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STRUCTURE OF $Ni_{60}Nb_{40}$ METALLIC GLASS STUDIED BY COMBINED X-RAY AND NEUTRON DIFFRACTION

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АННОТАЦИЯ

Определены парциальные структурные факторы $S/Q/_{NiNi}$, $S/Q/_{NiNb}$ и $S/Q/_{NbNb}$ в быстроохлажденных образцах металлического стекла $Ni_{60}Nb_{40}$. Комбинированным методом рентгеновской и нейтронной диффракции; последний метод применялся для образцов с изотопным замещением. Рассчитаны функции парциального распределения. Даны подробные данные атомных расстояний и координационных чисел пар Nb-Nb.

KIVONAT

Gyorshütött $Ni_{60}Nb_{40}$ fémüveg minták $S(Q)_{NiNi}$, $S(Q)_{NiNb}$ és $S(Q)_{NbNb}$ parciális struktura faktorait határoztuk meg kombinált röntgen- és neutrondiffrakciós mérésekkel, az utóbbit izotópos helyettesitésü mintákon. Kiszámitottuk a parciális eloszlási függvényeket. Részletes adatokat adunk a Ni-Ni, Ni-Nb és Nb-Nb párok atomtávolságára és koordinációs számára.

ABSTRACT

The partial structure factors $S(Q)_{NiNi}$, $S(Q)_{NiNb}$ and $S(Q)_{NbNb}$ were determined for splat cooled $Ni_{60}Nb_{40}$ metallic glass samples by combined X-ray and neutron diffraction experiments; the letter on isotope substituted samples. The partial distribution functions were calculated. Details are given on interatomic distances and coordination numbers for Ni-Ni, Ni-Nb and Nb-Nb pairs.

INTRODUCTION

In order to determine the partial correlation functions of a binary amorphous system without neglections or a priori models, three independent diffraction experiments are needed. Independent diffraction measurements may be neutron diffraction on several samples with isotope substitution or using polarized neutrons in the case of magnetic samples; X-ray diffraction using several primary wavelengths for which the anomalous scattering correction of the component atoms are different [1]; a suitable combination of neutron diffraction and X-ray diffraction. Nowadays, diffraction methods are sometimes completed with EXAFS measurements. So far there is little information in the literature on the determination of the partial structure factors of metallic glasses /see e.g. Co-P [2], Ni-P [3], Cu-Zr [1,4], Ni-Nb [1]/.

In the present paper we provide details of our results obtained by combined X-ray and neutron diffraction experiments on samples of rapidly quenched $Ni_{60}Nb_{40}$ metallic glass with natural Ni and with Ni^{58} isotope; our results are compared with those of previous authors.

EXPERIMENTAL

Two samples of the same chemical composition $Ni_{60}Nb_{40}$ but with different isotopes, natural Ni and Ni^{58}, were made by rapid quenching from the melt in the form of ribbons with cross-section 3mm x 30 μm [5]. The density of the samples was found by the Archimedes method to be $\rho_o = 8.80 \pm 0.08$ gcm^{-3}.

Neutron diffraction /n.d./ measurements were made at the WWRS-M reactor in Budapest. The wavelength of the monochromatic beam was $\lambda_o = 1.067$ Å with $\lambda/2$ contamination of less than 1%. The samples of 21.5 g total weight were wound on a 40 mm long vanadium tube of Ø5 mm, to give an overall diameter of 11 mm.

For X-ray measurements monochromated Mo-Kα radiation /$\lambda_o = 0.71$ Å/ was used and the sample was positioned in transmission arrangement /one layer thickness, irradiated area 1 x 10 mm/.

Important parameters of the two types of diffraction measurements were agreed: e.g. resolution, step lengths ΔQ and the preset number of counts yielding uniform counting statistics with an error less than 1%.

DATA PROCESSING

Procedures for correcting and normalizing the measured intensities to obtain the total sturcture factors S(Q)-see *Fig.1* - by the three independent measurements were described earlier /for n.d see [6] and for X-ray d. see [7]/.

