The very small first peak in $G_{NiNi}$ shows that contact of Ni—Ni atoms doesn't exist very often. The rather large difference 0.56 of the electro-negativities of Ni and Dy apparently leads to preference of Ni—Dy contacts. This is expressed in a rather strong first $G_{NiDy}$ maximum. In so far, there exists a striking similarity to Ni$_{33}$Y$_{67}$, too.

From the RDF's the partial coordination numbers $Z_{NiNi} = 3.0$, $Z_{DyDy} = 12.4$, and $Z_{NiDy} = 10.8$ were obtained yielding a relative Cargill-Spaepen short range order parameter $\eta_{NiDy}^{rel} = 2.3\%$. Thus the chemical range order is about half of that obtained in [3] for Ni$_{33}$Y$_{67}$.

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Acknowledgement

Thanks are due to the ILL, Grenoble, and its staff for the support during the performance of the diffraction experiments.