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PROCEEDINGS

Local Von Mises Stress Change in CuZr Metallic Glass as an Indicator of the Stress Response

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ABSTRACT

Revealing the origin of the mechanical properties of metallic glasses (MG) is a long-standing problem. MGs respond to the external strain with the activation of collective atomic motion, but the triggers of such motions are not revealed yet, in contrast to the well-defined dislocations in crystals. In the present study we show that the change of atomic Von Mises stress is one of the key local parameters to indicate the stress response to a shear strain in metallic glass. Four random Cu50%Zr50% structures were prepared in first-principles molecular dynamics cooling process. Structures were then put under the shear strain from 0.5 to 8.0%. To study this collective atomic response in detail, we use the atomic stress calculations in the first-principles framework [1]. We analyze the system's transformation between the affine and relaxed states and find a significant deviation from elastic behavior. By comparing atomic Von Mises stress to the xy component of the stress matrix we show that the former surves as a better parameter. As the atomic Von Mises stress change indicates, the xy shear strain invokes atomic stress response in other shear components. Other local parameters, such as charge transfer, atomic displacements, and atomic strain, are also discussed.

KEYWORDS

Metallic glass; first-principles atomic stress; CuZr; shear softening

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References

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