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M. Laridjani, P. Leboucher, D. Raoux, J. Sadoc. X-RAYS DIFFRACTION STUDY OF BINARY METALLIC Cu-Y GLASSES USING ANOMALOUS DISPERSION. Journal de Physique Colloques, 1985, 46 (C8), pp.C8-157-C8-161. 10.1051/jphyscol:1985821 . jpa-00225164

**HAL Id: jpa-00225164**

**<https://hal.science/jpa-00225164>**

Submitted on 4 Feb 2008

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# X-RAYS DIFFRACTION STUDY OF BINARY METALLIC Cu-Y GLASSES USING ANOMALOUS DISPERSION

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**Résumé** - La méthode de diffraction anormale des rayons X a été utilisée pour déterminer les fonctions de distribution radiale partielles pour un alliage amorphe Cu-Y.

**Abstract** - Anomalous X-ray diffraction method has been used to obtain partial radial distribution functions for an amorphous alloy Cu-Y.

The information about environment of each component in an alloy can be obtained from partial distribution function of the specific atomic species. The partial function is determined by different technique (1) one of these techniques, which has been developed recently (2,3), is the X-ray diffraction, in which the anomalous dispersion effects. In this technique the partial radial distribution function can be obtained by using the variation of atomic scattering as the function of photon energy near the absorption edge. Generally, the total atomic scattering factor ( $f$ ) is complex. The total atomic scattering can be written as :

$$f(k, \omega) = f_0(k) + f'(K, \omega) + i f''(k, \omega)$$

Here  $f_0$  is the atomic scattering factor for radiation with a frequency much higher than the absorption edge. It is only a synchrotron radiation source that provides a powerful flux on the adjustable wavelengths either close or away from the absorption edge.

In this paper the results of our resonance X-Ray diffraction study of sputter deposited amorphous  $\text{Cu}_5\text{Y}$  and  $\text{Cu}_2\text{Y}$  are discussed.

In order to obtain the different total interference function which can be obtained by modifying the total scattering factor ratio, in the case of a binary alloy, three experiments with three different wavelengths must be done.

The total interference function can be defined by :

$$J(K, \omega) = \frac{C_{\text{Cu}}^2 [f_{\text{Cu}}(K) + \Delta f_{\text{Cu}}(K, \omega)]^2}{A^2} Y_{\text{Cu-Cu}} + \frac{C_{\text{Y}}^2 [f_{\text{Y}}(K) + \Delta f_{\text{Cu}}(K, \omega)]^2}{A^2} Y_{\text{Y-Y}} + C_{\text{Y}} C_{\text{Cu}} \left\{ \frac{[f_{\text{Y}}(K) + \Delta f_{\text{Y}}(K, \omega)] [f_{\text{Cu}}(K) + \Delta f_{\text{Cu}}(K, \omega)]^*}{A^2} + \text{Conj.} \right\} Y_{\text{Cu-Y}} \quad (1)$$

$$\Delta f(K, \omega) = f'(K, \omega) + i f''(K, \omega)$$

$$\text{and } A^2 = \left| C_{\text{Cu}} [f_{\text{Cu}}(K) + \Delta f(K, \omega)] + C_{\text{Y}} [f_{\text{Y}}(K) + \Delta f_{\text{Y}}(K, \omega)] \right|^2$$

The three independant partial functions are defined in the conventional way (3). The best is to obtain  $J(K, \omega)$  from three different energies : one far away from the absorption edges, one very

close to the Y absorption K-edge, and one very close to the Cu absorption K-edge. But it is known that a good resolution on a P.D.R. function needs a short wavelength in order to have a large  $K$  value. A wavelength close to the Cu K-edge only allows  $K_{\max}$  of the order of  $9 \text{ \AA}^{-1}$  which gives a weak resolution. In the case of  $\text{Cu}_5\text{Y}$  alloy it was possible to by-pass this limitation. The low value of the Yttrium content leads to a contribution of  $Y_{Y-Y}$  partial function which is always very small. So it is possible to neglect this contribution or to suppose a very simple Y function and to derive the other partial functions. In this case only two experiments are needed both with high energies.

