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Comparison of the atomic structure of Zr-Cu amorphous alloys and the effect of Al, Ti, and Ni addition using synchrotron radiation in transmission

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Abstract – The atomic structure of Zr-Cu binary amorphous alloys was studied using real space pair distribution functions (PDF) derived from X-ray diffraction. The structure can be modeled by an ideal solution approximation because of relatively weak Cu-Zr atomic interactions. Addition of Al to Zr-Cu metallic glasses modifies the atomic structure in the short (SRO) and medium range order (MRO) because of the strongly attractive interaction between Al and Zr atoms. These interactions generate strong deviations from the ideal solution behavior. Ti addition has a minor influence on the local atomic structure of Cu-Zr based metallic glasses.

Zr-Cu based liquid alloys form metallic glasses with good thermal stability and high mechanical strength. For this reason this family of materials is of significant interest from fundamental research and application points of view. While binary Cu-Zr alloys form glasses upon cooling from the liquid state, the critical cooling rate for suppression of crystallization is still rather high such that the thickness of a crystallite-free metallic glass obtained by copper-mold casting is limited to just over 1 mm. However, addition of aluminum reduces the critical cooling rate such that thicker bulk metallic glasses can be obtained by copper-mold casting. Important steps towards a better understanding of the atomic structure in the glassy state have been carried out recently [1-3]. In the case of weakly interacting Cu-Zr atoms, an ideal solid solution behavior has been suggested for the binary Zr-Cu metallic glass [4].

The atomic structure of Zr–Cu binary glasses and the effect of Al additions were investigated using real space pair distribution functions (PDFs) derived from high precision x-ray diffraction data acquired at the ID11 of the European Synchrotron Radiation Facility (ESRF). It was found that the structure of the binary Zr-Cu metallic glasses can be modeled by an ideal solution approximation because of relatively weak Cu-Zr atomic interactions. Addition of Al strongly modifies the atomic structure because of the strongly attractive interaction between Al and Zr atoms, which generate strong deviations from the ideal solution behavior (fig. 1) [5]. With Al atomic size intermediate between those of Cu and Zr, formation of a large number of Al-Zr nn pairs results in a broader dispersion of 1st nearest neighbor (nn) interatomic distances apparently leading to a higher packing efficiency. Addition of Ti has a minor influence on the local atomic structure. On the other hand, substitution of Cu by Ni modifies drastically the local atomic structure of Zr-Cu-Al metallic glasses, especially in the first nn shell, while the changes in the medium range order (MRO) are less pronounced.

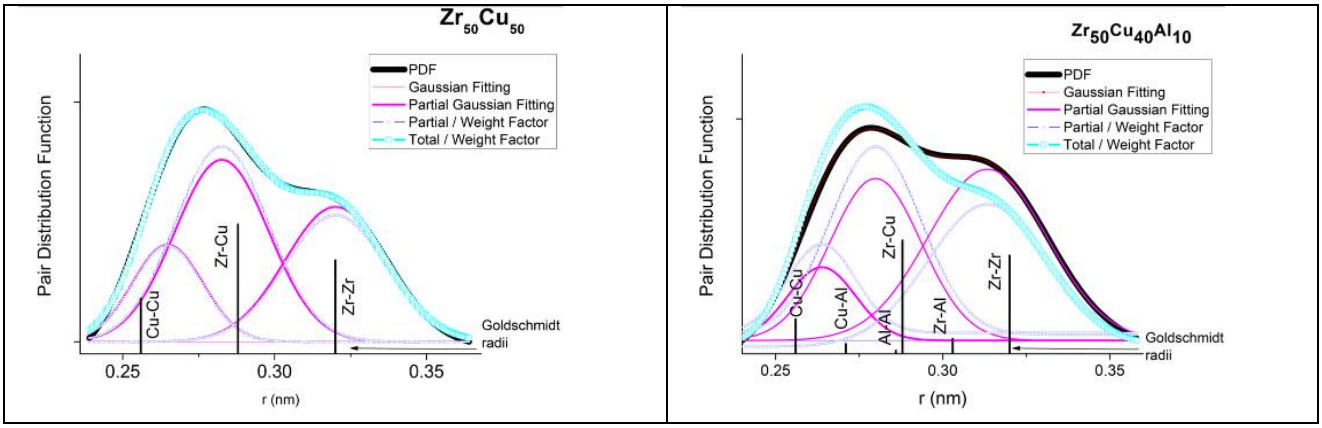

Figure 1: *Gaussian fitting of the first PDF peak for a $Zr_{50}Cu_{50}$ and b) $Zr_{50}Cu_{40}Al_{10}$ metallic glasses. Thick continuous black curves correspond to the experimental PDF, thin red continuous curves correspond to partial PDFs derived from the deconvolution of the experimental PDF into three Gaussians corresponding to Cu-Cu, Zr-Cu and Zr-Zr partial PDFs. Thin blue discontinuous curves represent the Gaussian partial PDFs if they are scaled to the weight factors of an ideal solution and the thick discontinuous bluish curves represent the expected total PDFs based on the weight factors. [5].*

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