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New framework for constitutive modeling and numerical simulation of energetic crystals

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New framework for constitutive modeling and numerical simulation of energetic crystals

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Abstract

The central goal of this research is to respond to the need to realistically predict accumulated plastic deformation in low symmetry energetic crystals undergoing dynamic events. A realistic description of plastic deformation during dynamic events can only be achieved only if accurate plasticity models are available at the crystal scale. In order to describe the initiation of energetic material through the occurrence of local hot spots induced by plastic dissipation at the crystal scale, a new computationally-efficient framework has been developed using appropriate multiscale techniques in conjunction with the new formulation for the description of the constituent crystal behavior. This new numerical framework will enable accurate predictions of the influence of loading history on the accumulation of plastic deformation in energetic material and as such be more readily applicable to predict local initiation.

The novel and creative solution put forward is a new description of the energetic crystal behavior, which respects the inherent symmetry of the lattice structure. During this research effort, a new single crystal plasticity model with yielding accounting for the specific tetragonal crystalline symmetry of the PETN crystal was developed. Furthermore, analytical expressions that allow the calibration of the single crystal yield criterion have been derived. The single crystal parameters can be identified analytically based on four uniaxial compression test. Therefore it was possible to obtain a parametrization based on available data for PETN crystal. Moreover, F.E. Simulation of dynamic collapse of a circular pore inside an energetic crystal described by the new model under plane strain loading condition have been performed for different orientations of the PETN crystal. It was predicted that the temperature depends of the single crystal orientation. Also the maximum temperature and the spatial temperature field are strongly influenced by the orientation of the single

crystal. During the dynamic collapse of a pore inside a PETN crystal, the rise of temperature induced by the plastic dissipation can vary by 60% depending on the orientation of the crystal surrounding the void.

Furthermore, a multi-scale numerical framework has also been developed to perform large scale F.E. simulations of high rate loading of energetic aggregates. This numerical framework enables large-scale simulations of dynamics events and predictions of the overall mechanical behavior of the energetic aggregate, while also providing means to monitor the local fields (e.g. plastic dissipation, local rise in temperature at the grain level). To demonstrate the performance of the new framework, simulation of dynamic densification assuming a PETN aggregate containing millions of crystals have been performed. Finally, this new numerical framework associated with the newly developed yield criterion for the PETN energetic crystal has been extended to account for the interaction between the casing material and the energetic aggregate during the impact event.

1. Introduction

Despite extensive efforts from both theoretical and numerical standpoints, it is generally accepted that the mechanical response of explosive materials subjected to severe plastic loadings is poorly predicted. While it is generally recognized that ignition in energetic materials is due to the rise of local temperature due to energy dissipation phenomena, models accounting for the inherent symmetry of the crystal structure are lacking. Prediction of initiation within low symmetry energetic materials under impact loading remains a formidable challenge. While various numerical frameworks have been developed, using either an Eulerian formulation (Tran and Udaykumar (2006)) or Lagrangian formulation (Barua and Zhou (2012)), none of these account for the plastic anisotropic behavior of energetic crystals. Even when the anisotropic plastic behavior of the energetic crystal is considered, Schmid law, developed for cubic crystalline structure, is commonly used (see Clayton and Becker (2012), Wang and al. (2016)). Due to the fact that occurrence of local hot spots depends strongly on the orientation of the crystal and the lattice structure, improvement of the prediction of initiation in energetic materials can only be achieved through a more appropriate description of the plastic behavior at the mesoscale level.

2. New anisotropic yield criterion for PETN tetragonal crystal

Constitutive models that account for the specific symmetry of the PETN crystal do not currently exist. It is possible to develop a new plasticity model for energetic crystal with orthorhombic structure using a generalized invariants methodology developed by Cazacu and Barlat (2001). The plasticity model should be a scalar function of such generalized invariants. Furthermore, this function ought to be independent of the hydrostatic pressure. The generalized invariants representing a given single-crystal behavior should respect the symmetry properties associated to their respective microstructure (see also Cazacu et al. (2018), Cazacu et al. (2019) and Cazacu and Revil-Baudard (2020)).

