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Studying the Enhanced Ductility of Bimodal Nanocrystalline Copper Using a Coarse-Grained Model GUO-JIE JASON GAO, Natl Taiwan Univ, YUN-JIANG WANG, Chinese Academy of Sciences, SHIGENOBU OGATA, Osaka University — Viewing a bimodal configuration of nanocrystalline copper as composed of soft grains containing stiff cores, we proposed a coarse-grained model with systematically tunable stiffness of grains to study the enhanced ductility of bimodal nanocrystalline copper [Y. Wang, M. Chen, F. Zhou, and E. Ma, Nature 419 (2002) 912]. Using molecular dynamics simulations, we shear our model quasistatically. Our results not only qualitatively confirms that a bimodal configuration could behave more ductile than a monomodal one but also predicts there exists a range of ratio of soft/stiff domains that best minimizes shear localization. Moreover, our model indicates that a bimodal configuration could sometimes exacerbate shear localization and therefore jeopardize ductility if the ratio of soft/stiff domains is not properly chosen. This may explain why some experimental results are hard to be reproduced.

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