Computer simulations of nanoindentation in Mg-Cu and Cu-Zr metallic glasses - DTU Orbit

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The formation of shear bands during plastic deformation of Cu0.50Zr0.50 and Mg0.85Cu0.15 metallic glasses is studied using atomic-scale computer simulations. The atomic interactions are described using realistic many-body potentials within the effective medium theory, and are compared with similar simulations using a Lennard-Jones description of the material. The metallic glasses are deformed both in simple shear and in a simulated nanoindentation experiment. Plastic shear localizes into shear bands with a width of approximately 5 nm in CuZr and 8 nm in MgCu. In simple shear, the shear band formation is very clear, whereas only incipient shear bands are seen in nanoindentation. The shear band formation during nanoindentation is sensitive to the indentation velocity, indenter radius and the cooling rate during the formation of the metallic glass. For comparison, a similar nanoindentation simulation was made with a nanocrystalline sample, showing how the presence of a polycrystalline structure leads to a different and more spatially distributed deformation pattern, where dislocation avalanches play an important role.

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