X-ray Diffraction Study of Amorphous $Ni_xZr_{(100-x)}$-Alloys Prepared by Melt-Spinning

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Amorphous Ni-Zr-alloys can be prepared by melt-spinning within a wide range of composition. Studies by X-ray diffraction yielded structure factors, pair correlation functions, total coordination numbers and atomic distances in dependence on the nickel concentration in the range of 25 up to 45 atomic percent. The change of the total coordination number and atomic distances turned out to be linear with the composition in this range. This is in good agreement with the linear composition dependence of the superconducting transition temperature, magnetic susceptibility, crystallization temperature, and electrical resistivity in the investigated range of composition.

1. Introduction

In the present paper we investigate the short range structure of amorphous $Ni_xZr_{(100-x)}$-alloys ($25 \leq x \leq 45$; $\Delta x = 1$) and focus on the question whether there is a linear dependence of the atomic distances and total coordination numbers on the composition.

2. Theoretical

We refer to references [1, 2] concerning the theoretical fundamentals of structural investigations and the definition of the Faber-Ziman structure factor $S^{FZ}(Q)$, where $Q = 4\pi(\sin\Theta)/\lambda$, λ = wavelength, and 2Θ = scattering angle. The same stands for the pair correlation function $G(R)$, the pair distribution function $g(R)$, and the total coordination number

$$Z_{tot} = 4\pi\varrho_0 \int_{R_L}^{R_U} R^2 g(R)\, dR\,, \qquad (1)$$

where

ϱ_0 = mean microscopic number density,
R_L = lower integration limit,
R_U = upper integration limit.

The determination of the total coordination number can be done by fitting Gaussians to the pair distribution function within the first coordination shell

$$g(R) = \sum_i g_{0i} \exp\left\{-\frac{(R-R_{0i})^2}{2\tau_i^2}\right\}, \qquad (2)$$

where

i = number of Gaussian,
g_{0i} = height of Gaussian i,
R_{0i} = position of Gaussian i,
τ_i = distance from R_{0i} to the point of inflection of the Gaussian i.

3. Experimental

We used amorphous $Ni_xZr_{(100-x)}$-alloys with a nickel concentration of 25 up to 45 atomic percent by changing the atomic fraction of nickel in steps of one atomic percent. Melt spinning was done in He-atmosphere (100 mbar). The Cu-zylinder with a diameter of 30 cm rotated with $50\ s^{-1}$. The melt was contained in quartz cylinders with 0.45 to 1 mm ejection hole diameter at a distance of 2 to 10 mm from the cylinder. The amorphous ribbons were 20 to 30 μm thick and 0.5 to 2 mm wide.

X-ray diffraction was done using molybdenum radiation with the instrument D 500 (Fa. Siemens) in transmission mode.

4. Results and Discussion

Figure 1 shows the total structure factors according to Faber-Ziman of all measured $Ni_xZr_{(100-x)}$-alloys. With increasing Ni-content we observe a change of three features:
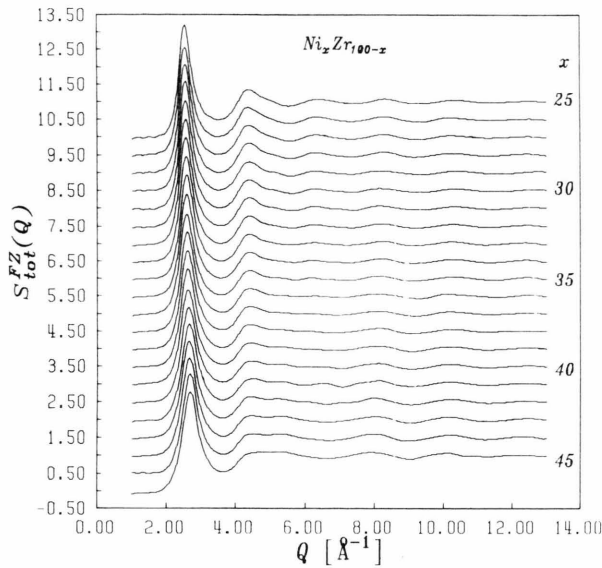
i) The main maximum is shifted towards higher Q-values.