For a crystal there exist, in the undeformed state, preferred directions. Associated with each crystal class is a group of symmetry transformations, g , also called crystallographic point group. When subjected to one of these transformations, the crystal is carried into a configuration which is undistinguishable from its initial one. In particular, these crystal symmetry requirements place restrictions on the form of yield function $\Phi(\boldsymbol{\sigma})$, namely that it should be form-invariant under the group of transformations g associated with the respective crystal class, i.e.

$$\Phi(\mathbf{Q} \boldsymbol{\sigma} \mathbf{Q}^T) = \Phi(\boldsymbol{\sigma}), \quad (1)$$

for any stress $\boldsymbol{\sigma}$ and any orthogonal transformation $\mathbf{Q}$ belonging to the symmetry group g . Let's denote by $R_{\mathbf{n}}^{\phi}$ the proper rotation (i.e. $\det R_{\mathbf{n}}^{\phi} = 1$) through an angle ϕ about an axis in the direction of the unit vector $\mathbf{n}$. For a material having rhombic symmetry, there exist three preferred directions that are mutually perpendicular. Let us denote Oxyz, the Cartesian coordinate system associated with these directions. According to theorems on representation of scalar-valued functions of symmetric tensors, for a polynomial $P(\boldsymbol{\sigma})$ to be form-invariant to any transformations belonging to the rhombic system, it must be expressible as a polynomial in the invariants of $\boldsymbol{\sigma}$, $N_1 \boldsymbol{\sigma}$, and $N_2 \boldsymbol{\sigma}$, which are:

$$tr(N_1 \boldsymbol{\sigma}), tr(N_2 \boldsymbol{\sigma}), tr(N_3 \boldsymbol{\sigma}), tr(N_1 \boldsymbol{\sigma}^2), tr(N_2 \boldsymbol{\sigma}^2), tr(\boldsymbol{\sigma}^3) \quad (2)$$

Relative to the Oxyz coordinate system associated with the symmetry axes, the set of irreducible invariants is:

$$\sigma_{xx}, \sigma_{yy}, \sigma_{zz}, \sigma_{xy}^2, \sigma_{yz}^2, \sigma_{xz}^2, \sigma_{xy}\sigma_{xz}\sigma_{yz}, \quad (3)$$

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Thus, any polynomial $P(\boldsymbol{\sigma})$ must be of the form:

$$P = P(\sigma_{xx}, \sigma_{yy}, \sigma_{zz}, \sigma_{xy}^2, \sigma_{yz}^2, \sigma_{xz}^2, \sigma_{xy}\sigma_{xz}\sigma_{yz}) . \quad (4)$$

To develop a new yield criterion accounting for the specificities of the crystalline tetragonal structure, the polynomial $P(\boldsymbol{\sigma})$ should respect the symmetries associated with the tetragonal classes. For the crystal classes of the tetragonal system, the symmetry generators are: $R_{[100]}^\pi$ and $R_{[001]}^{\pi/2}$ (see also Figure 1), i.e to respect the tetragonal symmetry, the yield criterion should respect the following invariance properties

- Invariance with rotation of $\pi/2$ about the axis [001]
- Invariance with rotation of π about the axis [100].

It follows that for a polynomial $P(\boldsymbol{\sigma})$ to respect the symmetries associated with these crystal classes, it should be of the form given by Eq.(4), and in addition be invariant to the following permutations :

$$P(\sigma_{xx}, \sigma_{yy}, \sigma_{zz}, \sigma_{xy}^2, \sigma_{yz}^2, \sigma_{xz}^2, \sigma_{xy}\sigma_{xz}\sigma_{yz}) = P(\sigma_{yy}, \sigma_{xx}, \sigma_{zz}, \sigma_{xy}^2, \sigma_{xz}^2, \sigma_{yz}^2, \sigma_{xy}\sigma_{xz}\sigma_{yz}) \quad (5)$$

with the **c**-axis of the tetragonal crystal being along the **z**-axis, (i.e. **z** is along [001]).

Assuming that the mechanical response in tension and compression is the same; in the coordinate system Oxyz associated with the <100> crystal axes (with the **z**-axis along the **c**-axis of the tetragonal crystalline structure), a quadratic yield criterion for a tetragonal crystal should be necessarily of the form:

$$\left\{ \frac{a_1}{6} \left[(\sigma_{xx} - \sigma_{zz})^2 + (\sigma_{yy} - \sigma_{zz})^2 \right] + \frac{a_3}{6} (\sigma_{xx} - \sigma_{yy})^2 + a_4 \sigma_{xy}^2 + a_5 (\sigma_{xz}^2 + \sigma_{yz}^2) \right\} = k^2, \quad (6)$$

where k denotes the yield limit in simple shear in the (100) or (010) crystallographic planes.