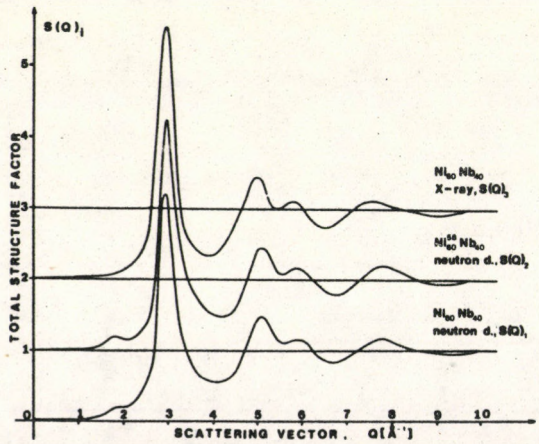

Fig. 1. Total structure factors $S(Q)_1$, $S(Q)_2$ and $S(Q)_3$ from the two neutron d. and X-ray d. experiments

In order to obtain the partial structure factors $S(Q)_{ab}$ we need to solve the matrix equation

$$[S(Q)]_i = [w_{i,ab}][S(Q)]_{ab} , \qquad (1)$$

where the subscripts i=1,2,3 refer to n.d with natural Ni, n.d. with Ni^{58} and X-ray d. measurements, a and b denote the two components Ni and Nb, respectively. The matrix elements w_{ab} are the weighting factors defined by $w_{aa}=c_a^2 b_a^2/\langle b\rangle^2$, $w_{ab}=2c_a c_b b_a b_b/\langle b\rangle^2$ and w_{bb} is analogous to w_{aa}. Here c represents the concentration and b the scattering amplitudes of the atoms and $\langle b\rangle$ is the avaraged scattering amplitude of the system. The numerical values are listed in Table 1.

Weighting factors of the partial structure factors $S(Q)_{ab}$ for the three experiments — Table 1.

	Ni-Ni	Ni-Nb	Nb-Nb
n.d. with Ni^{nat}	32.23%	43.14%	9.91%
n.d. with Ni^{58}	56.64%	37.23%	6.11%
X-ray d.	27.34%	49.89%	22.70%

The determinant of $w_{i,ab}$'s has usually a very low value /e.g. $|W|=0.005$/ and eqs. (1) cannot be solved directly with desirable accuracy. Some iterative algorithms to extract more reliable $S(Q)_{ab}$'s have been used by several authors [1,4,8].

We adopted the following procedure:

1/ The direct solution of eqs.(1) was calculated;

2/ A reduced system for the two n.d. structure factors was solved for $S(Q)_{NiNi}$ and $S(Q)_{NiNb}$ neglecting the terms of $S(Q)_{NbNb}$ as a first approximation;

3/ $S(Q)_{NiNi}$ as obtained from step 2/ was replaced into eqs.(1) which was then solved for $S(Q)_{NiNb}$ and $S(Q)_{NbNb}$;

4/ $S(Q)_{NiNb}$ as obtained from step 2/ replaced into 1/ which was solved for $S(Q)_{NiNi}$ and $S(Q)_{NbNb}$;

5/ From the solution of step 1/ to 4/ a set of consistent partial structure factors $S(Q)'_{ab}$ was constructed;

6/ The $S(Q)'_{ab}$ were replaced into eqs(1); the total structure factors were recalculated and compared with the experimental functions. The deviations were utilized for optimalizing the partial structure factors. Finally, the deviations nowhere exceeded 3%.

Reduced partial distribution function $G(r)_{ab}$ and partial distribution functions $RDF(r)_{ab}$ were calculated by Fourier transformation from the $S(Q)_{ab}$'s as follows:

$$G(r)_{ab} = \frac{2}{\pi} \int_0^\infty Q[S(Q)_{ab} - 1]\sin Q \, dQ$$

$$RDF(r)_{ab} = [4\pi r^2 \rho_o + rG(r)_{ab}]c_b$$

The partial coordination numbers n_{ab} were determined as the areas under the first peak of the corresponding $RDF(r)_{ab}$.

