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ATOMIC-SCALE STRUCTURE OF AMORPHOUS (Ni-Co)-(Zr-Hf) ALLOYS

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Résumé.- Les structures des alliages amorphes $Ni_{35}Zr_{65}$ et (Ni-Co)-(Zr-Hf) ont été déterminées en employant la méthode de l'angle 2θ variable pour les rayons X et la technique de la longueur d'onde variable pour les neutrons. Les fonctions partielles d'interférence (facteurs partiels de structure) $I_{ij}(K)$ ont été évaluées en utilisant la méthode de substitution isomorphe.

Abstract.- The structures of amorphous $Ni_{35}Zr_{65}$ and (Ni-Co)-(Zr-Hf) alloys have been determined employing the variable 2θ angle X-ray method and the variable wavelength neutron technique. The partial interference functions (structure factors) $I_{ij}(K)$ have been evaluated using the isomorphous substitution method.

Introduction.- The atomic-scale structure of metallic glasses can be determined from their x-ray and neutron scattering patterns. However, the analysis of the scattering experiments yields only a one-dimensional description of the three-dimensional distributions of the atoms in the amorphous alloys. In binary alloys, the total coherent scattering is a weighted sum of the three partial atomic pair (AP) structure factors (also called interference functions) $I_{ij}(K)$ or the number-concentration partial structure factors $S_{N-C}(K)$, i.e, [1]

$$I_N(K)=N\{\langle f^2\rangle + c_1f_1^2\,[I_{11}(K)-1] + c_2^2f_2^2\,[I_{22}(K)-1] + 2\,c_1c_2f_1f_2\,[I_{12}(K)-1\} \qquad (1)$$

or

$$I_N(K)=N\{\langle f^2\rangle + \langle f\rangle^2\,[S_{NN}(K)-1] + 2\Delta f\langle f\rangle\, S_{NC}(K) \qquad (2)$$

$$+ c_1c_2(\Delta f)^2\{[S_{CC}(K)/(c_1c_2)]-1\}$$

where $K = (4\pi/\lambda)\sin\theta$, f_i and c_i are the coherent scattering amplitude and atomic concentration, respectively, of element i, $\langle f\rangle = c_1f_1 + c_2f_2$, $\langle f^2\rangle = c_1f_1^2 + c_2f_2^2$, $\Delta f = f_1-f_2$, and N is the number of atoms in volume V. It can be readily shown that $I_{ij}(K)$ and S_{N-C} are related [2].

It is customary to introduce the total structure factor (or interference function) I(K) or S(K) defined as: [1]

$$I(K)-1 = \{[I_N(K)/N]-\langle f^2\rangle\}/\langle f\rangle^2 \qquad (3)$$

$$S(K)-1 = \{[I_N(K)/N]-\langle f^2\rangle\}/\langle f^2\rangle \qquad (4)$$

The Fourier transform of K[I(K)-1] yields the reduced atomic distribution function G(r), i.e.,

$$G(r) = (2/\pi)\int_0^\infty K[I(K)-1]\sin Kr\, dK \qquad (5)$$

It is readily seen that the differential correlation function D(r) is related to G(r) [Eqn. (5)] and $G_S(r)$, the Fourier transform of K[S(K)-1] by [1]

$$D(r) = \langle f(o)\rangle^2 G(r) = \langle [f(o)]^2\rangle G_S(r)$$

$$= 4\pi r[\sum_i \sum_j c_i c_j f_i(o) f_j(o) \rho_{ij}(r)/c_j] - 4\pi r\rho_o \langle f(o)\rangle^2 \qquad (6X)$$

where $\rho_{ij}(r)$ is the partial atomic distribution function, which represents the number of j-type atoms per unit volume at the distance r from an i-type atom and ρ_o is the average atomic density. The Fourier transforms of $K(I_{ij}(K)-1]$, $K[S_{NN}(K)-1]$, $KS_{NC}(K)$ and $K\{[S_{CC}(K)/(c_1c_2)]-1\}$ yield the reduced atomic correlation functions $G_{ij}(r)$, $G_{NN}(r)$, $G_{NC}(r)$ and $G_{CC}(r)$, respectively.

The goal of the scattering experiments is the evaluation of the partial atomic pair structure factors $I_{11}(K)$, $I_{22}(K)$ and $I_{12}(K)$ or the number-concentration structure factors $S_{NN}(K)$, $S_{NC}(K)$ and $S_{CC}(K)/(c_1c_2)$ of a binary amorphous alloy. This can be accomplished, in principle, by performing three separate scattering experiments in each of which the weight factor $W_{ij}(K) = c_i c_j f_i f_j/\langle f\rangle^2$ has been changed [3]. In this investigation, the combination of isomorphous substitution of Zr by Hf and Ni by Co was employed in x-ray and neutron scattering.

