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EXAFS STUDIES OF GLASSY METALLIC ALLOYS

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Abstract.- The near neighbor correlations have been obtained from EXAFS measurements at Stanford Synchrotron Radiation Laboratory for a series of metal-metal glassy alloys. In particular, the structures of $\text{Mo}_{50}\text{Ni}_{50}$ alloy in amorphous and crystalline states are presented. The structure of the a-MoNi may be described by a more or less dense random packing of binary spheres in contrast to the c-MoNi which is described by a distorted bcc structure.

Introduction

During the past two decades, from its birth in 1960 to the present, vast improvements in both fabrication techniques and glass properties of metallic glasses have been achieved. The first metallic glasses, ill-formed flakes of expensive alloys, have given way to uniform ribbons of inexpensive steel alloy compositions. This progress has required, and will continue to require, simultaneous attention to both the fabrication methods and the alloy compositions. The impetus for this effort has long since changed from scientific curiosity to interest in application of the unique properties of metallic glasses.

Metallic glasses not only exhibit technologically interesting properties, such as high fracture strength, good soft magnetic behavior, excellent corrosion resistance, and catalytic properties, but also constitute ideal materials for the studies of low temperature transport, critical phenomena and electrical properties of disordered metals⁽¹⁾

These unique properties arise from the unique structure of the glassy state, namely the absence of translational periodicity and structural and compositional homogeneity. A detailed knowledge of the atomic arrangement in glassy metal is apparently necessary for the understanding of their unique properties.

Partial distribution functions characterizing the structure, particularly the short range structure of binary alloy glasses have been extracted either from a combination of X-ray and neutron diffractions, or from anomalous X-ray scattering measurements.

These measurements provide only qualitative information regarding the short-range order for a limited class of metallic glasses because of inherent drawbacks of these methods. For example, neutron diffraction requires large samples $\sim 1 \text{ cm}^3$ which are not often attainable in amorphous state, while anomalous X-ray scattering method with conventional sources often limits the measurable maximum k value of only $\sim 10 \text{ \AA}^{-1}$ which is insufficient for resolving very short range structure. Another disadvantage of X-ray measurements is the difficulty in differentiating two elements which lie close to each other in the periodic table, e.g. Fe and Ni or Co, as well as in distinguishing the minor constituents of lighter elements from the heavier atoms, e.g. metalloid atoms (P, B, Si, C) from transition metals (Fe, Co, Ni and Cu) in metal-metalloid glasses.

In contrast, Extend X-Ray Absorption Fine Structure (EXAFS) spectroscopy can be used to probe either the K or L-absorption edge of constituents separately such that three pair correlations of binary alloys can be extracted thus providing important information for the understanding of the alloying effects on formation, stability, and properties of glassy metal alloys.

Recently, we have been involved in the EXAFS studies of (1) $\text{Zr}_{100-x}\text{Cu}_x$ glassy alloys with $x = 35, 50$ and 65 and (2) a $\text{Mo}_{50}\text{Ni}_{50}$ alloy in both amorphous and crystalline states. Only the results for the MoNi alloys are presented here

Experimental Results

The amorphous film about $25 \mu\text{m}$ thick was prepared by high-rate

sputter deposition onto a Cu substrate at 78 K. The amorphous structure was verified by X-ray diffraction. The crystalline specimen was obtained by annealing the sputtered film at 1000 K for 1 hr. The crystalline phases were identified as a mixture of a MoNi_3 phase and b.c.c. structure. EXAFS measurements were carried out at the Stanford Synchrotron Radiation Laboratory (SSRL) using the facility at Wiggler beam line IV. The measurements in transmission mode were made on both the amorphous and crystalline materials at room temperature and near liquid nitrogen temperature at the Ni K edge (8340 eV) and Mo K edge (19980 eV). Measurements were also made on standard Mo metal.

The data were analyzed via standard procedures described in the literature.⁽²⁻⁵⁾ Fig. 1 shows the Ni K edge (at 8340 eV) absorption spectrum of amorphous $\text{Mo}_{50}\text{Ni}_{50}$ at room temperature. Fig. 2 shows the EXAFS modulation after removing the smooth μ_0 background and choosing $E_0 = 8340$ eV. The resulting $\chi(k)$ curve has been multiplied by k^3 .

The Fourier transform of the curve in Fig. 2 is shown in Fig. 3. The large peak is the contribution from either Ni or Mo at the first shell of Ni atoms. The dashed line in Fig. 3 is a smooth filter window-function applied to the Fourier transform of $\chi(k)$ to isolate the EXAFS from the first shell. Fig. 4 illustrates the inverse transform which contains information about the first neighbor coordination number, the kind of atoms involved and the distribution of interatomic distances.

