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Hydrostatic compression effects on metallic glasses -a combined XAFS and simulation study

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Metallic glasses (MGs) are amorphous alloys that lack the regular atomic structure typical of crystalline metals. The stability of MGs against crystallization is attributed to their high atomic packing density, which, despite the absence of long-range periodicity, displays significant short- and medium-range order. The atomic packing efficiency of MGs can be further enhanced by applying external hydrostatic pressure. Recent findings suggest that, under compression, MGs adapt to external load through complex structural reorganization involving electronic effects.

In this study, we investigate the high-pressure atomic and electronic structures of binary Zr-Cu and Zr-Ni MGs using X-ray absorption spectroscopy and theoretical modeling. Our results show that compression induces the development of atomic icosahedral short-range order, involving crystallographically forbidden five-fold symmetry [1, 2]. This structural reconfiguration is primarily driven by the preferential straining of mechanically soft Zr-Zr pairs. Additionally, as suggested by molecular dynamics simulations [3] and confirmed experimentally by X-ray absorption data, an unexpected collapse in the Zr atomic radius occurs around 50 GPa. Density functional theory calculations indicate that this effect is related to a pressure-induced change in the electronic configuration of Zr [4].

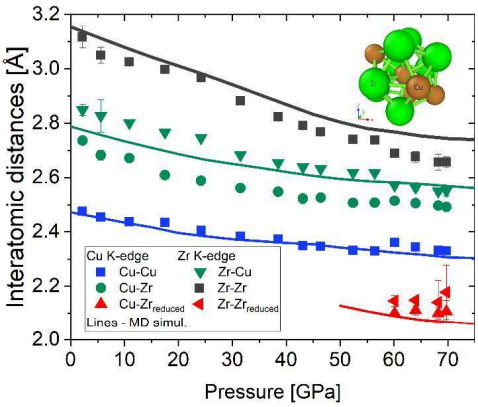

Figure 1. *Pressure dependence of interatomic distances during hydrostatic compression of $Zr_{67}Cu_{33}$ metallic glass derived from EXAFS fitting (symbols). Solid lines represent the results of the molecular dynamics simulations.*

References

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