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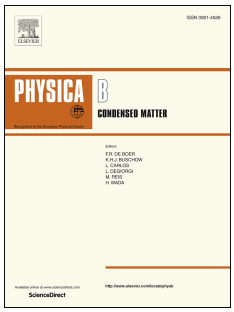

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Effect of cooling rate on structures and mechanical behavior of $Cu_{50}Zr_{50}$ metallic glass: a molecular-dynamics study

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Abstract

In this paper, the molecular dynamics simulations are utilized to study the cooling rate effect and to understand the relationship among the local atomic structure, free volume, and mechanical property in $Cu_{50}Zr_{50}$ metallic glass. The radial distribution function, bond pair analysis technique, and Voronoi tessellation are performed to characterize the structure evolution and local atomic configurations during the cooling process. The results demonstrate that a faster cooling rate results in a higher glass transition temperature and less amount of icosahedra-like clusters. It has been recognized that the concentration of free volumes presents a strong evidence of upward trends as the cooling rate increases. The analyses for the free volume and Voronoi polyhedron indicate that icosahedral-like clusters show a lower free volumes as compared with the rest clusters, revealing that well-developed icosahedra-like clusters in $Cu_{50}Zr_{50}$ make the system densely packed and lower free volume structure. In addition, the simulated alloy obtained at a lower cooling rate exhibits a higher yield strength and elastic modulus, all of which may attribute to the structure with more densely icosahedral-like clusters and less free volumes.

Key words: cooling rate; free volume; icosahedra-like; $Cu_{50}Zr_{50}$