Molecular Dynamics Study of Shear Transformation Zones in Metallic Glasses

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Shear bands in metallic glasses have been extensively studied using molecular dynamics (MD), but many aspects of these materials are not well understood yet, for instance, the atomistic mechanisms behind their plasticity. The objective of this research was to verify the influence of the size of the simulation box, the boundary conditions and the test type (tension or compression) on the formation of shear transformation zones and shear bands using MD. For this study it was used a $Cu_{45}Zr_{45}Al_{10}$ alloy, because this alloy exhibits extensive plastic deformation *via* multiple shear banding. This system is also a typical model system for metallic glasses. First, a simulation box containing 54000 atoms was amorphized; Then, it was submitted to a compression test, using periodic boundary conditions. Based on the similation results it was possible to verify which simulation box best allows for a clear visualization and characterization of the shear bands. The simulation results also showed that the periodic boundary conditions may have induced artifacts in the form of shear bands being formed by the very periodic condition. Therefore, semi-periodic conditions may be more suitable to induce defornation localization without the appearance of artficious shear bands. Finally, for the same simulation box and boundary conditions, tensile and compression tests were simulated to verify its inlfuence on the formation of shear transformation zones. !