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Atomic structure of Cu-Zr metallic glass assessed by EXAFS method and molecular dynamics simulations

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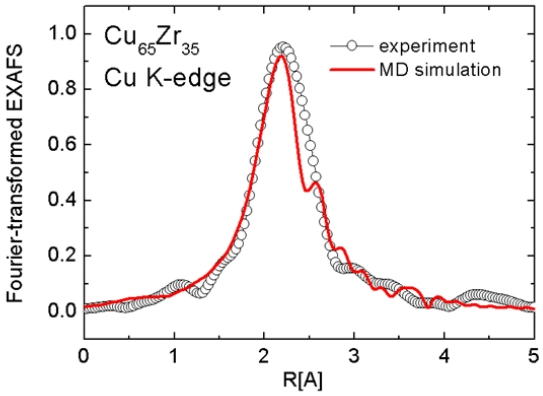

We report on atomic structure study of $Cu_{65}Zr_{35}$ amorphous alloy (metallic glass) by means of extended X-ray absorption fine structure (EXAFS) method and molecular dynamics (MD) simulations. The limitations and applicability of EXAFS technique exploited for resolving the local structure of metallic glasses are discussed. In order to verify the reliability of EXAFS analysis method we use two kinds of approach: *ab-inito* EXAFS signal simulation from equilibrium MD configuration and standard experimental EXAFS signal fitting. Copper K-edge EXAFS spectra of melt-spun glassy ribbons were measured in transmission mode at liquid nitrogen temperature to reduce thermal disorder. The MD simulations for system of 128.000 atoms were based on a tight binding in the second moment approximation model adopted for Cu-Zr glasses. Direct modeling of EXAFS spectra from MD configuration was performed using FEFF8 code [1]. We demonstrate how the variety of local atomic icosahedral-like environments contribute to the global EXAFS signal. The final spectra were obtained by averaging the EXAFS oscillations originating from individual absorbing atoms. It was found that due to atomic disorder the averaging over at least 1000 atoms is required for satisfactory results. The averaged EXAFS spectra are in very good agreement with the experimental ones indicating that MD reproduces the true atomic structure of the amorphous alloy. Independently we apply a different approach based on fitting of experimental EXAFS data using VIPER software [2]. The fitting parameters were: coordination number, interatomic distances and mean square atomic displacement. The resulting values were compared with those derived from the MD configuration. In all cases the fitted values were consistent with the MD data indicating high reliability of the EXAFS fitting approach [3].

References:

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