Given that the criterion given by Eq. (6) is a homogeneous function in stresses, the yielding response is the same if the coefficients a_1, a_3, a_4, a_5 are replaced by $\beta a_1, \beta a_3, \beta a_4, \beta a_5$, with β being an arbitrary positive constant. Therefore, without loss of generality one of the parameters, for example a_1 , can be set equal to unity. Accordingly, the effective stress, $\bar{\sigma}$, associated to the new tetragonal single-crystal criterion is:

$$\bar{\sigma} = \left\{ \frac{a_1}{6} \left[(\sigma_{xx} - \sigma_{zz})^2 + (\sigma_{yy} - \sigma_{zz})^2 \right] + \frac{a_3}{6} (\sigma_{xx} - \sigma_{yy})^2 + a_4 \sigma_{xy}^2 + a_5 (\sigma_{xz}^2 + \sigma_{yz}^2) \right\}^{1/2}. \quad (7)$$

Remark:

Note that the tetragonal energetic crystal yield criterion involves exactly three independent parameters: a_3, a_4, a_5 . The coefficient a_4 has a clear physical significance being directly expressible in terms of the ratio between the yield limits in uniaxial tension along $\langle 100 \rangle$ directions and the yield limit in simple shear i.e. k . The remaining coefficients a_3, a_5 can be determined from for example uniaxial tests along two different orientations.

3. Effect of loading orientation on yielding in uniaxial compression according to the proposed yield criterion

The stereographic projection of a tetragonal crystal is shown in Figure 1. Due to the symmetries of the tetragonal single crystal, to quantify the effect of the loading orientation on yielding for uniaxial loadings, it is sufficient to conduct tests along directions belonging to the basic stereographic triangle with corners along $[001]$, $[110]$ and $[100]$ (red triangle in Figure 1.c). Note also that for a direction $\mathbf{f}$ to be in this stereographic triangle, its latitude angle φ and its longitude angle θ should be in the following range: $0 \leq \varphi \leq \pi/4$ and $0 \leq \theta \leq \pi/2$ respectively.

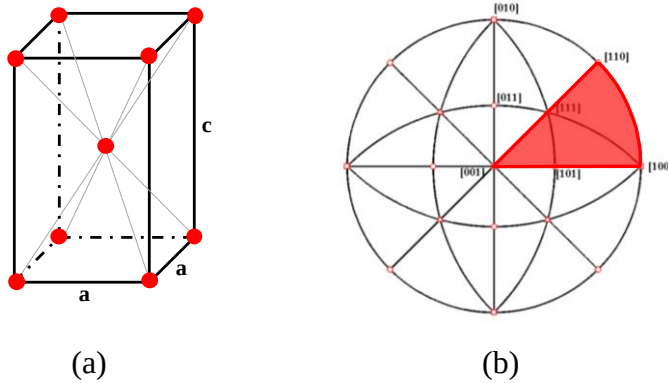


Figure 1 (a) Tetragonal crystal lattice; and (b) Basic stereographic triangle for tetragonal symmetry

Let us denote Y_f the yield limit under uniaxial loading along any given direction $\mathbf{f}$ given by the Miller indices $[\alpha\beta\gamma]$. Thus, in the Oxyz coordinate system associated with the crystal axes, with (c/a) being the characteristic ratio for the tetragonal crystal structure:

$$\mathbf{f} = \frac{\alpha \mathbf{e}_x + \beta \mathbf{e}_y + \gamma (c/a) \mathbf{e}_z}{\sqrt{\alpha^2 + \beta^2 + \gamma^2 (c/a)^2}}. \quad (8)$$

Under uniaxial loading along the direction $\mathbf{f}$, at yielding the stress tensor is $\boldsymbol{\sigma} = Y_f (\mathbf{f} \otimes \mathbf{f})$.

Therefore, in the Oxyz coordinate system, the stress is given by the matrix:

$$\boldsymbol{\sigma} = \frac{Y_f}{\alpha^2 + \beta^2 + \gamma^2 (c/a)^2} \begin{bmatrix} \alpha^2 & \alpha\beta & \alpha\gamma(c/a) \\ \alpha\beta & \beta^2 & \beta\gamma(c/a) \\ \alpha\gamma(c/a) & \beta\gamma(c/a) & \gamma^2 (c/a)^2 \end{bmatrix}_{(\mathbf{e}_x, \mathbf{e}_y, \mathbf{e}_z)} \quad (9)$$

Substituting Eq. (9) into the expression of the effective stress corresponding to the new yield criterion given by Eq.(7), we obtain the value of Y_f , the yield stress under uniaxial loading along the direction $\mathbf{f}$.

