Ultra Fine structure of the short range order of the $Cu_{65}Zr_{35}$ and $Cu_{35}Zr_{65}$ Metallic Glasses

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We present Molecular Dynamics simulations (MD) results referring to the microstructure of two representatives CuZr Metallic Glasses (MG) ($Cu_{65}Zr_{35}$ and $Cu_{35}Zr_{65}$). From the microscopic analysis of the glassy structures of both systems we found that they are mainly composed by small Icosahedral-like clusters (ICO) that are interconnected and/or interpenetrating, in agreement with previous studies. The detailed exploration of their possible interconnections revealed that the structural characteristics of the systems may be satisfactorily reproduced by considering only 13 and 15-atom ICO clusters that are interpenetrating with predefined ways, thus explaining the existence of the short range order which is a typical characteristic of these MGs. The approach is based on geometrical considerations for the possible combinations of the ICO-like clusters in conjunction with the restriction of the systems' composition. Several polyicosahedral superclusters (PSC) are thus predicted and subsequently verified by the analysis of the MD equilibrium configurations. It turns out that there are "magic" numbers for the PSCs that are dictated from the combination of both the geometry of the interpenetrating ICOs and the stoichiometry of the system and that these numbers are identical for both compositions, the only difference being their relative amplitudes. Interestingly, the radial distribution function calculated by considering only the central atoms of the participating ICOs in the PSCs reproduces very well the experimental data. The energetic and electronic stability of some representative small free standing PSCs were further investigated and verified by means of calculations based on the Density Function Theory. We believe that the present results elucidate the microstructure of these MGs and that they could be of use for the description of more complex systems and possibly for the design of new MGs with improved properties.

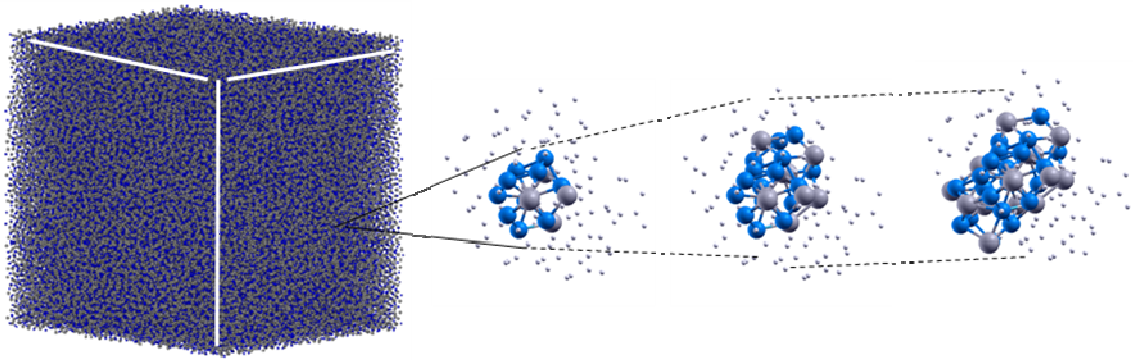

Figure. Polyicosahedral superclusters within the metallic glass

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