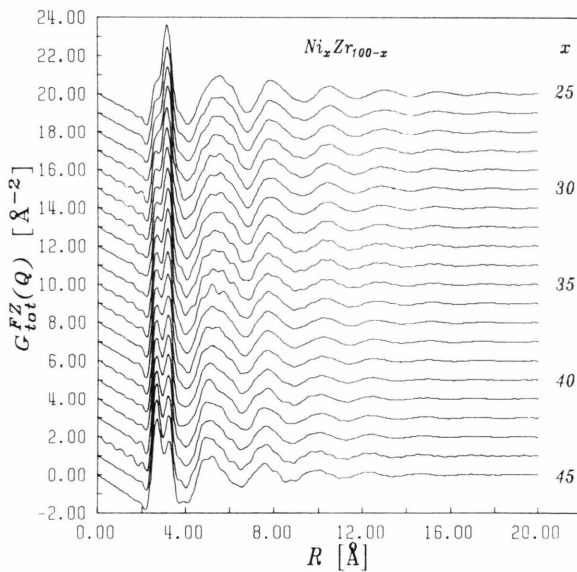Fig. 1. Amorphous $Ni_xZr_{(100-x)}$. Total structure factors according to Faber-Ziman.

Fig. 2. Amorphous $Ni_xZr_{(100-x)}$. Total pair correlation functions according to Faber-Ziman.

ii) At the right hand side of the second maximum a shoulder grows.

iii) The intensity of the left part of the second maximum decreases.

By Fourier transformation we obtained the total pair correlation functions according to Faber-Ziman
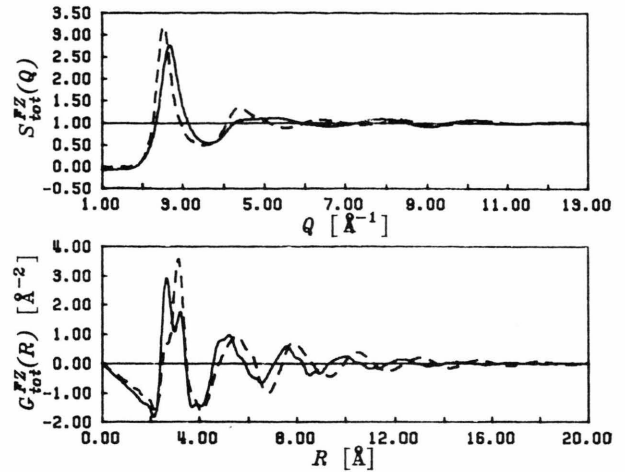

Fig. 3. Amorphous $Ni_{25}Zr_{75}$ (– – –) and $Ni_{45}Zr_{55}$ (——). Total structure factors $S_{tot}^{FZ}(Q)$ (above) and total pair correlation functions $G_{tot}^{FZ}(R)$ (below).

as shown in Figure 2. With increasing Ni-concentration we can state the following features:

i) The shoulder on the lower R side of the main maximum at about 2.64 Å grows. It finally becomes a separate peak. At $x = 41$ atomic percent it shows the same peak height as the peak which forms the main maximum at its right hand side (~ 3.18 Å). The latter peak is present at each concentration and decreases with increasing Ni-content.

ii) The intensity of the maxima at high R-values decreases with increasing Ni-concentration.

iii) Maxima at high R-values shift to lower R-values when the Ni-content increases, i.e. the structure becomes compressed. This behaviour is expected since with increasing Ni-content the number of smaller atoms increases ($\phi_{Ni} < \phi_{Zr}$). Thus, less volume is required to built up the amorphous matrix. As a consequence, the mean microscopic number density ϱ_0 increases from 0.0495 Å^{-3} ($x = 25$) to 0.0576 Å^{-3} ($x = 45$).

For a more distinct survey of the structural variation during increasing Ni-concentration between 25 and 45 atomic percent we present in Fig. 3 the total structure factors $S_{tot}^{FZ}(Q)$ (above) and total pair correlation functions $G_{tot}^{FZ}(R)$ (below) of amorphous $Ni_{25}Zr_{75}$ (– – –) and $Ni_{45}Zr_{55}$ (——). The features i)–iii) mentioned above are clearly evidenced.

