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THE STRUCTURE OF AMORPHOUS Ni-Zr ALLOYS

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Resume: Les structures des alliages Ni-Zr avec 55, 60, 65 et 70 at% Zr, et avec des additions mineures de Co et Fe ont été déterminées en employant la technique de l'angle 2θ variable pour les rayons X et de la longueur d'onde variable pour les neutrons. Les facteurs partiels de structures (fonctions partielles d'interférence) $I_{ik}(Q)$ et $S_{nc}(Q)$ ont été réévalués, et leurs transformations de Fourier indiquent qu'il y a peu de voisins NiNi dans l'alliage amorphe $Ni_{35}Zr_{65}$.

Abstract: The structures of amorphous Ni-Zr alloys with 55, 60, 65 and 70 at%Zr, and small additions of Co and Fe, have been determined employing the variable 2θ x-ray and the variable wavelength neutron techniques. The partial structure factors (partial interference functions) $I_{ik}(Q)$ and $S_{nc}(Q)$ have been reevaluated and their Fourier transforms indicate that there are few NiNi neighbors in the amorphous $Ni_{35}Zr_{65}$ alloy.

I. - INTRODUCTION

The structure of multi-component, non-crystalline materials is still not well understood. The problem lies in the diffuse nature of the scattering patterns which permit us to determine only a weighted average of the partial atomic distribution functions [1]. The weight factors in this average depend on the scattering of the individual components in the non-crystalline materials. They can be changed by using different radiation probes (e.g. x-rays and neutrons), and by isomorphous and isotopic substitution of one or both alloying elements in binary systems.

The total, coherently scattered intensity per atom $I_a(Q)$ can be expressed in terms of the atomic pair partial structure factors $I_{ik}(Q)$ or the number-concentration structure factors $S_{nc}(Q)$ as a function of the length of the diffraction vector Q , i.e.

$$Q = (4\pi/\lambda)\sin\theta = (4\pi m/h)(L/t)\sin\theta \quad (1)$$

where λ is the wavelength, m is the mass of the neutron, h is Planck's constant, L is the total path traveled by the neutrons in the time t . For binary alloys, we can write:

$$I_a(Q) = \langle f^2 \rangle + (c_1 f_1)^2 [I_{11}(Q) - 1] + (c_2 f_2)^2 [I_{22}(Q) - 1] + 2c_1 f_1 c_2 f_2 [I_{12}(Q) - 1] \quad (2)$$

$$I_a(Q) = \langle f^2 \rangle + \langle f \rangle^2 [S_{nn}(Q) - 1] + 2\Delta f \langle f \rangle S_{nc}(Q) + c_1 c_2 (\Delta f)^2 \{ [S_{cc}(Q) / (c_1 c_2)] - 1 \} \quad (3)$$

where $f_i(Q)$ and c_i are the coherent scattering amplitude and atomic concentration, respectively, of element i , $\langle f \rangle = \sum c_i f_i(Q)$, $\langle f^2 \rangle = \sum c_i [f_i(Q)]^2$ and $\Delta f = f_1(Q) - f_2(Q)$.

It can be readily shown that the factors $I_{ik}(Q)$ and $S_{nc}(Q)$ are related [1].

The total structure factors $I(Q)$ and $S(Q)$ are defined as follows:

$$I(Q)-1 = [I_a(Q) - \langle f^2 \rangle] / \langle f \rangle^2 = \sum \sum W_{ik}(Q) [I_{ik}(Q) - 1] \quad (4)$$

$$S(Q)-1 = [I_a(Q) - \langle f^2 \rangle] / \langle f^2 \rangle = \sum \sum W_{ik}(Q) [\langle f \rangle^2 / \langle f^2 \rangle] [I_{ik}(Q) - 1] \quad (5)$$

$$\text{where } W_{ik}(Q) = c_i f_i(Q) c_k f_k(Q) / \langle f(Q) \rangle^2 \quad (6)$$

The Fourier transforms of $Q[I(Q)-1]$ and $Q[S(Q)-1]$ yield the total, reduced atomic distribution functions $G_I(r)$ and $G_S(r)$, respectively. It can be readily shown that the total correlation function $T(r)$ is given by:

$$T(r) = \langle f(0) \rangle^2 G_I(r) + 4\pi r \rho_0 \langle f(0) \rangle^2 = \langle [f(0)]^2 \rangle G_S(r) + 4\pi r \rho_0 \langle f(0) \rangle^2 \quad (7)$$

where ρ_0 is the average atomic density of the amorphous alloy. $T(r)$ is related to the partial correlation functions $T_{ik}(r)$, i.e.,

$$T(r) = \sum \sum c_i f_i(0) c_k f_k(0) T_{ik}(r) \quad (8)$$

$$\text{where } T_{ik}(r) = 4\pi r \rho_{ik}(r) / c_k = G_{ik}(r) + 4\pi r \rho_0 \quad (9)$$

