# Atomic structure in amorphous YNi2

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# Atomic structure in amorphous $YNi_2$

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**Résumé.** — La diffusion des rayons X et des neutrons a été mesurée sur un alliage amorphe non magnétique $YNi_2$. Bien que la symétrie locale soit très basse, on observe un ordre préférentiel des atomes qui rappelle celui de l'état cristallisé.

**Abstract.** — X-ray and neutron scattering experiments were performed on the non-magnetic a-$YNi_2$ alloy. Although the local symmetry is very low, a preferential ordering of Y and Ni atoms related to the crystalline arrangement is observed.

1. **Introduction.** — X-ray and neutron scattering results have been previously obtained on amorphous alloys such as $GdFe_2$ and $TbFe_2$ [1, 2, 3]. The present work involves a joint X-ray and neutron scattering experiment on the non-magnetic a-$YNi_2$ alloy. The radial distribution functions (RDF) have been deduced by Fourier transformation of the data. They are compared to those calculated in a structural model which has been recently proposed for amorphous $ErCo_2$ [4].

2. **Experiment and results.** — The amorphous alloy $YNi_{1.85}$ was prepared by D.C. sputtering. The X-ray scattering data were obtained using the $MoK_\alpha$ and $K_\beta$ radiations. A solid state detector was used as counter in order to avoid fluorescence. The neutron experiment ($\lambda_n = 1.218$ Å) was performed on the $D_{1B}$ diffractometer at ILL (Grenoble) and the multidetector aperture was 80°. The maximum $k$-values were 10 and 15 $Å^{-1}$ respectively in the neutron and X-ray experiments. The average atomic density $\rho_0$ was measured to be $6.8 \pm 0.1$ g/cm$^3$ compared to 7.38 g/cm$^3$ in crystalline $YNi_2$.

After correction for background and Laue scattering the diffracted X-ray intensities $I(k)$ were used to obtain the reduced interference function

$$F(k) = k[I(k) - 1]$$

shown in figure 1. The Fourier transform of $F(k)$ is the reduced RDF (figure 2) :

$$W(r) = \frac{1}{2\pi^2 \rho_0} r\left[\frac{\rho(r)}{\rho_0} - 1\right].$$

The diffracted neutron intensities were corrected for background, multiple scattering [5] incoherent and Laue scattering. The associated functions $F(k)$ and $W(r)$ are presented respectively in figures 1 and 2.

The general features of the X-ray and neutron interference functions are very similar with a first main peak centered at $k \sim 2.8$ $Å^{-1}$ and a second peak at about 5 $Å^{-1}$. In the case of neutrons a small peak is observed at $k = 1.5$ $Å^{-1}$. This peak is remi-

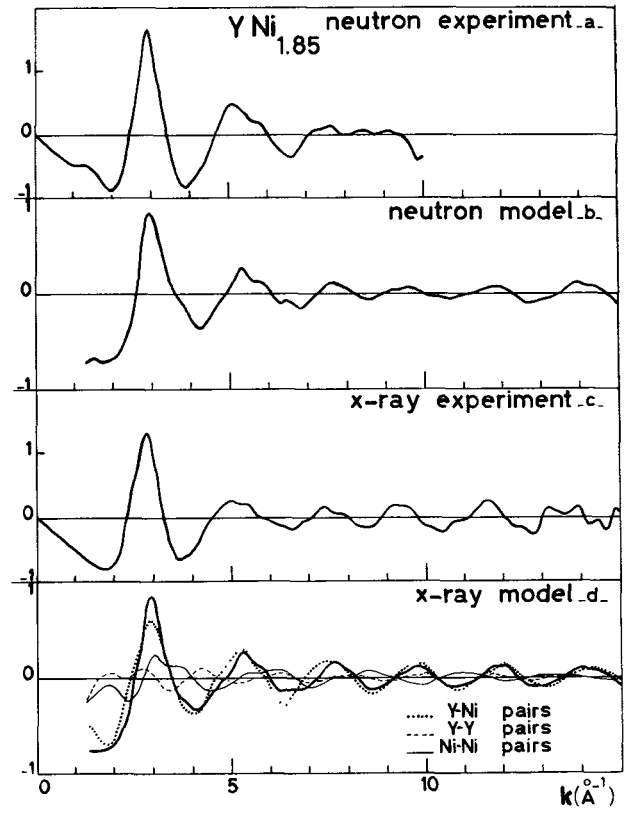


Fig. 1. — Experimental and calculated interference functions $F(k)$.

niscent of a superstructure peak in the crystalline state and must be attributed to a preferential ordering between Y and Ni atoms. It is only obtained in the neutron experiment due to the value of the ratio between the Ni and Y Fermi lengths. The large maximum value of $k$ in the X-ray experiment leads to a better resolution of the peaks in the X-ray RDF than in the neutron one.