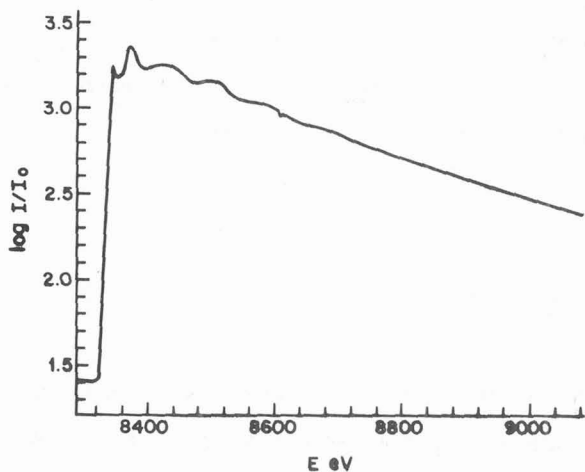


Fig. 1. The Ni K edge at 8340 eV absorption spectrum of $\text{a-Mo}_{50}\text{Ni}_{50}$ at R T.

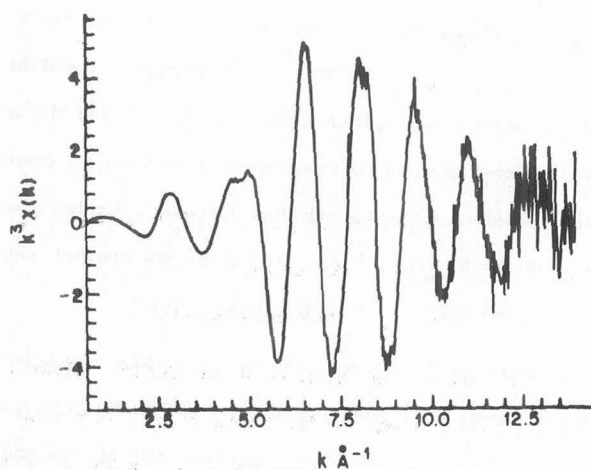


Fig. 2. The EXAFS modulation of Fig. 1, after background removal.

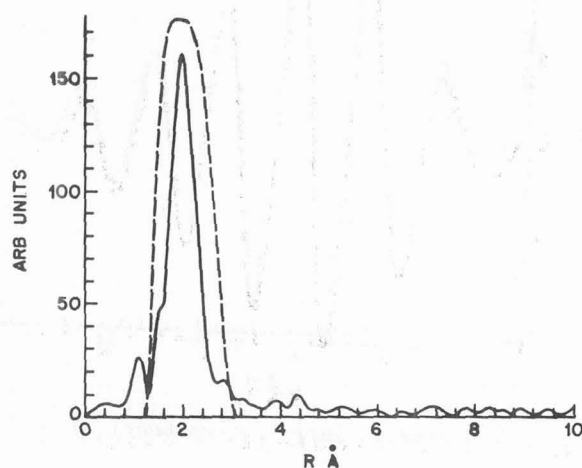


Fig. 3. The Fourier transform of the curve in Fig. 2.

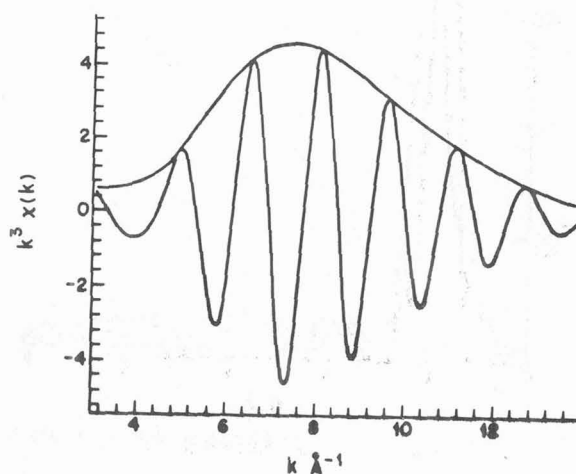


Fig. 4. The inverse transform of the first peak in Fig. 3.

Since we did not know, a priori, the nature of the first shell distance, we attempted to fit the Fourier-filtered data with Ni-Ni, Ni-Mo, and a combination of both. For the Ni edge we found the first shell contains two kinds of neighboring atoms (Ni and Mo) at slightly different distances via a least-squares curve fitting procedure (using theoretical amplitude and phase functions⁵) detailed elsewhere in the literature.²⁻⁴ An excellent fit was obtained with $r_{\text{Ni-Ni}} \cong 2.36 \text{ \AA}$ and $r_{\text{Ni-Mo}} \cong 2.59 \text{ \AA}$ as shown in Fig. 5.

