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Rotational defects and plastic deformation in molecular crystal RDX[1] ANIRBAN PAL, CATALIN PICU, Rensselaer Polytechnic Institute — Defects in molecular crystals differ in many aspects from their atomic counterparts. Molecules in the crystal lattice can undergo conformational changes or twist and rotate into various configurations during deformation. These processes play an important role in the mechanics at a larger scale by controlling critical parameters like dislocation mobility. We present a computational study of such processes in cyclo-trimethylene-trinitramine (RDX), an energetic molecular crystal. Conformational changes, rotational defects and their role in the deformation mechanics of RDX is investigated using molecular dynamics simulations. Structure and mobility of dislocations are also presented and role of conformational and rotational defects in dislocation mobility is discussed.

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