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Studying the enhanced ductility in bimodal nanocrystalline metals using a model with tunable crystallinity and crystallite stiffness GUO-JIE JASON GAO, Department of Mechanical Engineering, National Taiwan University, YUN-JIANG WANG, Institute of Mechanics, Chinese Academy of Sciences, SHIGENOBU OGATA, Department of Mechanical Science and Bioengineering, Osaka University — We propose a polycrystalline model composed of small and large particles, where crystallinity and stiffness of each crystallite can be separately tuned by varying the number ratio of small/large particles [H. Shiba et al., Phys. Rev. E. 81, 051501 (2010)], and implementing a pairwise interparticle n-6 Lennard-Jones (L-J) potential [Z. Shi et al. J. Chem. Phys. 135, 084513 (2011)], respectively. This simple model resembles the molecular structure of bimodal nanocrystalline metals containing crystallites of two sizes, where crystallite stiffness inversely proportional to its size. We conduct 2D molecular dynamics (MD) simulations to study the shear deformation of the model consist of stiff crystallites, soft crystallites, or stiff and soft crystallites. We find the flow stress increases monotonically with increasing crystallite stiffness, and it can be systematically adjusted via changing the ratio of soft/stiff crystallites. We address applying the results of our study to explain the enhanced ductility found in bimodal nanocrystalline metals, where shear localization and propagation are presumably weakened due to crystallites of two properties.

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