

Medium-range order, formation of back-bone of amorphous alloys and its effect on the initiation of plastic flow : A molecular dynamics viewpoint study

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Abstract

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 relation of the amorphous alloys. In this study, we propose new types of structural organization, i.e. icosahedral medium-range order (I-MRO) and its backbone that affect the mechanical properties, plasticity in particular. Using a combination of molecular dynamics simulations and weighted-Voronoi tessellation, we demonstrate the three-dimensional configuration of I-MROs and its backbone elucidate how these icosahedral orders are evolving under shear deformation. It was observed that the structural stability of the icosahedral orders relies largely on how they are linked via percolation and is explained here in details.

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

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