A series of samples of $(Ni\text{-}Co)_{35}(Zr\text{-}Hf)_{65}$ metallic glasses were prepared by the melt spinning process, and their scattering patterns were determined by the X-ray variable 2θ method and the neutron variable λ method. The neutron experiments were carried out at Argonne and Los Alamos National Laboratories. Attempts were made to evaluate the partial structure factors $I_{ij}(K)$ and $S_{NC}(K)$.

Results and Discussion. - The total interference function or structure factor I(K) of the seven $Ni_{35}Zr_{65-x}Hf_x$ alloys are shown in Fig. 1, and the corresponding reduced distribution G(r) are presented in Fig. 2. Although the functions I(K) for different Hf concentrations are remarkably similar, their reduced distribution functions do show the effect of the weight factor $W_{ij}(o) = c_i c_j f_i(o) f_j(o)/\langle f(o)\rangle^2$ which are given in Table 1.

Table 1. Weight factors $W_{ij}(o) = c_i c_j f_i(o) f_j(o)/\langle f(o)\rangle^2$ for Ni-Zr-Hf alloys

Radiation	Neutrons	X-Rays	X-Rays	X-Rays
Ni-Zr-Hf	35-65-0	35-65-0	35-50-15	35-35-30
$W_{11}(o)$	0.195	0.077	0.060	0.048
$2W_{12}(o)$	0.493	0.401	0.370	0.342
$W_{22}(o)$	0.311	0.522	0.570	0.610

The first peak in G(r) is split into two maxima, one at $r_1^1 = 2.68$A and another at $r_1^2 = 3.19$A. Since the second maximum of the X-ray curves increases in height with increasing Hf content, in the same way as $W_{22}(o)$, and its position is close to the atomic diameter of Zr and Hf atoms, it is reasonable to conclude that it represents the position of the first (Zr,Hf)-(Zf,Hf) neighbors. In the neutron pattern, the second peak is lower than the first as it should according to $W_{22}(o)$ in Table 1. The first maximum must predominently contain the Ni-Zr neighbor pairs because the weight factor $W_{NiNi}(o)$ is very small in the X-ray case.

Substitution of Ni by Co does not affect the values of $W_{ij}(o)$, and as a consequence the X-ray scattering patterns of $(Ni\text{-}Co)_{35}Zr_{65}$ are practically identical as shown in Fig. 3. Thus, the Ni-Co-Zr samples can be used for neutron scattering experiments where the small scattering amplitude of Co ($b = 0.25\times10^{-12}$ cm) will

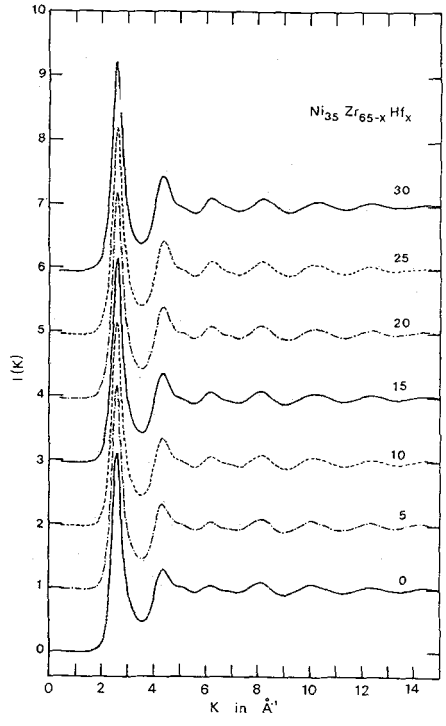

Fig. 1 Total structure factor I(K) of amorphous Ni-Zr-Hf alloys

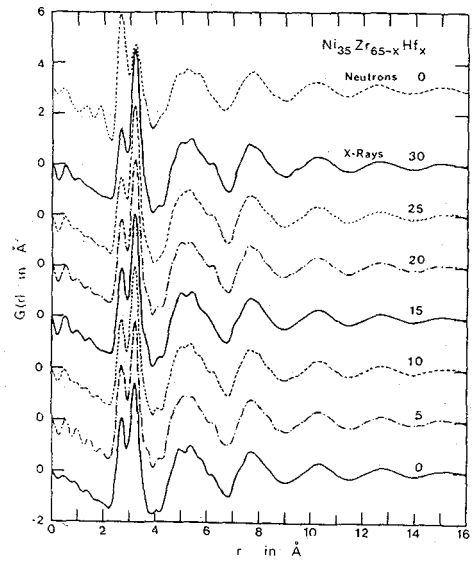

Fig. 2 Reduced atomic distribution function $G(r)=4\pi r[\rho(r)-\rho_o]$ of amorphous Ni-Zr-Hf alloys

partially offset the large value of $b = 1.03 \times 10^{-12}$ cm for Ni. The neutron structure factor I(K), shown in Fig. 3 for the $Ni_{35}Zr_{65}$ alloy exhibits a different shape for $K<5$ Å^{-1}, and even exhibits a prepeak at 1.8 Å^{-1} usually associated with chemical short-range order in the amorphous alloy [1,2,4,5].

