Plastic flow of amorphous carbon and the activation of shear transformations

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Eyring proposed in 1936 to interpret flow of fluids and solids as activated processes. Modern theories for deformation of amorphous materials employ this concept to formulate rates for triggering of shear transformations, the fundamental carrier of plastic deformation in glasses. A direct connection between a molecular model of a glass and the activation of a shear transformation zone is however still elusive. We here use molecular dynamics calculations of amorphous carbon to study plastic flow and extract phenomenological yield surfaces. By identifying individual shear transformations, we show for this single component network glass that a shear transformation is the breaking of an individual bond. By forcing breaking of these bonds in auxiliary calculations we directly extract energy barriers for the activation of shear transformations as a function of stress. Our results are a first direct observation Eyring's proposition in disordered materials and allows parametrization of mesoscopic models of plastic flow.