Molecular dynamics study of structural evolution, tensile deformation and nanoindentation of monatomic metallic glasses

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Abstract

Metallic glasses are attracting tremendous attention because of their fundamental significance and great potential to be used as structural or functional materials in engineering applications. Significant efforts have been devoted to studying their unique properties as well as their disordered nature. Metallic glasses possess much higher strength and elastic strain limit than their crystalline counterparts. Maximum allowed size of metallic glass products is being increased continuously as new alloy compositions with high glass forming ability are developed. However, the glassy structure and the mechanical behavior of metallic glasses are still far from thoroughly understood. This is partly due to the chemical complexity of multi-component metallic glasses that are examined in most studies. Newly discovered monatomic metallic glasses, such as Ta metallic glass, could bring new insights since they are consisted of only one type of element. This thesis thus focuses on investigating the atomic structure and mechanical properties of monatomic metallic glasses using molecular dynamics simulations. Comparisons are made to multi-component metallic glasses, represented by a specific Cu-Zr binary alloy.

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