$\rho_{ik}(r)$ is the partial atomic distribution function which represents the number of k -atoms per unit volume at the distance r from an i -type atom, and $G_{ik}(r)$ is the Fourier transform of the partial structure factor $I_{ik}(Q)$:

$$G_{ik}(r) = (2/\pi) \int Q [I_{ik}(Q) - 1] \sin Qr \, dQ \quad (10)$$

II. - EXPERIMENTAL TECHNIQUES.

The amorphous alloys of Ni-Zr with 55, 60, 65, and 70 at% Zr, and 5 and 18 at% Co or 5 at% Fe, were produced by the melt-spinning process. The x-ray specimens were prepared by mounting several small ribbons next to each other over the opening in Al sample holders. The neutron samples consisted of about 5 g of ribbons for each composition. The ribbons were wound in such a way as to produce cylindrical specimens, 60 mm in height and 5 mm in diameter. The x-ray measurements were carried out with the variable 2θ technique using Ag-K α radiation and a Si solid state detector. The neutron measurements were performed on the pulsed spallation source at Argonne National Laboratory, using the variable λ technique.

III. - RESULTS AND DISCUSSION.

The total structure factors $I(Q)$ [equation (4)] of the $(\text{Ni-Co-Fe})_x\text{Zr}_{1-x}$ glasses, measured with x-rays, are shown in Fig. 1, and the corresponding total correlation functions $T(r)/\langle f(0) \rangle^2$ [equation (6)] are presented in Fig. 2. The equivalent neutron data are shown in Fig. 3. Although the structure factors $I(Q)$ are rather similar for the concentration range studied, the corresponding correlation function $T(r)$ clearly show the effect of the different Zr concentrations. The first peak in $T(r)$ is split into two maxima, one positioned at $r_1=2.69$ Å, and the other at $r_2=3.15$ Å. The latter peak changes in height with varying Zr content in the same way as the values of the weight factor $[c_{\text{Zr}} f_{\text{Zr}}(0)]^2 / \langle f(0) \rangle^2$ do [see equations (6) and (8)]. Thus, it is reasonable to assume that the peak at $r_2=3.15$ Å is due to the Zr-Zr first neighbors in the metallic glass [2].

Substitution of Co (up to 25 at%) or Fe (5 at%) for Ni did not change the x-ray scattering patterns of the $\text{Ni}_{35}\text{Zr}_{65}$ glasses. The x-ray total $I(Q)$ shown in Fig. 1 is the composite curve of the data taken with specimens containing 5 and 18 at% Co and 5 at% Fe, respectively. Since the x-ray weight factors $W_{ik}(Q)$ [equation (6)] are little affected by the substitution of Fe or Co for Ni, it is reasonable to assume that Co can be readily substituted for Ni, and that 5 at% Fe substitution did not change the structure within the accuracy of the experiment.

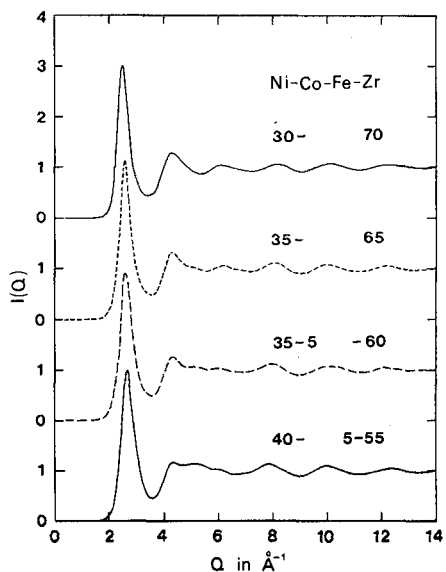


Fig. 1 Total structure factors $I(Q)$ of amorphous (Ni-Co-Fe)-Zr, measured with x-rays.

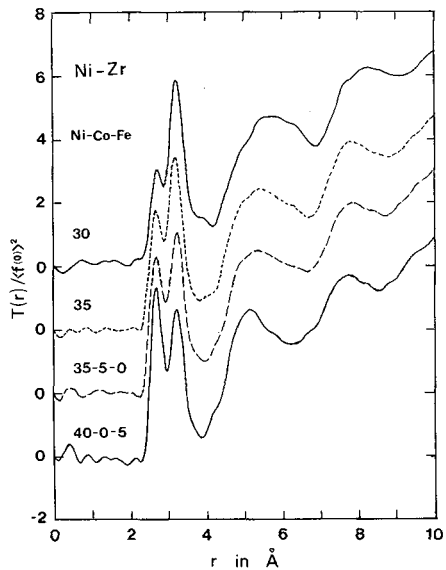


Fig. 2 Total correlation functions $T(r)$ of amorphous (Ni-Co-Fe)-Zr alloys.