RESULTS AND DISCUSSION

The partial structure factors $S(Q)_{NiNi}$, $S(Q)_{NiNb}$ and $S(Q)_{NbNb}$ are shown in *Fig. 2*. Some general features of these and also of the total structure factors in *Fig. 1* are similar: a main peak

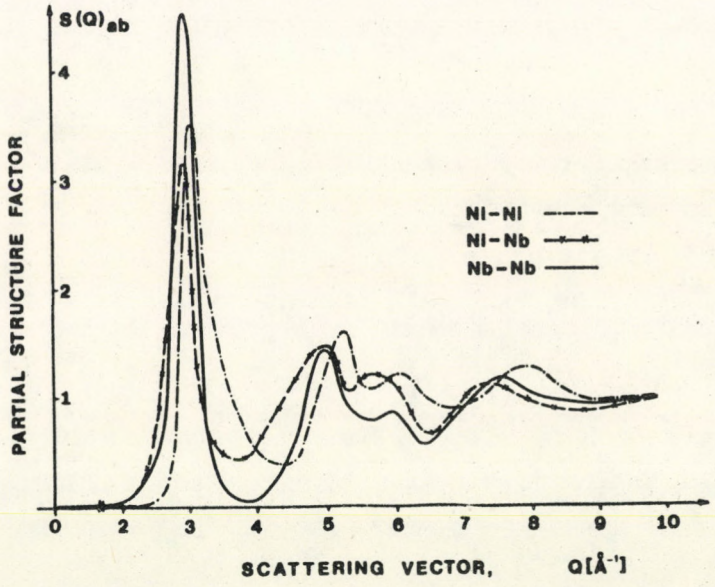

Fig. 2. Partial structure factors $S(Q)_{ab}$

around $Q=3\text{Å}^{-1}$ followed by a "double peak" between Q=4 and 6.5 Å^{-1}; only peak positions and heights in the three partial structure factors are slightly different /see Table 2/. Atten-

Peak positions from $S(Q)_{ab}$ and $G(r)_{ab}$ /error:±0.03/ Table 2.

	$S(Q)_{ab}$			$G(r)_{ab}$				
ab	Q_1	Q_2	Q_3	r_1	r_2	r_3	r_2/r_1	r_3/r_1
Ni-Ni	3.05	5.22	6.10	2.52	4.16	5.00	1.65	1.98
Ni-Nb	2.86	5.00	5.70	2.72	4.58	5.35	1.68	1.97
Nb-Nb	2.92	4.95	5.80	2.70	4.55	5.20	1.68	1.93

tion is drawn to the small, yet definite peak before the main peak: a so-called "pre-peak" at 1.8 Å^{-1} in both n.d. S(Q) curves, but missing from the X-ray d. curve. A similar pre-peak was found in the structure factor of some other amorphous and liquid alloys by neutron diffraction, this originated from chemical short-range order [9,10]. Detailed analyses of this pre-peak are currently being carried out.