Attempts were made to evaluate the partial structure factors $I_{ij}(K)$ and $S_{N-C}(K)$ from the three x-ray patterns of the $Ni_{35}Zr_{65}$, $Ni_{35}Zr_{50}Hf_{15}$ and $Ni_{35}Zr_{35}Hf_{30}$ alloys. [6].

The AP partial structure factors are shown in Fig. 4.

The partial structure factors $I_{ij}(K)$ were used to evaluate the number-concentration structure factors $S_{NN}(K)$, $S_{NC}(K)$ and $S_{CC}(K)/(c_1c_2)$, which are shown in Fig. 5. Also shown is the $S_{NC}(K)$ curve for the hard-sphere Percus-Yevick model [7] which agrees very well with the experimental $S_{NC}(K)$. The Fourier transforms of the number-concentration structure factors, i.e., the number concentration correlation functions $G_{N-C}(r)$, are shown also in Fig. 5. $G_{NN}(r)$ shows the splitting of the first peak with $r_1^1 = 2.68$ A and $r_1^2 = 3.20$ Å similar to G(r) in Fig. 2. The function $G_{CC}(r)$, however, possesses a deep minimum at $r_1 = 2.68$ A indicating a preference for unlike nearest neighbors at that distance, which consequently must correspond to Ni-Zr neighbors.

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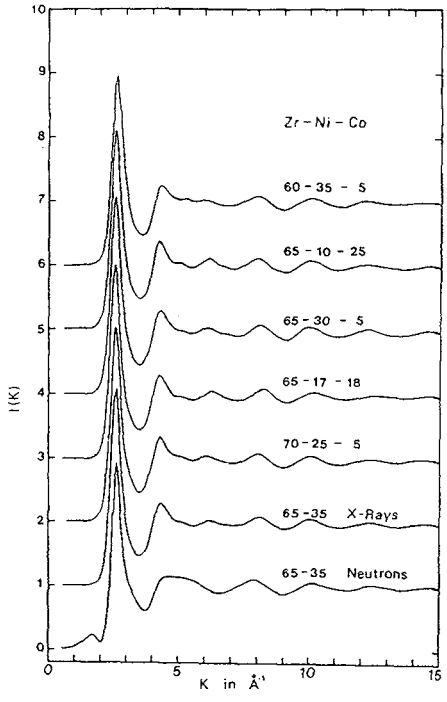

Fig. 3 Total structure factor I(K) of amorphous Ni-Co-Zr alloys

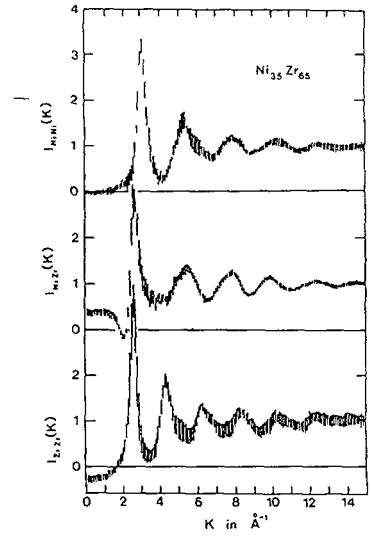

Fig. 4 Partial structure factors $I_{ij}(K)$ of amorphous $Ni_{35}Zr_{65}$

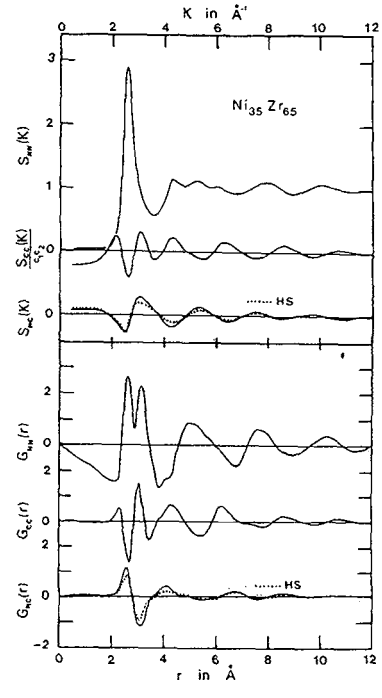

Fig. 5 Partial number-concentration structure factors $S_{N-C}(K)$ and partial reduced correlation functions $G_{N-C}(r)$ of amorphous $Ni_{35}Zr_{65}$. H.S. is the hard-sphere NC curve.

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