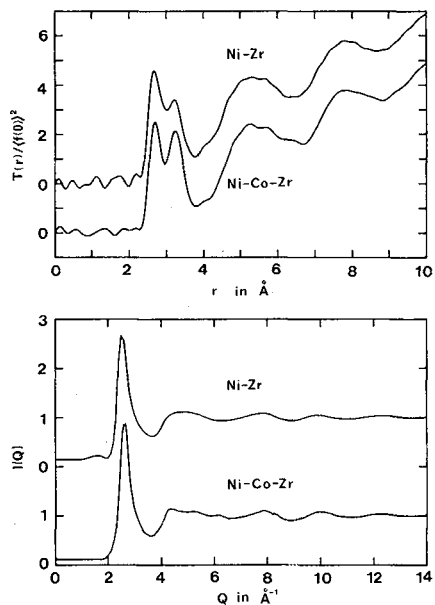


Fig. 3 Neutron structure factors $I(Q)$ and correlation functions $T(r)$ of amorphous (Ni-Co-Fe)-Zr.

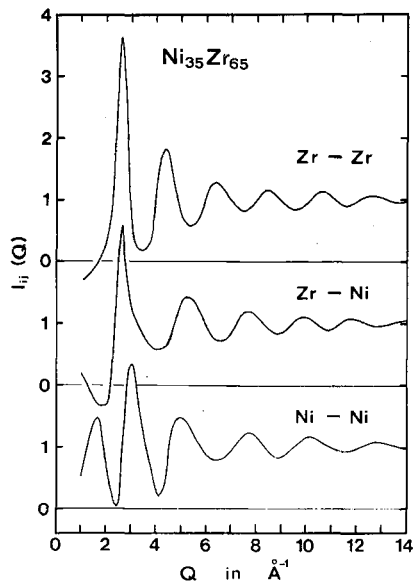


Fig. 4. Partial atomic pair structure factors $I_{ik}(Q)$ of amorphous $\text{Ni}_{35}\text{Zr}_{65}$.

The neutron measurements on the $Ni_{35}Zr_{65}$ were recently repeated at Argonne National Laboratory, and showed a lower background than the previous data [3,4]. Therefore, it was felt that a reevaluation of the partial structure factors would be desirable. We used the x-ray data of the $Ni_{35}Zr_{65}$ and $Ni_{35}Zr_{35}Hf_{30}$ alloys and the neutron data of the $Ni_{35}Zr_{65}$ and $Ni_{17}Co_{18}Zr_{65}$ alloys in the recalculation. The atomic pair partial structure factors $I_{11}(Q)$, $I_{22}(Q)$ and $I_{12}(Q)$ are shown in Fig. 4. These data are in very good agreement with those published previously [4], but their weighted sum [equation (4)] produced a much better fit with the total structure factor $I(Q)$, measured with neutrons.

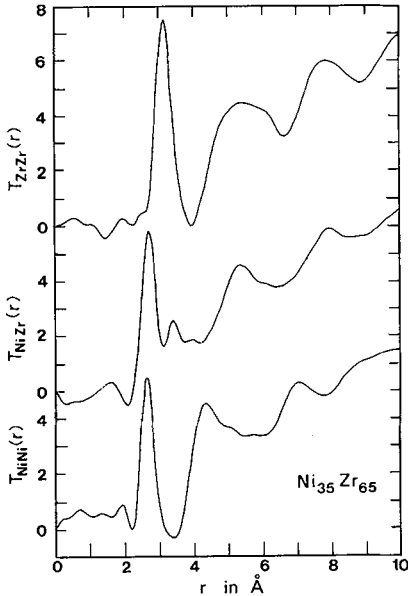


Fig.5 Partial pair correlation functions $T_{ik}(r)$ of amorphous $Ni_{35}Zr_{65}$.

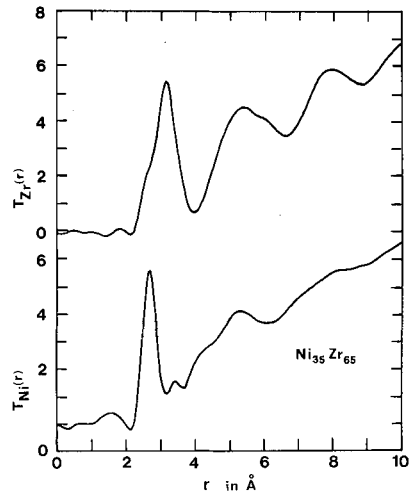


Fig. 6 Atomic pair correlation functions $T_i(r) = \sum c_k T_{ik}(r)$ of amorphous $Ni_{35}Zr_{65}$.

