Asymmtrical shear responses of grain boundaries

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Abstract

The breaking of symmetry always leads to intriguing physical properties. While extensive research has been conducted on tension-compression asymmetry at the nanoscale in metallic materials, there is a lack of attention on the possibility of shear asymmetry. In this work, we introduce the concept of shear asymmetry in grain boundaries (GBs) and systematically investigated the positive and negative shear responses of 157 symmetric and asymmetric tilt grain boundaries using molecular dynamics (MD) simulations. Our findings reveal that GBs with asymmetric structures have distinct shear responses under opposite shear directions. Furthermore, the extent of shear asymmetry corelates positively with the shear modulus difference across GBs, arising from materials anisotropy. To explain this phenomenon, we proposed a new disconnection-based theoretical model. This discovery of shear asymmetry offers valuable insights into the plastic mechanics of materials and offers potential implications for material design and understanding.

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