In particular, if Y_{100} denotes the yield stress under uniaxial loading along the $[100]$ crystallographic direction, then according to the new yield criterion (7), the following relation holds:

$$\frac{Y_{100}}{k} = \sqrt{\frac{6}{a_1 + a_3}}. \quad (10)$$

It is worth noting that the new criterion automatically respects the symmetries of the tetragonal lattice and as such predicts the same yield limit under uniaxial loading along the $[010]$, $[\bar{1}00]$, $[0\bar{1}0]$ directions, respectively.

If Y_{110} denotes the yield stress under uniaxial loading along the $[110]$ crystallographic direction, then according to the new yield criterion (7) predicts:

$$\frac{Y_{110}}{k} = \sqrt{\frac{12}{a_1 + 3a_4}}. \quad (11)$$

Similarly, if Y_{001} is the yield stress under uniaxial loading along the $[001]$ crystallographic direction, then according to the criterion (7):

$$\frac{Y_{001}}{k} = \sqrt{\frac{3}{a_1}}. \quad (12)$$

It is worth noting that for tetragonal crystals, unlike cubic single crystals (see Cazacu and Revil-Baudard (2020)), the yield stress along the $[001]$ direction is different than the yield stress along $[100]$ direction (compare Eq.(10) and Eq.(12)). Indeed, $Y_{001} = Y_{100}$ if and only if $a_1 = a_3$.

If Y_{101} denotes the yield stress under uniaxial loading along the $[101]$ crystallographic direction, then according to the criterion (7):

$$\frac{Y_{101}}{k} = \sqrt{\frac{6(1+(c/a)^2)^2}{a_1 + a_3 - 2a_1(c/a)^2 + 2a_1(c/a)^4 + 6a_5(c/a)^2}}. \quad (13)$$

It is to be noted that the yield criterion (7) predicts the same yield limit under uniaxial loading along the orientations $[011]$, $[\bar{1}0\bar{1}]$, $[0\bar{1}\bar{1}]$, which is a direct consequence of the criterion being form-invariant to the tetragonal crystal symmetries.

Another crystallographic orientation of interest is $[111]$ for which the yield criterion predicts that the yield in uniaxial compression, Y_{111} , is:

$$\frac{Y_{111}}{k} = \sqrt{\frac{3(2+(c/a)^2)^2}{a_1 + 3a_4 + 2(c/a)^2(3a_5 - a_1) + a_1(c/a)^4}}. \quad (14)$$

3.1. Identification procedure for the parameters of the yield criterion for tetragonal energetic crystals

If we impose that the proposed yield surface (see Eq. (7)) passes through the yield point in uniaxial compression along the orientation $[100]$, the criterion is expressed as:

$$\frac{6}{a_1 + a_3} \left\{ \frac{a_1}{6} \left[(\sigma_{xx} - \sigma_{zz})^2 + (\sigma_{yy} - \sigma_{zz})^2 \right] + \frac{a_3}{6} (\sigma_{xx} - \sigma_{yy})^2 + a_4 \sigma_{xy}^2 + a_5 (\sigma_{xz}^2 + \sigma_{yz}^2) \right\} = Y_{100}^2 \quad (15)$$

Setting $a_1 = 1$, the remaining coefficients, a_3, a_4, a_5 can be expressed in terms of the uniaxial yield stresses along any three different orientations among $[001]$, $[111]$, $[101]$ and $[110]$ directions by making use of the following relations:

$$\begin{aligned}
\left(\frac{Y_{001}}{Y_{100}}\right)^2 &= \frac{a_1 + a_3}{2a_1} \\
\left(\frac{Y_{110}}{Y_{100}}\right)^2 &= \frac{2a_1 + 2a_3}{a_1 + 3a_4} \\
\left(\frac{Y_{111}}{Y_{100}}\right)^2 &= \frac{(a_1 + a_3)(2 + (c/a)^2)^2}{2a_1 + 6a_4 + 2(c/a)^2(6a_5 - 2a_1) + 2a_1(c/a)^4} \\
\left(\frac{Y_{101}}{Y_{100}}\right)^2 &= \frac{(a_1 + a_3)(1 + (c/a)^2)^2}{a_1 + a_3 - 2a_1(c/a)^2 + 2a_1(c/a)^4 + 6a_5(c/a)^2}
\end{aligned} \tag{16}$$

Remark: It is also worth noting that the parameters of the new tetragonal yield criterion depend on the characteristics of the tetragonal lattice structure, namely the ratio c/a (see Eq. (16)).

