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Non-Schmid effect of pressure on plastic deformation in molecular crystal HMX. ANIRBAN PAL, CATALIN PICU, Rensselaer Polytechnic Institute — The energetic molecular crystal HMX is a key constituent in common plastic bonded explosives. Its plastic deformation under shock conditions is important in reaction initiation and detonation. Here we study the effect of high pressure on dislocation slip using isothermal-isobaric atomistic simulations. We consider two slip planes, (011) and (101), that are reported to be most active under ambient conditions. For all slip systems considered, the effect of pressure is to increase the critical resolved shear stress for dislocation slip. Pressure may fully inhibit dislocation-based plasticity if the resolved shear stress is not increased in proportion. On the other hand, at sufficiently high shear stresses the crystal loses shear stability. Therefore, in a broad range of shock conditions, plastic deformation takes place by a combination of dislocation glide in some slip systems and localization in some other systems, with dislocation activity being gradually inhibited as the shock pressure increases. This provides new data on the physical basis of plastic deformation in HMX, indicating that mesoscale representations of plasticity must include shear localization which is more important under these conditions than dislocation plasticity.

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