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Detection of plasticity mechanisms in an energetic molecular crystal through shock-like 3D unidirectional compressions : A Molecular Dynamics study PAUL LAFOURCADE, CHRISTOPHE DENOUAL, JEAN-BERNARD MAILLET, CEA-DAM,DIF — TATB crystal structure consists in graphitic-like sheets arranged in the a-b plane where a, b and c define the edge vectors of the unit cell. This type of stacking provides the TATB monocrystal very anisotropic physical, chemical and mechanical properties. In order to explore which mechanisms are involved in TATB plasticity, we use a Molecular Dynamics code in which the overall deformation is prescribed as a function of time, for any deformation path. Furthermore, a computation of the Green-Lagrange strain tensor is proposed, which helps reveal various defects and plasticity mechanisms. Through prescribed large strain of shock-like deformations, a three-dimensional characterization of TATB monocrystal yield stress has been obtained, confirming the very anisotropic behavior of this energetic material. Various plasticity mechanisms are triggered during these simulations, including counter intuitive defects onset such as gliding along transveral planes containing perfect dislocations and twinning. Gliding in the a-b plane occurs systematically and does not lead to significant plastic behavior, in accordance with a previous study on dislocation core structures for this plane, based on a coupling between the Peierls-Nabarro-Galerkin method and Molecular Dynamics simulations.

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