The total and partial distribution functions - see *Fig. 3* -

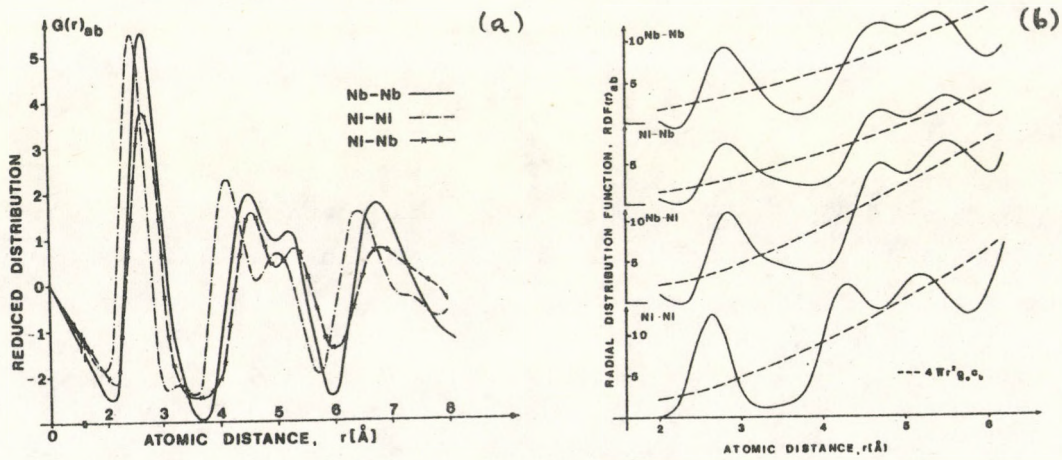

Fig. 3. Reduced partial distribution functions $G(r)_{ab}$ /a/ and partial radial distribution functions $RDF(r)_{ab}$ /b/

also exhibit a strong first peak corresponding to the first neighbour distances and partially overlapping second /higher/ and third /lower/ maxima, for details see Table 2. The atom pair distances as read from the first peak positions of $G(r)_{ab}$ functions are somewhat different from the results of ref.[1]. On the other hand, the measured density of our sample is significantly higher than that in ref[1] but in accordance with ref[11] which suggests that the packing of atoms in the two samples is slightly different.

The partial coordination numbers and their fractions to the total number of first neighbour atoms are summarized in Table 3. It can be seen that the contributions of components reflect the chemical composition of the sample. The total number of first neighbours of both Ni and Nb as central atom is 12 within the accuracy limit which is equal to the weighted sum of the partial coordination numbers. The mean coordination numbers obtained from the total RDF(r)'s are also about 12.

Partial coordination numbers n_{ab} /error: $\pm$ 0.5/ Table 3.

	Ni	Nb	total
Ni	7.3/62%/	4.5/38%/	11.8
Nb	6.8/56%/	5.4/44%/	12.2

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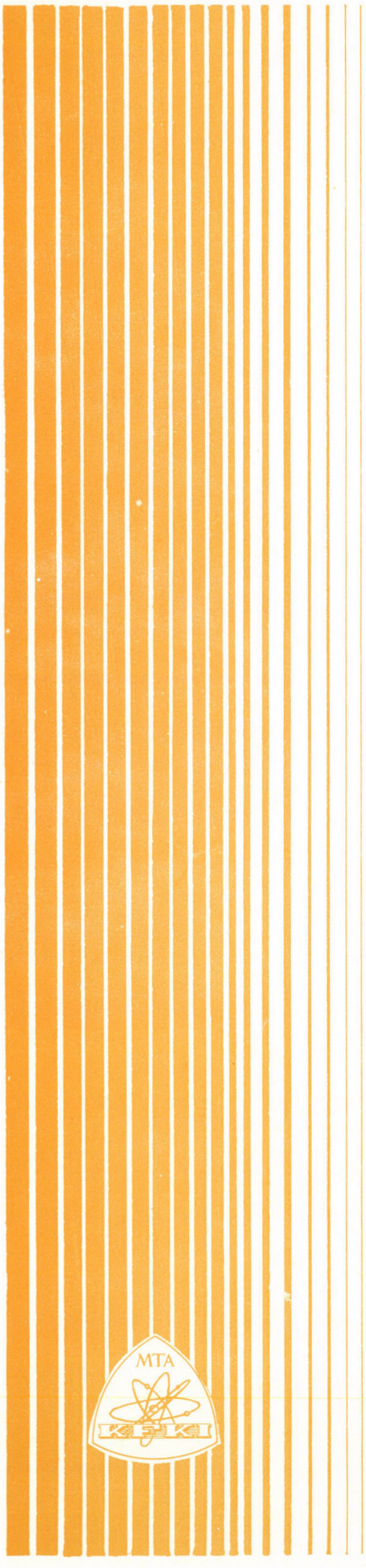

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