The partial atomic pair correlation functions $T_{11}(r)$, $T_{22}(r)$ and $T_{12}(r)$ are shown in Fig. 5, and the corresponding pair correlation functions $T_1(r) = c_1T_{11}(r) + c_2T_{12}(r)$ and $T_2(r) = c_1T_{21}(r) + c_2T_{22}(r)$ are presented in Fig. 6. It is clear from this figure that the distribution of atoms about a Ni atom is quite different from atomic distribution about a Zr atom. The individual partial coordination numbers N_{ik} , were evaluated from the area under the first peak in $rT_{ik}(r)$, centered at $(r_1)_{ik}$. The following values were obtained: $(r_1)_{NiNi} = 2.66 \text{ \AA}$, $(r_1)_{NiZr} = 2.69 \text{ \AA}$, $(r_1)_{ZrZr} = 3.15 \text{ \AA}$, $N_{NiNi} = 2.3$, $N_{NiZr} = 7.9$, and $N_{ZrZr} = 9.1$. It is possible to calculate the partial coordination numbers $N_{i1} = N_{i1} + N_{i2}$ from these data, i.e., $N_1 = 10.2$ and $N_2 = 13.4$. These numbers are in reasonable agreement with those calculated directly from Fig. 6.

In order to see the effect of chemical ordering in this amorphous alloy, the chemical short-range order (CSRO) parameter α_1 was calculated using the relation [5]:

$$\alpha_1 = 1 - N_{12} / (c_2 N_w) \tag{11}$$

where $N_w = c_2 N_1 + c_1 N_2 = 11.3$ (12)

Equation (11) yields a value of $\alpha_1 = -0.08$. However, it is also possible to evaluate

the CSRO parameter directly from the number-concentration correlation functions $T_{n-c}(r)$ which are the Fourier transforms of the number-concentration structure factors $S_{n-c}(Q)$, which are shown in Figs. 8 and 7, respectively.

If we define the number-concentration coordination numbers $N_{n-c}(r)$ as a function of the upper limit of integration of the correlation functions $rT_{n-c}(r)$, we can define the CSRO parameter $\alpha_1(r)$ as follows:

$$\alpha_1(r) = N_{CC}(r)/N_W(r) = 1 - N_{12}(r)/\{c_2[c_2N_1(r)+c_1N_2(r)]\} \quad (13)$$

The values of the coordination numbers $N_{ik}(r)$ are given in Table 1 as a function of the upper limit of integration r , together with the CSRO parameter $\alpha_1(r)$.

Table 1. Partial coordination numbers $N_{ik}(r)$ and CSRO parameter $\alpha_1(r)$ in $Ni_{35}Zr_{65}$

r (Å)	3.0	3.2	3.4	3.6	3.8	4.0
N-NiNi(r)	2.2	2.3	2.2	2.2	2.3	2.8
N-NiZr(r)	4.9	5.6	6.7	7.7	8.6	9.2
N-ZrZr(r)	2.1	5.0	7.5	8.7	9.1	9.1
$\alpha_1(r)$	-0.20	-0.09	-0.07	-0.09	-0.11	-0.11

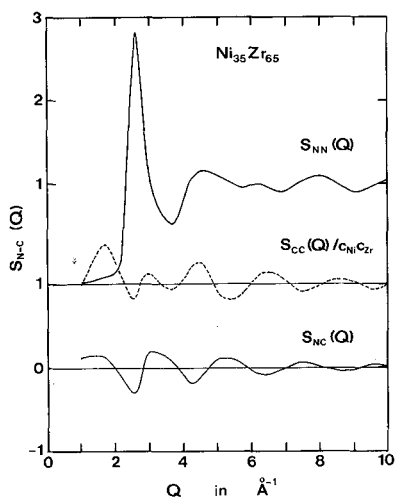


Fig 7 Number-concentration structure factors $S_{n-c}(Q)$ of $Ni_{35}Zr_{65}$.

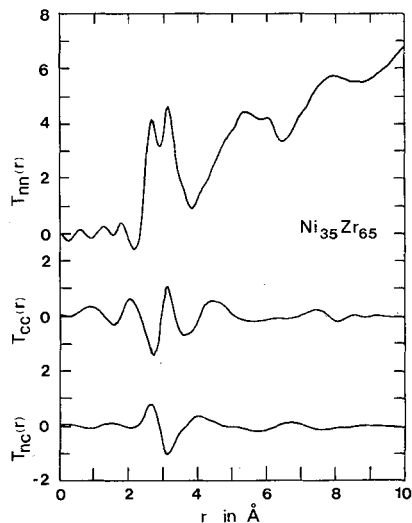


Fig. 8 Number-concentration functions $T_{ik}(r)$ of $Ni_{35}Zr_{65}$.

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