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Shear deformation of naocrystal-metallic glass composites: A computational analysis PENGFEI GUAN, MICHAEL L. FALK, Johns Hopkins University — Due to the shear strain localization, the limited ductility becomes the major drawback for the application of metallic glass materials, and the introducing of crystalline phase has been regarded as the effective method for improving the ductility of these materials. Here, we systematically investigate the nanocrystal-metallic glass composites by using Molecular Dynamic (MD) simulations. The three–dimension (3D) atomic configurations with different crystalline grain sizes and factions are constructed based on the ZrCu EAM potential. The phase diagram based on the crystalline grain size-fraction is established between single nanocrystal phase and amorphous phase. The mechanical responses of these materials are investigated by applying the shear deformation, and the relationships between the mechanical properties and atomic structure information (crystalline fraction, grain size ?) are established.

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