Icosahedral medium to extended-range orders of Cu-Zr binary amorphous alloys

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Abstract

Plasticity and strength of amorphous alloys are composition-dependent. And the differences in these properties are due to their different atomic-scale structures. The local structural states of amorphous alloys have been depicted previously via short-range orders (SROs). However, the concept of SROs alone is inadequate and sometimes insufficient to explain the structure-property relationship of the amorphous alloys. We propose new types of structural organization, i.e. icosahedral medium-range orders(I-MROs) that influence the properties of the amorphous alloys. Using a combination of molecular dynamics simulations and weighted-Voronoi tessellation technique, we demonstrated a detailed 3-D configuration of I-MROs and its extended-range orders, which form different icosahedral backbone structures depending on different composition.

Keywords: amorphous alloy, short(medium)-range order, backbone, plasticity, molecular dynamics

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