#### THE EXPERIMENTAL PROCEDURE

The ductile amorphous foils of  $\text{Cu}_5\text{Y}$  was prepared by D.C. triod sputtering using Al. Substrate.

The experiment was carried out at a beam line D1 at LURE, which is equipped with a channel-cut Si (220) single crystal as a monochromator with an energy resolution of 10 eV at 17000 eV. The DCI ring was operated at 1.72 and 1.85 GeV.

The diffraction intensity  $I(K)$  was measured at two energies below and on the Cu and Y, K absorption edges. In order to avoid fluorescence the scattered beam was recorded by an energy dispersive detectors, of lithium-drifted silicon, connected with a pulse processor. The detail of the experiment is described elsewhere (3)

#### RESULTS AND DISCUSSION

As the energy resolution of the solid state detector is about 180 eV, for a photon energy near 8000 eV, it was sufficient to resolve the fluorescence lines  $K_{\alpha}$  and  $K_{\beta}$  of Y but not adequate enough to resolve  $K_{\beta}$  from the elastically scattered photon.

The fluorescence line intensities are very important when the incident beam energy is over the absorption edge, but even when it is below the absorption edge the intensities still persist. This is due to Raman resonant effect, but also to a small amount of second harmonic energy in the incident beam.

An accurate estimation of the K intensity is necessary to be subtracted from the diffracted intensity. We have supposed a ratio between the  $K_{\beta}$  and  $K_{\alpha}$  intensities independant of the excitation energy. A precise measurement of the two fluorescent lines with an excitation energy well resolved from  $K_{\beta}$  gives  $K_{\beta Y}/K_{\alpha Y} = 0.235$  and  $K_{Cu}/K_{Cu} = 0.16$

The diffracted intensities were normalized with the incident beam or with the fluorescence intensity of  $\text{Cu-K}_{\alpha}$  in order to take in account the time decrease of the beam.

According to the above corrections and normalisations  $J(K)$  functions are obtained with a satisfactory reproductibility for different experiments performed at the same energy.

So the variations in the features of the two  $J(K, \omega)$  functions related to anomalous dispersion are significant.

In order to normalize the scattered intensity, the value of  $f'$  at  $E = 17036 \text{ eV}$  was assumed  $f' = -6$ . This was obtained from the theoretical value, calculated in the reference (4). They have used Cromer and Liberman relations.

Fig. (1) shows two reduced interference functions  $F(K) = K (J(K)-1)$  which have been derived from two energy measurements :  $E = 17036 \text{ eV}$  (near the absorption edge of Y) and  $E = 15800 \text{ eV}$  (below the absorption edge).

The reduced radial distribution function  $W(R)$  is the Fourier transform of the  $F(K)$  function (Fig. 2). They have characteristic features of amorphous metallic radial distribution function with two well resolved first interatomic distances. At first sight it seems reasonable to consider the first peak as the Cu-Cu first distance, and the second peak to Cu-Y.

#### THE PARTIAL INTERFERENCE AND DISTRIBUTION FUNCTION

For a diluted alloy such as  $\text{Cu}_5\text{Y}$  as it was mentioned above, the contribution of  $\text{Y}_\text{y-y}$  is weak in both cases of energy. Therefore this function can be taken as an adjustable parameter ; and by inversion, the linear system can be solved with the two unknown functions  $\text{Y}_{\text{Cu-Cu}}$  and  $\text{Y}_\text{y-Cu}$ .

Fig. (3) shows the two partial interference functions for the amorphous alloy  $\text{Cu}_5\text{Y}$  evaluated from the independent functions as it was mentioned above.

But the information on the atomic distribution functions in real space is given by the Fourier transformation of each partial interference function.

Fig. (4) shows the two partial radial distribution functions  $w(R)$  of Cu-Cu and Cu-Y. These functions permit us to find distances occurring in Cu-Cu and Cu-Y pairs. The first peak of the Cu-Cu partial function corresponds to a distance at 2.50 Å. At the foot of this peak there is another distance at 3.32 Å which can be interpreted as a second site for Cu atoms. On the other function, corresponding to Cu-Y distances, the first peak is at 3.0 Å. The atomic radius of Cu is 1.28 Å and the atomic radius of Y is 1.78 Å : experimental distances are slightly contracted if we refer to atomic radius. Other distances appear in Fig. 4 ; similar distances in the crystalline phase  $\text{Cu}_5\text{Y}$  are presented in table 1. Coordination numbers obtained from these functions are given in table 2.

