Onset of plasticity and its relation to atomic structure in CuZr metallic glass nanowire: A molecular dynamics study

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We present a computational tensile test which shows the evolution of the atomic structure of a Cu50Zr50 metallic glass nanowire at 300 K as the applied strain increases. The system consists of a parallelepiped composed by 1.008.000 atoms interacting by means of an embedded atom potential. The local structure of the atoms is analyzed using the Voronoi polyhedral technique and the nucleation and propagation of the shear band by monitoring the local atomic shear strain. Our results clearly reveal three regimes: an elastic regime below 4% of strain, a homogeneous deformation, where the shear band begins to form, and an inhomogeneous deformation regime, above 10% of strain, where the shear band is formed. Each regime is characterized by a typical bimodal polyhedra distribution, except at 10% of strain, where the distribution is unimodal. A detailed atomic level study of the shear band shows that, in spite of the large displacement experimented by eac