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The effect of crystal orientation on shock loading of single crystal energetic materials

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ABSTRACT

Void collapse under shock loading has become a model problem to study the nucleation of hot spots in high energy density materials. While experimental observation of this phenomenon remains elusive, simulations can help identify the relevant physical mechanisms for heat generation and criticality. A finite element method approach to simulate shock waves that includes crystal plasticity, with a power-law slip rate, hardening law and an equation of state is presented. Numerical simulations of shock loading of single crystal β-HMX containing a cylindrical hole of diameter 10 μm are performed with different orientations and impact velocities in 3D and under plane strain conditions. The elastoplastic response, including the temperature increase due to plastic dissipation, is strongly affected by the crystal orientation. Specifically, the $(\bar{1}\ \bar{1}\ 1)$-oriented crystal shows the highest temperature increase. These results can guide the design of experiments to investigate processes at the micrometer length scales in energetic materials.

1. Introduction

Heat, impact or other form of thermomechanical stimulus may produce heating in localized regions [3,8]. The temperature and size of these localized regions known as “hot spots” [29,50] determine the ignition of energetic materials. Hot spots are nucleated due to dissipative mechanisms such as, inelastic deformation, fracture and frictional sliding [44,3,16]. Due to the important role attributed to voids in the nucleation of critical hot spots, void collapse under shock loading has become a model problem for atomistic and continuum simulations [54,42,41,4,43].

Simulations of the collapse of a 40 nm diameter void in RDX were performed by Wood et al. [54,53] under a 2 km/s impact shock leading to a deflagration wave. Eulerian [42,41,26] and Lagrange-Eulerian [5,4] approaches have been used at the continuum level to study void collapse in HMX. Rai et al. [42] focused on the sensitivity of elongated voids subjected to shock loading. Their simulations show how the orientation and aspect ratio enhance initiation. Barton et al. [5,4] described a 2D void collapse in HMX induced by shock loading. The shock velocity in these simulations is in the range 1–1.5 km/s and the void size is 0.5–1 μm [4]. Their model accounts for thermal/mechanical responses and chemical reactions that are driven by the temperature field. Shear bands are found to be an important mode of localization growing out of the pore region and serving as potential ignition sites.

The anisotropic plastic behavior of energetic materials has consequences on the deformation field, the mechanical work and the resulting temperature increase. Since polymer-bonded explosives are constituted of crystalline grains with random orientations embedded in a matrix, the orientation dependence of the dissipation mechanisms is of key importance for ignition sensitivity and has been studied with atomistic [61] and continuum simulations [18]. The effect of anisotropy and microstructure on polycrystalline HMX is investigated by Hardin et al. [18]. Their results show that crystalline anisotropy induces significant heterogeneity in the stress and thermal fields. However, a systematic study of the crystal orientation dependence of the energy dissipated during void collapse has not been carried out.

In this paper, a Lagrangian model to describe the elasto-plastic behavior of β-HMX single crystals at high strain rates is developed and used to study plastic deformation under shock loading. The single crystal plasticity model is based on a power-law slip rate and hardening law [39], and implemented in a finite element solver, as explained in Section 2. The crystal plasticity model is coupled to an equation of state introduced in Section 2.2. The different deformation mechanisms are compared in Section 3. The response of β—HMX with a 10 μm diameter cylindrical hole under shock loading is studied in Section 4, where the stress and temperature fields due to plastic energy dissipation are discussed as a function of the crystal orientation.

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Table 1
Material and model parameters used in the simulations [5,4,6,60,56].

Reference bulk modulus (K_0)	12.4 GPa
Bulk modulus pressure derivative (K'_{T0})	10.4
Equation of state exponent (n)	6.6
Reference density (ρ_0)	1.9 g/cm^3
Reference sound speed (c_0)	3.5 km/s
Reference temperature (T_0)	293 K
Plastic strain rate coefficient ($\dot{\gamma}_0$)	0.001 ns^{-1}
Plastic strain rate exponent (m)	0.1
Phonon drag strain rate limit ($\dot{\gamma}_{0,pd}$)	0.0025 ns^{-1}
Hardening matrix ($h_{s_i s_j}$)	9.34 MPa
Hardening exponent (a)	2.5
Initial slip resistance ($g_s(t=0)$)	103.03 MPa
Saturation slip resistance (g_{sat})	155.73 MPa
Bulk viscosity coefficient (C_0)	0.1
Bulk viscosity coefficient (C_1)	0.1
Specific heat (C)	1576.3 J/(kg K)
Thermal conductivity (k)	0.31 W/(m K)
Volumetric thermal expansion coefficient (α)	$2.1 \cdot 10^{-4}$ K^{-1}

2. Material model

While β-HMX is brittle at ambient pressure [40], plastic deformation becomes important at higher pressures [52,5,15,61]. Molecular dynamics (MD) simulations have been of key importance to determine the plastic response in HMX and RDX single crystals during shock loading [23,10], showing the nucleation of dislocations and a transition to shear bands at higher impact velocities. In this section the elasto-plastic and shock response models of β-HMX single crystals are presented. The Cauchy stress $\boldsymbol{\sigma}$ is calculated and the conservation of linear momentum:

$$\rho \frac{\partial^2 \mathbf{u}}{\partial t^2} = \nabla \cdot \boldsymbol{\sigma}, \tag{1}$$

is solved, where ρ is the density and $\mathbf{u}$ the displacement vector. All the model parameters used in the following simulations are reported in Table 1.