The new yield criterion developed for tetragonal crystals has been applied to a PETN crystal. For a PETN single crystal, Conroy et al. (2007) have reported the following yield ratios : $Y_{001}/Y_{100} = 1.85$, $Y_{101}/Y_{100} = 0.85$, $Y_{111}/Y_{100} = 0.85$ and $Y_{110}/Y_{100} = 1.09$. It has to be noted that for PETN single crystal, the ratio c/a is equal to 0.7143. As mentioned, the parameters can be expressed analytically in terms of 3 yield ratios. Using the reported Y_{001}/Y_{100} , Y_{111}/Y_{100} and Y_{110}/Y_{100} and $a_1 = 1$, it follows that $a_3 = 5.90$, $a_4 = 3.57$ and $a_5 = 6.08$. The reported yield ratio Y_{101}/Y_{100} which has not been used for the determination of the parameters involved in the tetragonal yield criterion (7) can serve for validation purposes. For this direction, using Eq. (16)₄, we obtain $Y_{101}/Y_{100} = 0.8$ against $Y_{101}/Y_{100} = 0.85$ reported by Conroy et al. (2007).

Figure 2 shows the projection of the yield locus according to the new yield criterion for the PETN crystal in the biaxial planes $(\sigma_{xx}, \sigma_{yy})$ and $(\sigma_{xx}, \sigma_{zz})$. It is to be noted that if the crystallinity of the tetragonal energetic crystal is neglected and the yielding of the crystal is described by the isotropic von Mises yield criterion. To visualize the influence of neglecting the crystallinity of the tetragonal energetic crystal, in Figure 2 is also plotted the yield surface according to the von Mises material. It is worth noting that the proposed yield criterion is in very good agreement with the data, while the isotropic yield criterion (i.e. neglecting the crystallinity of the material) cannot account for the influence of the loading orientation on the plastic behavior of the PETN crystal. The maximum

difference between yielding according to the proposed criterion (7) and the isotropic yield criterion of von Mises is for loadings in the $(\sigma_{xx}, \sigma_{zz})$ biaxial plane. It is important to note that if the von Mises yield criterion is used to describe the PETN single crystal, the predicted rise in temperature induced by plastic dissipation would be the same irrespective of the orientation of the PETN crystals with respect to the applied loading. However, using the proposed yield criterion, which has been derived using rigorous theorems that enable to account for the intrinsic symmetry of the energetic crystal, the predicted plastic dissipation will depend on the relative orientation of the crystal axes and loading axes.