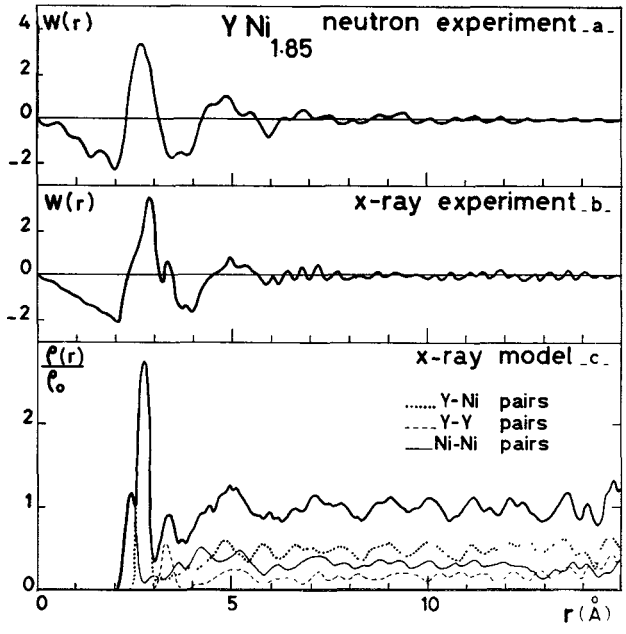


Fig. 2. — Experimental $W(r)$ functions and calculated $\rho(r)/\rho_0$ functions.

3. **Discussion.** — The RDFs exhibit a main broad peak centered around 2.8 Å with a shoulder at 2.45 Å and an other smaller peak at 3.4 Å. These peaks are logically attributed to Y-Ni, Ni-Ni and Y-Y first neighbour distances which are compared to those observed in the cubic Laves phase $YNi_2$ and to the Goldschmidt diameters in table I.

The shortest Ni-Ni distance is close to the Ni Goldschmidt diameter. The first distance between Y atoms occurs at a greater distance than the very short Y-Y spacing in crystalline $YNi_2$, but it is less than the Y Goldschmidt diameter. Finally, the first Y-Ni distance is shorter than the average of the Y-Y and Ni-Ni distances.

The interference and pair correlation functions have been calculated using a model [4] based on the observed experimental distances (figures 1 and 2). To fit the experimental results, one must assume that three Y atoms cannot be in contact. This condition tends to favor unlike pairs of atoms, i.e. to create a preferential atomic ordering and leads to the existence of a small peak at 1.5 $Å^{-1}$ in the calculated neutron interference function. Below 6 Å, the second and third neighbour distances in the partial pair correlation functions are in good agreement with the experimental data (figure 2). The coordination numbers deduced from the model are close to those of the crystalline state rather than those associated with a random distribution of atoms (table I). This suggests that the local atomic arrangement in the amorphous state resembles that of the crystalline state. Such an arrangement minimizes the energy since the associated local density is increased.

4. **Conclusion.** — The amorphous short-range order resembles that of the crystalline state; however, this does not imply that the cubic Laves phase symmetry is kept, as shown by the very low symmetry of the crystal field found in magnetic amorphous alloys [6].

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Table I

| | First-neighbour distances Å | | | Coordination numbers | | |
|---|---|---|---|---|---|---|
| | Crystal | Amorphous | Goldschmidt diameter | Crystal | Amorphous model | Statistical $YNi_{1.85}$ |
| Y-Y | 3.11 | 3.40 | 3.60 | 4 | 4 | 5.6 |
| Y-Ni | 2.98 | 2.80 | 3.04 | 12 | 12 | 10.4 |
| Ni-Y | | | | 6 | 5 | 4.2 |
| Ni-Ni | 2.54 | 2.45 | 2.48 | 6 | 5.5 | 7.8 |

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