2.1. Single crystal plasticity model

The mechanical response model is based on the finite strain formalism, in which a multiplicative decomposition of the deformation gradient into an elastic, $\mathbf{F}_e$, and plastic, $\mathbf{F}_p$, parts is used:

$$\mathbf{F} = \mathbf{F}_e \cdot \mathbf{F}_p. \tag{2}$$

The plastic deformation gradient $\mathbf{F}_p$ deforms the crystal lattice in an intermediate stress-free configuration, which in turn is deformed into the current configuration by $\mathbf{F}_e$ [45]. The time evolution of the plastic strain is calculated following standard single crystal plasticity models [45]. The rate of the plastic deformation gradient is the sum of the plastic strain rate on each slip system:

$$\mathbf{L}_p := \dot{\mathbf{F}}_p \mathbf{F}_p^{-1} = \sum_{i=1}^{N_s} \dot{\gamma}_{pl,s_i} \hat{\mathbf{b}}_{s_i} \otimes \hat{\mathbf{n}}_{s_i}, \tag{3}$$

where N_s is the number of slip systems, $\dot{\gamma}_{pl,s}$ is the plastic strain rate, $\hat{\mathbf{b}}_s$ is the slip direction, and $\hat{\mathbf{n}}_s$ is the slip plane normal of the slip system s. The slip directions and slip plane normals of β-HMX single crystals are reported in Table 2 in Cartesian coordinates. They correspond to the slip systems given in $P2_1/c$ notation in [4].

The plastic strain rate $\dot{\gamma}_{pl,s}$ is calculated using a Hutchinson power-law model [39,24] as:

$$\dot{\gamma}_{pl,s_i} = \dot{\gamma}_0 \, sign(\tau_{s_i}) \left| \frac{\tau_{s_i}}{\tau_{th,s_i}} \right|^{\frac{1}{m}}, \tag{4}$$

where m is a constant [11], τ_s is the resolved shear stress, and $\tau_{th,s}$ the threshold resolved shear stress of the slip system s. The constant $\dot{\gamma}_0$ represents the characteristic rate at which dislocations overcome barriers by thermal activation. The absolute value of the plastic strain rate $\dot{\gamma}_{pl,s}$ of every slip system is limited to $\dot{\gamma}_{0,pd}$ due to phonon drag [5].

Table 2
β-HMX slip systems, slip plane normals and Burgers vectors written in Cartesian coordinates and strength ratios [5,4]. They correspond to the slip systems given in $P2_1/c$ notation in [4].

Slip system	$\hat{\mathbf{n}}$	$\hat{\mathbf{b}}$	r_i
s_1	(0 1 0)	[1 0 0]	1.0
s_2	(0 0.545 0.838)	[1 0 0]	0.963
s_3	(0 0.545 −0.838)	[−1 0 0]	0.963
s_4	(−0.660 0 0.751)	[0 1 0]	0.933
s_5	(0 0 1)	[1 0 0]	1.681
s_6	(−0.660 0 0.751)	[0.751 0 0.660]	0.376
s_7	(0 0.545 0.838)	[−0.348 −0.786 0.511]	0.931
s_8	(0 −0.545 0.838)	[0.348 −0.786 −0.511]	0.931
s_9	(0.844 0.500 −0.194)	[−0.224 0 −0.975]	0.701
s_{10}	(0.844 −0.500 −0.194)	[0.2241 0 0.975]	0.701

The threshold stress $\tau_{th,s}$ is calculated on every slip system and depends on the strength ratio r_s of the slip systems [4] as:

$$\tau_{th,s_i} = r_s g_{s_i}, \tag{5}$$

where g_{s_i} is a resistance function given by the power law [24]:

$$\dot{g}_{s_i} = \sum_{j=1}^{N_s} h_{s_i s_j} \left(1 - \frac{g_{s_j}}{g_{sat}}\right)^a \dot{\gamma}_{pl,s_j}, \tag{6}$$

where $h_{s_i s_j}$ is a hardening matrix, and g_{sat} is the saturation slip resistance and a is a constant. The resistance function represents the hardening due to forest dislocations piercing the slip system. The initial value of the slip resistance $g_{s_i}(t=0)$ and the saturation value g_{sat} for every slip system are taken from the constitutive model in [5], assuming a negligible initial dislocation density and a balance between dislocation generation and annihilation at saturation [35], which corresponds to a dislocation density of 10^{17} m^{-2}. This value of dislocation density is very high for a material with brittle response. However, no experimental study on the dislocation density is available on samples after deformation.

The coefficients $h_{s_i s_j}$ in Eq. (6) are all equal and determine the increase of the resistance function g_{s_i}, depending on the increase of the plastic strain $\Delta\gamma_{pl,s_j}$ on the slip systems. Therefore, the plastic strain increment to reach the saturation stress is of the order of $g_{sat}/h_{s_i s_j}$. The coefficients $h_{s_i s_j}$ are chosen to match the hardening behavior of the dislocation density model used in reference [5], in which a Taylor hardening law is used [2]. The crystal plasticity model was calibrated with gas gun experiments [5,15]. The calibration was done only for two different pressures (1.5 GPa and 2.4 GPa), while higher pressure experiments would be required to find a more accurate hardening law and to study the dislocation density at saturation. However, in the following simulations at 200 m/s impact velocity, hardening does not affect strongly the results because the plastic strain is typically smaller than 5%. Therefore, as shown in Fig. 1(a) and explained in Section 3.1, we expect a hardening of at most 10 MPa.

Finally, twinning is not considered in the present model. It is recognized as a mechanism for permanent deformation in β-HMX [15,59]. However, the present crystal plasticity model is calibrated without considering twinning. Therefore, the amount of plastic deformation is comparable with experiments, even if the amount of twinning cannot be predicted. Twinning in β-HMX is included in the model by Zamiri and De [57]; however, the plastic strain rate and hardening law are assumed to be the same for slip and twin systems. This is because of the lack of experimental knowledge about the twinning rate in β-HMX.