Fig. 6 shows the Fourier transform of the EXAFS modulation $\chi(k)k^3$ at the Mo K absorption edge of the a-MoNi. The first large peak is identified to be the contributions from both Mo-Mo and Mo-Ni pairs.

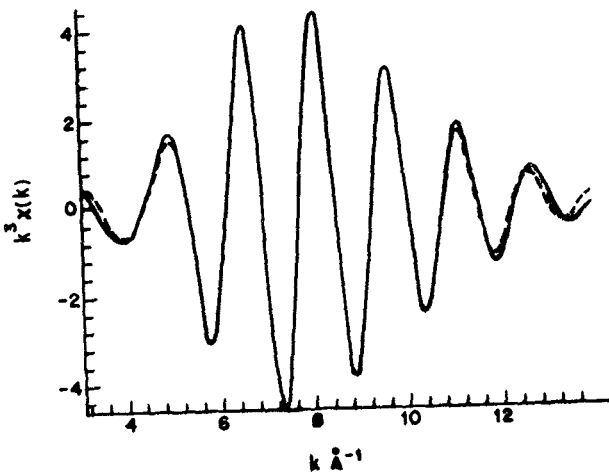


Fig. 5. Experimental data (—) fit with theory (----).

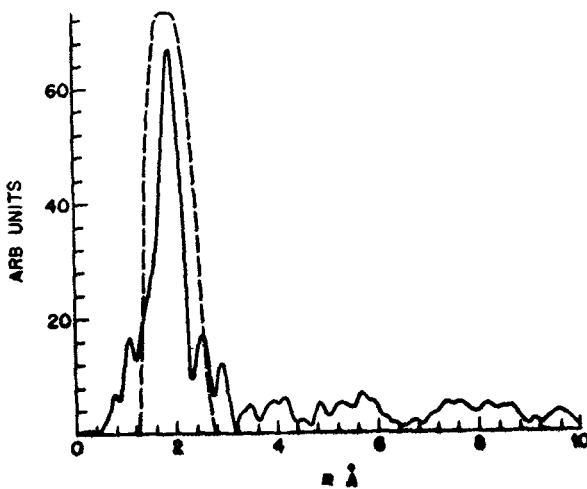


Fig. 6. Fourier transform of the EXAFS modulation at Mo K edge of the a-MoNi at R.T.

In contrast to the amorphous alloys, both the crystalline MoNi alloy and the Mo metal exhibit a distinct second peak at a distance which is about 0.5 \AA larger than the first peak in the Fourier transform of the EXAFS spectrum at Mo K edge. Curve fitting of the filtered EXAFS data yielded, for the Mo metal, the first and the second shell distances of 2.725 \AA and 3.147 \AA , respectively, which are in excellent agreement with the X-ray data. We also calculated the coordination numbers of the alloys with the scaling factor obtained from the Mo metal measurements. For a-Mo₅₀Ni₅₀, a factor of ~ 3 reduction in the EXAFS amplitude was observed. Table I lists the distances and coordination numbers of first and second shells at Mo atoms for the crystalline metals. It may be noted that for the first shell, the average distance ($\bar{r} = 2.64 \text{ \AA}$) and the average coordination number ($\bar{N} = 7$) of the alloy are very close to those in the Mo metal. In addition, the average distances of both the first and second shells in the alloy are $\sim 0.08 \text{ \AA}$ shorter than in the pure metal, apparently as a result of smaller Ni atoms replacing larger Mo atoms in the alloy. We may thus suggest that the coordination of the Mo atoms in the crystalline alloy resembles distorted bcc Mo structure with Ni atoms substituting Mo atoms.

Table 1. The distance r and coordination number (N) of the first and second shell at Mo atoms in crystalline Mo and Mo₅₀Ni₅₀.

c-Mo ₅₀ Ni ₅₀			
	$r_2(N_1)$	$\bar{r}_1(\bar{N}_1)$	$r_2(N_2)$ $\bar{r}_2(\bar{N}_2)$
Mo-Mo	2.81 Å (2)		3.16 Å (6)
		2.64 Å (7)	3.07 Å (12)
Mo-Ni	2.57 Å (5)		2.98 Å (6)
c-Mo			
	$r_1(N_1)$		$r_2(N_2)$
Mo-Mo	2.73 (8)		3.15 (6)

Table 2 lists the distance, Debye-Waller factor, and the coordination number of the first shell of a-Mo₅₀Ni₅₀ and c-Mo₅₀Ni₅₀. There is a discrepancy in the average distance of the MoNi pairs extracted from the Mo K edge and Ni K edge. The discrepancies