If we compare the present result with the first distance in the crystalline  $\text{Cu}_5\text{Y}$ , table (1), we find certain resemblances between the local order in amorphous and the crystalline phase. This resemblance is shown by the EXAFS methods also. Table (2) shows the coordination numbers of the two phases in which we cannot observed the indicated similarity.

We have checked these results with radial distribution functions obtained from interference functions measured with photon energy close to the Cu absorption edge. First and second distances agree with the Y edge results. Coordination numbers obtained from Cu-Cu and Cu-Y function also agree. But there is no hope to determine the y function by comparison of results obtained with photon energies corresponding to Y-edge and Cu-edge, because due to the small  $K_{\text{max}}$  value ( $K_{\text{max}} = 8 \text{ \AA}^{-1}$ ) nothing can be concluded on distances which contribute lightly to interference functions.

For obtaining the  $\text{Y}_\text{y-y}$  contribution we change the composition of the alloy to  $\text{Cu}_2\text{Y}$ . As it is mentioned. We did three independent experiments with three different energies near the absorption edge of Y. The analysis of the data is in progress.

Therefore, we believe that the important result of this work is to show useful aspects of anomalous dispersion effects for solving the structure problem in the disordered material.

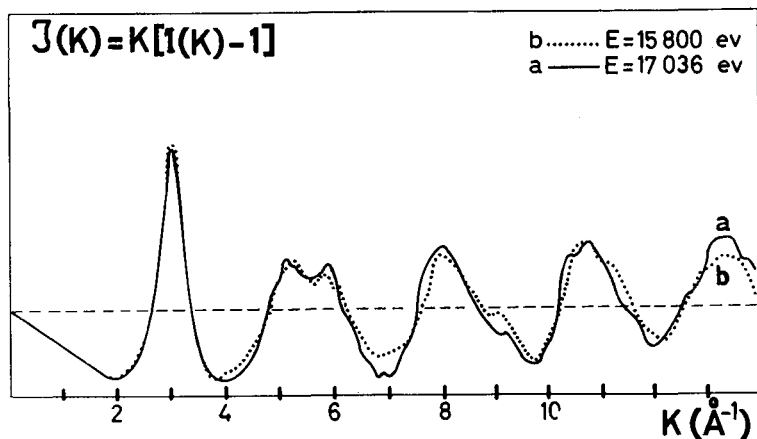


Fig (1) Interference functions for the amorphous alloy  $\text{Cu}_5\text{Y}$ .

a - near the yttrium k - edge  
b - Below the yttrium K-edge

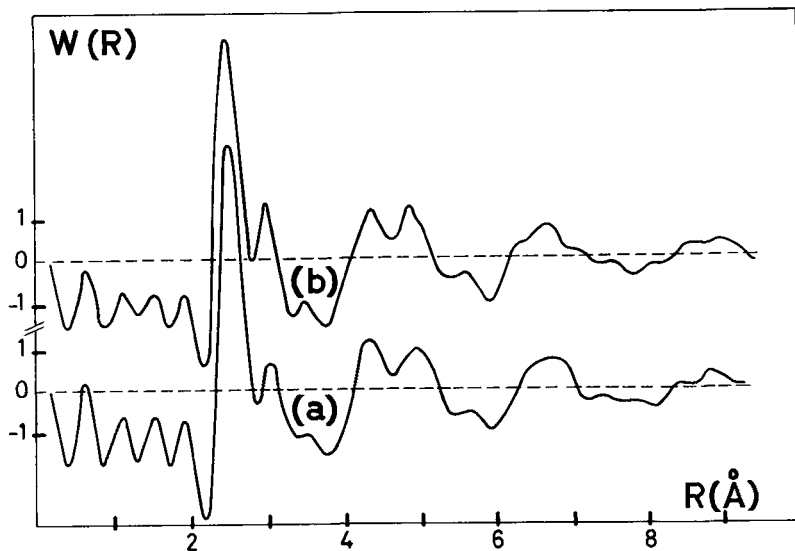


Fig. (2) The reduced radial distribution functions derived by Fourier transform from Fig. 1(a) and (b)