According to (2) we fit the split up main maximum of the total pair distribution functions $g(R)$ with two Gaussians. Their positions R_{01} and R_{02} yield the
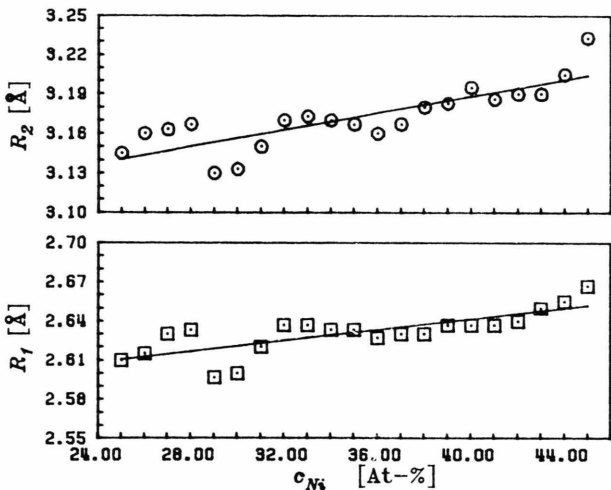
Fig. 4. Amorphous $Ni_xZr_{(100-x)}$. Atomic distances R_1 (below) and R_2 (above).
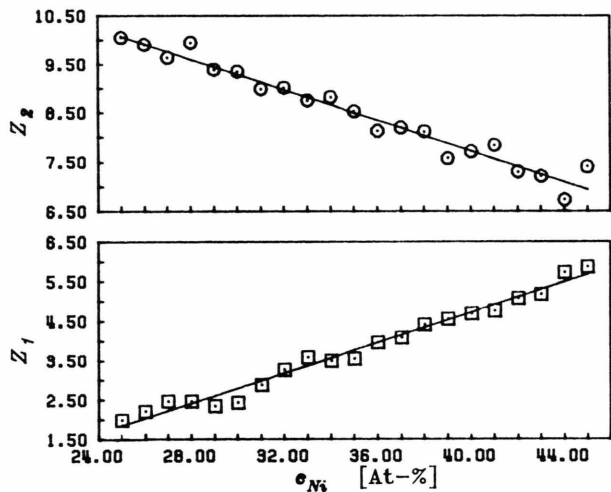

Fig. 5. Amorphous $Ni_xZr_{(100-x)}$. Coordination numbers Z_1 (below) and Z_2 (above).

R_1	2.61 Å	present	Table 1. Atomic
R_2	3.15 Å	work	distances in amorphous
			$Ni_{25}Zr_{75}$.
R_{NiNi}	2.63 Å	[1]	
R_{NiZr}	2.66 Å	[1]	
R_{ZrZr}	3.16 Å	[1]	

tances as obtained from partial pair distribution functions [1].

Evidently, the left hand side of the split up main maximum is caused by a superposition of the Ni–Ni- and Ni–Zr-correlations. The right hand side is caused mainly by Zr–Zr-nearest neighbors, involving a small contribution from Ni–Zr-pairs [1]. The values evaluated in the present work from the total functions are mean values of atomic distances and of partial coordination numbers.

We suppose that in all investigated samples R_1 and Z_1 are related to Ni–Ni- and Ni–Zr-pairs. R_2 and Z_2 represent Zr–Zr-pairs influenced by Ni–Zr-pairs.

Figure 4 shows the atomic distances R_1 and R_2 versus the Ni-content and Fig. 5 the coordination numbers Z_1 and Z_2 versus c_{Ni}. Apart from fluctuations at low Ni-contents in R_1 and R_2, which are caused by uncertainties during fitting the Gaussians, a linear concentration dependence of the atomic distances and the total coordination numbers can be stated.

5. Conclusion

In the investigated range of 25 to 45 atomic percent nickel in amorphous Ni–Zr-alloys a linear concentration-dependence of atomic distances and total coordination numbers is observed. This is in good agreement with results concerning the variation of the superconducting transition temperature [3–5], magnetic susceptibility [4, 6], crystallization temperature [7], and electrical resistivity [4] in the same concentration region. Therefore, we state that the variations in macroscopic physical parameters are directly related to changes in structure, i.e. to the distribution of atoms in the amorphous matrix.

atomic distances R_1 and R_2, respectively. Integration of the Gaussians according to (1) yields the two coordination numbers Z_1 and Z_2.

To decide which atomic pairs belong to these maxima, we compare in Table 1 for the case of amorphous $Ni_{25}Zr_{75}$ the distances R_1 and R_2 with atomic dis-

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