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A mesoscopic model with non-linear elasticity and phase transformation framework for the twinning-buckling behavior of TATB under dynamic loading: A Molecular Dynamics inferred constitutive law

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A mesoscopic modeling of 1,3,5-TriAmino-2,4,6-TrinitroBenzene, a very anisotropic energetic molecular crystal, is proposed and validated on MD simulations. The two dominant deformation modes observed at nanometric scale and limited stress (less than one GPa) are a buckling instability and a non-symmorphic twinning (irreversible) transformation.

A thermodynamically consistent continuum model is detailed, with a non-linear elasticity in pressure constructed to reproduce a cold equation of state. The twinning-buckling phase transition observed in MD is modeled by using a Phase-Field by Reaction-Pathway (PFRP) formalism. To validate the present constitutive law, we study the response of the single crystal under constant strain-rate uniaxial compressions for various directions in the basal plane and present one to one comparisons between both techniques. These comparisons are done by prescribing the same non-proportional strain tensor, insuring a strictly constant strain-rate. We then compare the Green-Lagrange strain tensor between PFRP and MD simulations, the latter obtained through a local least-square estimate.

Finally, an upscale is performed and simulations using the mesoscopic constitutive law are presented for time and space scales non reachable in MD. A large TATB polycrystal is generated and two types of loadings are considered: a hydrostatic compression and a shock compression at different impact velocities. We show that in each case, the twinning-buckling phase transition is activated and this phenomenom is explained in detail.

References

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