

Local icosahedral order in Cu-Zr metallic glasses studied by means of X-ray absorption fine structure and molecular dynamics simulations

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We have used X-ray absorption fine structure method and molecular dynamics (MD) simulations to characterize atomic order in Cu-Zr metallic glasses (MGs) [1]. The microstructure of these MGs is described in terms of interconnected icosahedral-like clusters (superclusters) which are basic building units reproducing the stoichiometry of the system [2]. The equilibrium MD configurations were used as an input for *ab-initio* calculations of the extended X-ray absorption fine structure (EXAFS) and X-ray absorption near-edge structure (XANES) spectra. The theoretical EXAFS and XANES spectra were compared with those measured for rapidly quenched glassy Cu-Zr alloys. We demonstrate that the experimental results are well reproduced by EXAFS modeling of the population of the superclusters derived from the MD configuration [3]. The average local structural motif can be approximated by Cu-centered icosahedral-like cluster satisfying the condition of maximal local packing efficiency and approximating the system stoichiometry. The simulated XANES exhibits good agreement with experiment, indicating that the atomic order of the MD configuration is consistent with that of the real alloy structure over distances of about 1 nm.

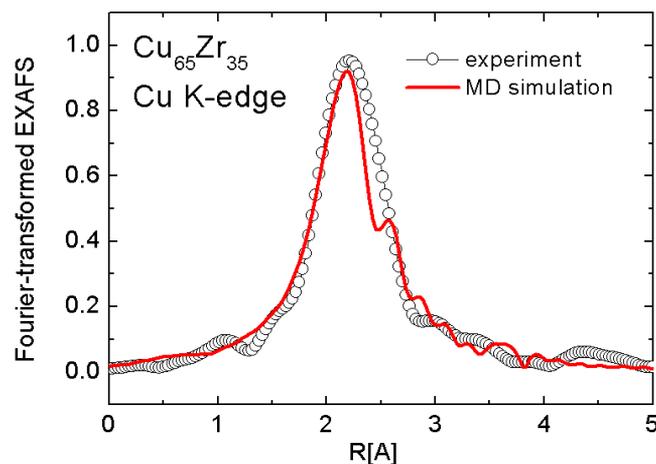


Figure 1. Experimental and simulated Fourier-transformed Cu K-edge EXAFS for Cu₆₅Zr₃₅ metallic glass.

References

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- [3] J. Antonowicz, A. Pietnoczka, T. Drobiazg, G.A. Almyras, D.G. Papageorgiou & G.A. Evangelakis (2012): Icosahedral order in Cu-Zr amorphous alloys studied by means of X-ray absorption fine structure and molecular dynamics simulations, *Philosophical Magazine*, DOI:10.1080/14786435.2012.659008.