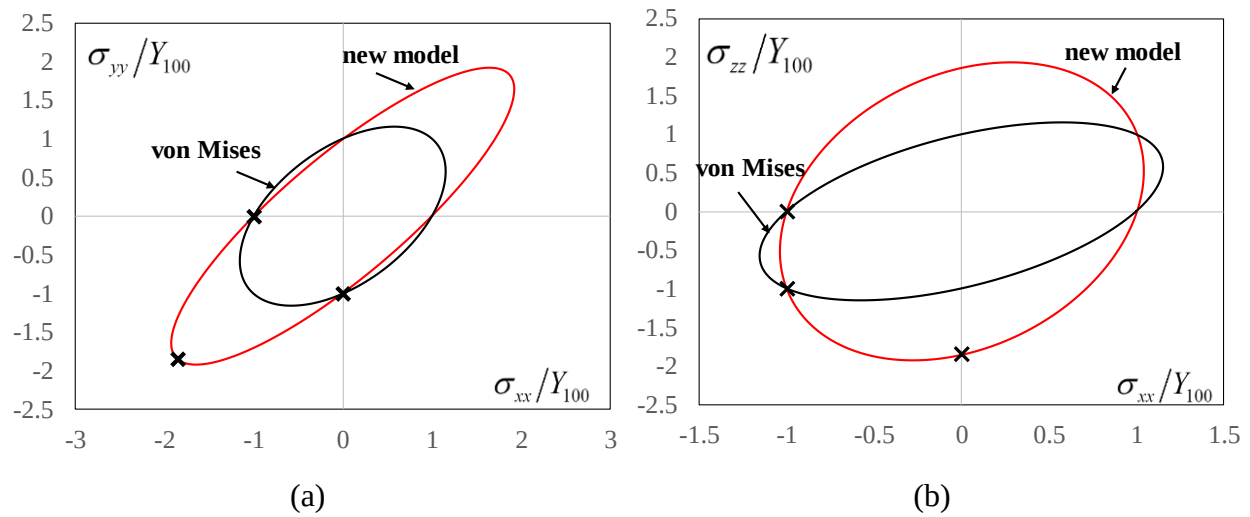


Figure 2. Projections of the yield surface according to the new anisotropic yield criterion accounting for the tetragonal symmetry of the PETN single crystal and the yield surface using the isotropic von Mises yield criterion (a) in the $(\sigma_{xx}, \sigma_{yy})$ plane (b) in the $(\sigma_{xx}, \sigma_{zz})$ plane. Data from Conroy et al. (2007) are represented by symbols.

3.2. Effect of loading orientation on yielding in uniaxial compression in several crystallographic planes

First let us analyze the effect of the orientation on yielding in uniaxial compression in the crystallographic planes of normal $\langle 010 \rangle$ (see Figure 3a). If Y_θ is the uniaxial yield stress along a direction at θ to the crystallographic axis $[001]$ ($\theta = 0$ represents the direction $[001]$ and $\theta = \pi/2$ is the direction $[100]$), then according to the criterion (6):

$$\frac{Y_\theta}{Y_{100}} = \sqrt{\frac{a_1 + a_3}{(\sin^4 \theta (a_1 + a_3) + 2a_1 \cos^4 \theta + 2\sin^2 \theta \cos^2 \theta (3a_5 - 2a_1))}} \quad (17)$$

Note that for $\theta=0$ (i.e. the direction $[001]$), Eq. (17) reduces to Eq.(16)₁ while for $\theta=\pi/2$ which correspond the direction $[100]$, Eq. (17) reduces to an identity.

Another crystallographic plane of interest is the plane of normal $\langle 1\bar{1}0 \rangle$ (see Figure 3b). Let us denote by $Y_{\langle 110 \rangle}(\theta)$ the yield stress in uniaxial compression along an arbitrary axis $\mathbf{f} = \sin\theta/\sqrt{2} \mathbf{e}_x + \sin\theta/\sqrt{2} \mathbf{e}_y + \cos\theta \mathbf{e}_z$ in this plane ($\theta=0$ corresponds to the direction $[001]$ and $\theta=\pi/2$ to the direction $[110]$, respectively). According to the new criterion (7),

$$\frac{Y_{\langle 110 \rangle}(\theta)}{Y_{100}} = \sqrt{\frac{a_1 + a_3}{2(\sin^4 \theta (a_1 + 3a_4)/4 + a_1 \cos^4 \theta + \sin^2 \theta \cos^2 \theta (3a_5 - a_1))}} \quad (18)$$

Note that for $\theta=0$, Eq. (18) reduces to Eq.(16)₁ and for $\theta=\pi/2$, Eq. (18) reduces to Eq.(16)₂.