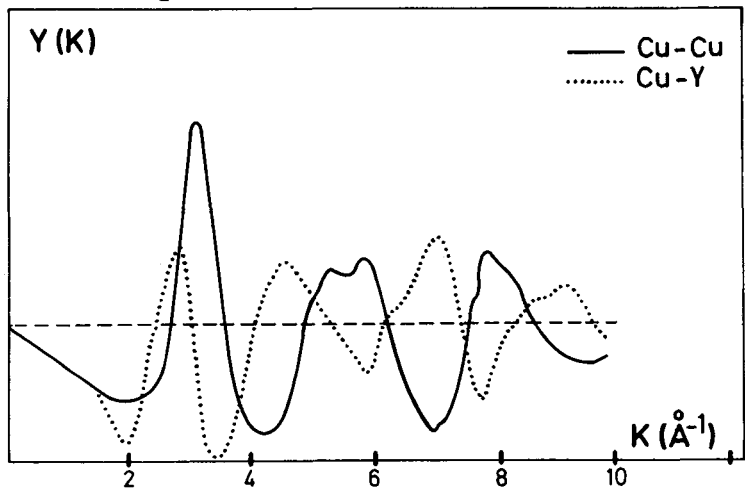


Fig. (3) The partial interference functions  $Y_{\text{Cu-Cu}}$  and  $Y_{\text{Cu-Y}}$  derived from  $J(K)$

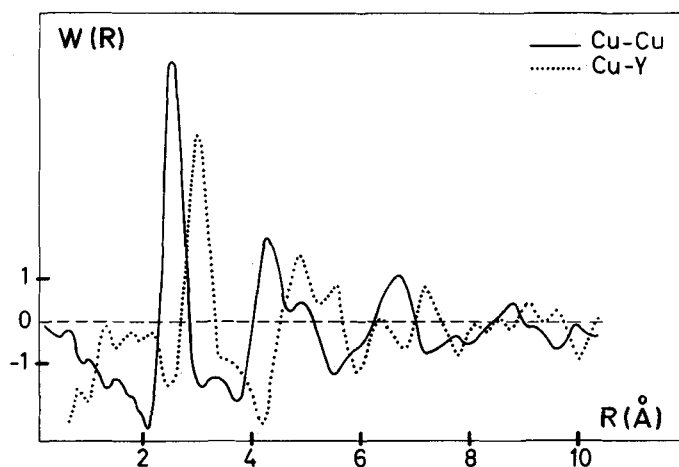


Fig. 4. : The reduced radial distribution function  $W_{\text{Cu-Cu}}$  and  $W_{\text{Cu-Y}}$

Table 1 - Interatomic first distances in the Crystalline  $\text{Cu}_5\text{Y}$  (5) and amorphous phase.

CRYSTALLINE PHASE						AMORPHOUS PHASE	
(Cu II - Cu II)	(Cu II - Cu I)	(Cu I - Cu I)	(Cu I - Cu Y)	(Cu Y - Cu Y)	(Cu - Cu)	(Cu - Cu)	(Cu - Y)
(2.49 Å)	(2.51 Å)	(2.88 Å)	(2.88 Å)	(3.23 Å)	(2.50 Å)	(3.32 Å)	(3 Å)

Table 2 -

	Atom taken as origin	number of Cu around it	number of Y around it	Total (Z)	mean coordination number (Z)
amorphous	Cu	7.4+3 = 10.3	2.8*	13.2 (0.5)	13.75
$\text{Cu}_5\text{Y}$	Y	14.39	2	16.5 (0.5)	
crystalline	Cu (I or II)	8 or 9 (8.33)	4 or 3 (3.66)	12	13.33
$\text{Cu}_5\text{Y}$	Y	18	2	20	

\* Hypothetical as in the crystal (Réf. 18).

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