# Modeling of Deformation Twinning of β-HMX with Jacobian-free Newton-Krylov Method

**Rahul* and Suvranu De†**

* Department of Mechanical, Aerospace and Nuclear Engineering
Rensselaer Polytechnic Institute, Troy, NY 12180, USA
e-mail: rahul@rpi.edu

† Department of Mechanical, Aerospace and Nuclear Engineering
Rensselaer Polytechnic Institute, Troy, NY 12180, USA
e-mail: des@rpi.edu

## ABSTRACT

β-HMX is an extensively used energetic material that exhibits Type II deformation twinning on (101) plane of its $P2_1/c$ monoclinic crystal structure [1]. Twinning allows low symmetry monoclinic crystal to accommodate large strain, which may have significant effect on the activation. We develop a thermodynamically consistent continuum twin/slip phase field model to study the deformation behavior of β-HMX. The order parameter is associated with the twinning shear. Dislocations, twins and phase transformations are distinguished and modeled within a crystal plasticity framework. The Landau potential is derived for the finite elastic deformation analysis. The equilibrium response of the externally stressed β-HMX single crystal is obtained by solving coupled continuum momentum equation and phase evolution equation using Helmholtz free energy functional, which consists of elastic potential energy and local interfacial energy that follows from the Cahn–Hilliard formalism [2]. This is a set of coupled nonlinear partial differential equations that is discretized using the finite element method. The resulting nonlinear algebraic system of equation is solved using a Jacobian-free Newton-Krylov (JFNK) iterative method. Not having to explicitly compute and store the Jacobian matrix of the coupled system at each Newton step reduces storage requirements and computational complexities and costs compared to efforts based on Jacobian formation at every Newton step. The computational efficiency of the JFNK iterations is enhanced using a matrix-free block-preconditioner [3]. Numerical example of twin nucleation and growth in a 3D sample of β-HMX molecular single crystal shows that twins form upon loading single crystals on the (011) face, which become thicker and more numerous with increasing load. On further loading twins become plastic and permanent twin from. Twin bands are not visible for loading on (010) face. These observations are consistent with experiments [4].

## REFERENCES

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