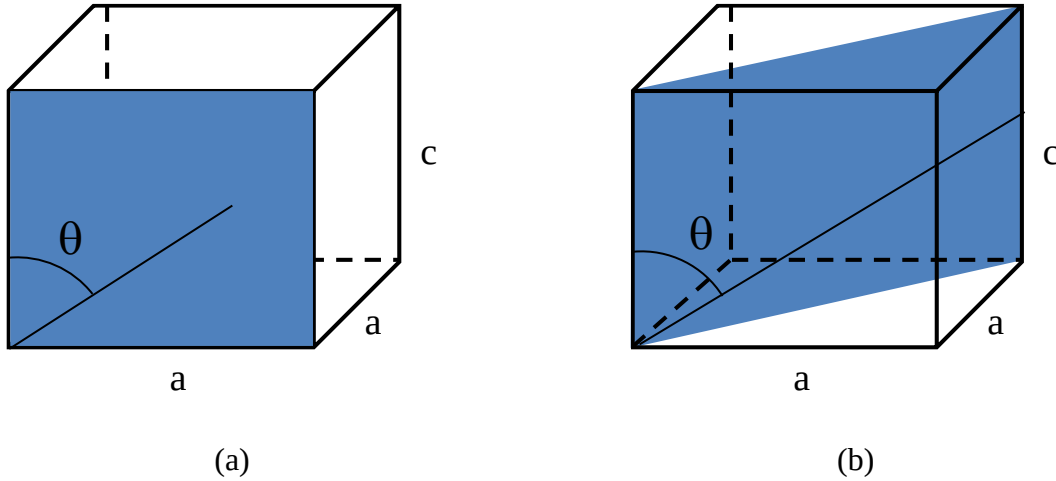


Figure 3. Representation of the crystallographic plane of normal : (a) $\langle 010 \rangle$; (b) $\langle 1\bar{1}0 \rangle$

The variation of the yield stress in uniaxial compression with the orientation θ in the planes of normal $\langle 010 \rangle$ and $\langle 1\bar{1}0 \rangle$ are shown in Figure 4 (a) and (b), respectively, along with the available data reported by Conroy et al. (2007). Note the good agreement between the model predictions and the data. In the plane of normal $\langle 010 \rangle$, the ratio Y_θ/Y_{100} varies between 1.85 for the orientation $[001]$, i.e. uniaxial compression along the $\mathbf{c}$ -axis and 0.78 for the an orientation close to the

orientation [506]. In the plane of normal $\langle 1\bar{1}0 \rangle$, the ratio $Y_{\langle 110 \rangle}(\theta)/Y_{100}$ varies between 1.85 for the orientation [001], i.e. uniaxial compression along the c -axis, and 0.8. for θ close to $\pi/4$.

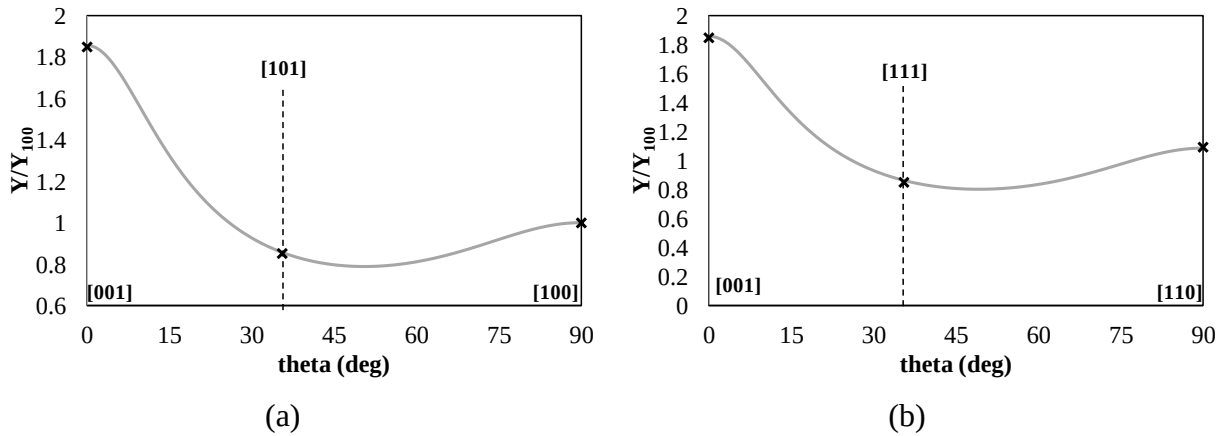


Figure 4. Variation of the normalized yield stress with the orientation θ (a) in the plane of normal $\langle 010 \rangle$ (b) in the plane of normal $\langle 1\bar{1}0 \rangle$ according to the new yield criterion in comparison with the data for a PETN crystal reported by Conroy et al. (2007) (symbols).

