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

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By neutron diffraction using the method of isotopic substitution with the amorphous alloy $Ni_{31}Dy_{69}$ the partial structure factors S_{NiNi}, S_{DyDy}, and S_{NiDy} 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 $Ni_{81}B_{19}$ (Ref. [1]) as well as $Ni_{80}P_{20}$ (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 $Ni_{33}Y_{67}$ (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

$$S^{F.Z.}(Q) = \frac{c_1^2 b_1^2}{\langle b\rangle^2} S_{11}(Q) + \frac{c_2^2 b_2^2}{\langle b\rangle^2} S_{22}(Q) + \frac{c_3^2 b_3^2}{\langle b\rangle^2} S_{33}(Q) + \frac{2 c_1 c_2 b_1 b_2}{\langle b\rangle^2} S_{12} + \frac{2 c_1 c_3 b_1 b_3}{\langle b\rangle^2} S_{13} + \frac{2 c_2 c_3 b_2 b_3}{\langle b\rangle^2} S_{23} \quad (1)$$

with

$$\langle b\rangle = c_1 b_1 + c_2 b_2 + c_3 b_3 . \quad (2)$$

From (1) follows that the contribution $S_{33}(Q)$ from deuterium (element 3) within the amorphous alloy formed by the elements 1 and 2 can be measured directly by one scattering experiment if

$$b_1 = b_2 = 0 . \quad (3)$$

Equations (1) and (3) then yield

$$S^{F.Z.}(Q) = S_{33}(Q) . \quad (4)$$

3. Experimental

Four melt spun amorphous alloys were put into V-containers and at room temperature diffraction experiments were performed at the instrument D4B at the high flux reactor of 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) $^{nat}Ni_{31}{}^{nat}Dy_{69}$; nat = natural isotopic abundance,
ii) $^{nat}Ni_{31}{}^{0}Dy_{69}$; ^{0}Dy = zero coherent scattering mixture of ^{nat}Dy and ^{162}Dy,
iii) $^{0}Ni_{31}{}^{nat}Dy_{69}$; ^{0}Ni = zero coherent scattering mixture of ^{60}Ni and ^{62}Ni,
iv) $^{0}Ni_{31}{}^{0}Dy_{69}$ + 10 a/o D; the deuterium was loaded under high pressure.

The densities of the ribbons were determined by the Archimedian method using Dibrome-ethane yielding for the mean atomic density ϱ_0 as average value finally $\varrho_0 = 0.0412$ 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 $^{0}Dy_{69}{}^{0}Ni_{31}$ 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 i, ii, and iii 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 ΔS_{DD} is shown in Fig. 1 in magnified scale. The distance between 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 ΔS_{DD} curve in Fig. 1 indeed shows a pronounced peak around 10 Å^{-1}. However, to correlate this with the existence of D_2-molecules within the $Ni_{31}Dy_{69}$ 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 $Ni_{33}Y_{67}$ (Ref. [3]) though the Δb-values in the present case are much more larger.

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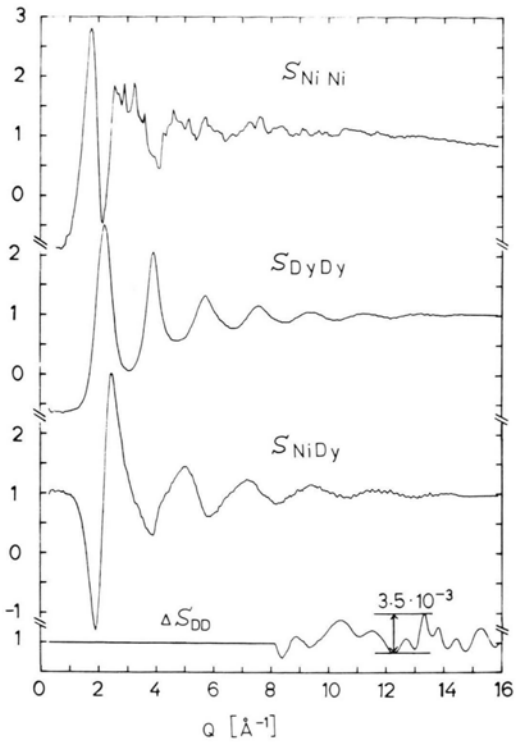

Fig. 1. a-$Ni_{31}Dy_{69}$: Partial structure factors S_{NiNi}, S_{DyDy}, and S_{NiDy}. a-$^{0}Ni_{31}{}^{0}Dy_{69}$ + 10 a/o D: Difference ΔS_{DD} showing the oscillating part of the partial DD structure factor.

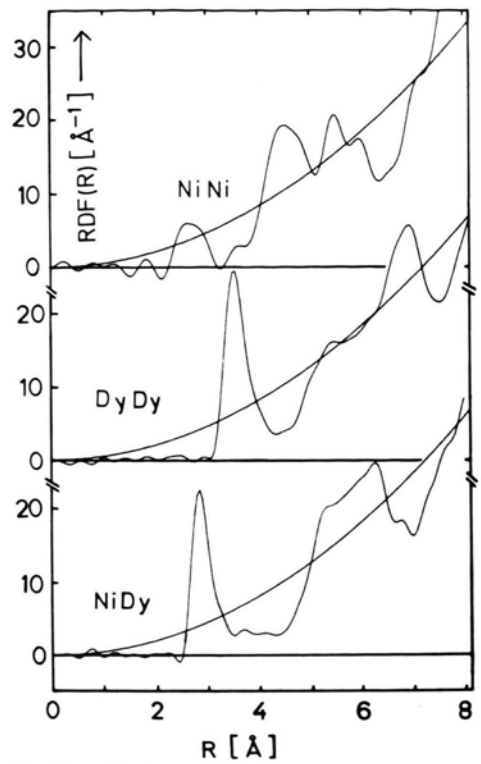

Fig. 2. a-$Ni_{31}Dy_{69}$: Partial radial distribution functions RDF_{NiNi}, RDF_{DyDy}, and RDF_{NiDy}.

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 $Ni_{33}Y_{67}$.

The similarity of all the partial functions of the $Ni_{33}Y_{67}$- and $Ni_{31}Dy_{69}$-alloys is not astonishing regarding the fact that the concentrations in both cases are nearly the same and that Y and Dy are elements with similar chemical behaviour. However, it is not selfunderstanding that the atomic species with the smaller concentration, i.e. in the present case the species Ni shows similar behaviour to the B–B or P–P partials, since those elements are very different from the chemical and topological point of view. The present results will be presented in a more comprehensive form (Ref. [6], [7]) containing also the Bhatia Thornton partial functions.

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