Abstract Submitted
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Plasticity of amorphous carbon[1] JULIAN VON LAUTZ, MICHAEL MOSELER, LARS PASTEWKA, Fraunhofer IWM — We use molecular dynamics simulations to probe the plastic response of representative bulk volumes of amorphous carbon at densities from 2.0 g cm^{-3} to 3.3 g cm^{-3} in simple and triaxial shear. After an initial elastic response the samples yield with only little strain hardening or softening. Individual plastic events in this network forming glass are strikingly similar to those observed for bulk metallic glasses: We find that plasticity is carried by fundamental rearrangements of regions of around 100 atoms, the shear transformation zone. In the simple shear geometry, those events coalesce to form a shear-band on longer time scales. During plastic deformation, the material changes its hybridization by transforming sp^3 carbon atoms to sp^2. We provide evidence that this transformation of the structural state occurs before the material yields, hence weakening the material.

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