MS01 Functional Materials: state of the art and advances

Short-range atomic structure of $Pd_{40}Cu_{30}Ni_{10}P_{20}$ metallic glass: insights from X-ray pair distribution function analysis in bulk and thin films

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Metallic glasses (MGs), in bulk form or as thin films, offer compelling routes for materials discovery enabling the design of non-crystalline metallic alloys with exceptional mechanical strength, elasticity, and corrosion resistance. These properties arise from their disordered atomic structure, which differs fundamentally from conventional crystalline metals, and therefore open opportunities for applications in extreme environments such as aerospace, energy, and the medical domain.

In this study, we investigate the Pd-based metallic glass alloy $Pd_{40}Cu_{30}Ni_{10}P_{20}$. We examine how different processing routes influence the short-range atomic ordering of the alloy in bulk form using laboratory-based X-ray Pair Distribution Function (PDF) analysis. Although the alloys remain fully amorphous after production, subtle variations in short-range order are observed depending on the processing conditions. The atomic structure is modeled using large-box simulations based on Reverse Monte Carlo methods revealing variations in the distribution of local polyhedral motifs within the amorphous network. In addition, a sample of this alloy was exposed outside the International Space Station (ISS) for one year (Dec. 2024-Dec.2025). The impact of the space environment, such as high temperature gradients, cosmic radiation, vacuum conditions, microgravity and their combination, will be studied and will give us the possibility to evaluate eventual changes of the atomic structure in the materials including defects.

In parallel, the same alloy was deposited as thin films using physical vapor deposition (PVD) by sputtering. The resulting coatings are homogeneous and exhibit short-range order similar to that of the bulk material. Reactive sputtering was also explored by introducing nitrogen during deposition. Preliminary results indicate that nitrogen incorporation modifies the amorphous structure. X-ray photoelectron spectroscopy (XPS) shows that nitrogen affects the chemical environment of Cu, Ni, and P, while Pd remains largely unchanged. Additionally, the crystallization activation energy increases with higher nitrogen content, suggesting an improvement in the thermal stability of the films.

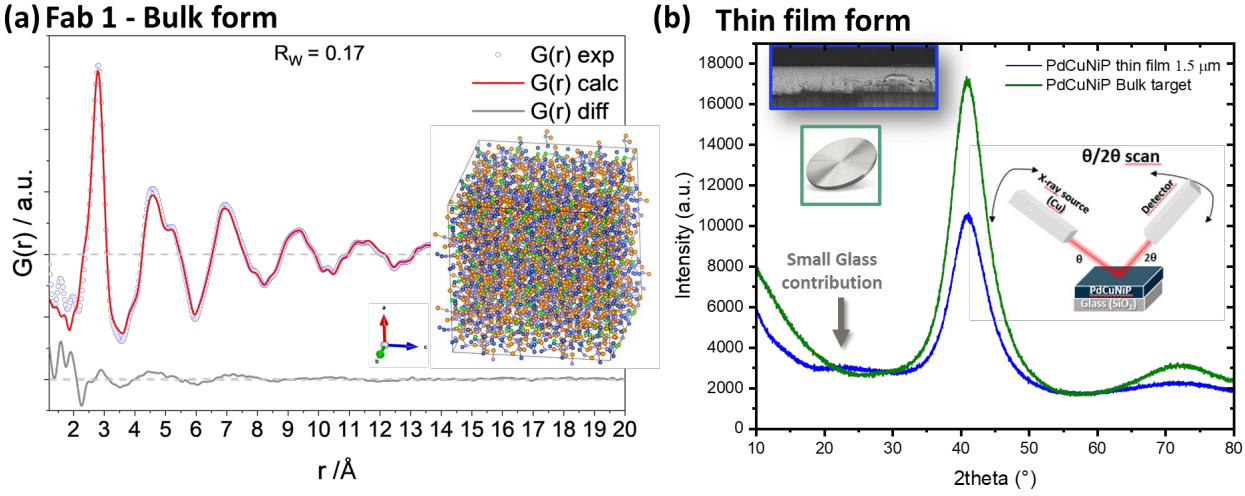


Figure 1- (a) *X-ray Pair distribution function and Reverse Monte Carlo fitting of bulk PdCuNiP alloy* ***(b)*** *XRD pattern of amorphous bulk sputtering target (green) and thin film (blue) of PdCuNiP alloy.*