As already discussed, due to the symmetries of the tetragonal single crystal, to fully represent the influence of the loading orientation on yielding under uniaxial compression, all the directions contained in the basic stereographic triangle with corners along [001], [110] and [100] (red triangle in Figure 1 .c) should be considered. In Figure 5 is presented the predicted yield stress normalized by the yield stress along [100] for uniaxial compression for the PETN single crystal. It is worth noting that the maximum yield stress ratio is 1.85 along [001], i.e. along the c axis, while the lowest predicted yield stress is 0.78 along an orientation closed to [506] (extremum value correspond to the extremum in the plane of normal $\langle 1\bar{1}0 \rangle$). Therefore, for the PETN single crystal, the maximum variation in yield stress in uniaxial compression is about 134%. As already mentioned to correctly describe the local rise in temperature in a PETN system (either single crystal or energetic aggregate), it is critical to correctly describe the anisotropy in yield stress of the constituent crystals. This is vital for the prediction of the nucleation sites of hot spots. ***The results presented that under uniaxial loading, the local rise of temperature can vary by as much as 134% depending on the orientation of the PETN single crystal. To be recalled, if the crystallinity of the energetic crystal is neglected, the yield stress in uniaxial compression will be the same irrespective of the loading orientation.***

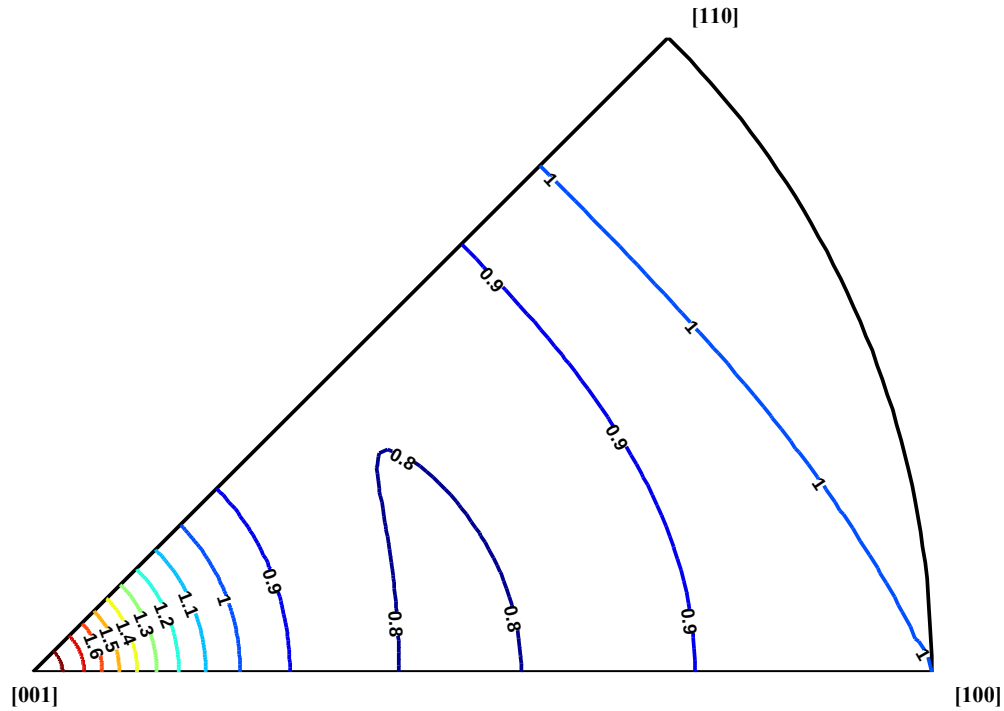


Figure 5. Anisotropy in yield stress ratio in uniaxial compression for a PETN single crystal according to the proposed yield criterion (Eq.(6)), identified based on the data reported by Conroy et al. (2007). Yield stress are normalized by the yield stress along [100]

Furthermore, the influence of the crystal orientation on the mechanical response and subsequent energy dissipation should also be investigated for multi-directional loading and 3-D loadings. It is important to note that the yield criterion is valid for any full 3-D loading. To further investigate the influence of the crystallinity of energetic crystals on the rise in temperature due to energy dissipation, the proposed yield criterion (6) has been implemented into a Finite Element (FE) software Abaqus using an implicit time-integration algorithm (Backward Euler algorithm) for solving the set of equations governing the elastic-plastic behavior. This algorithm has been developed in the framework of corotational algorithms established by Hughes (1984). Specifically, the constitutive equations are written in an appropriate orthogonal rotating frame. This enables the description of large deformations and transformations, in a form identical to their simpler small strains counterpart while verifying the objectivity principle (objectivity of the time derivatives, see Hughes, 1984). Specifically, an Abaqus User subroutine (UMAT) has been developed and used to perform numerical investigations on the influence of the crystallinity on the mechanical response of PETN crystals. More specifically, in the next section, we present F.E. simulations of void

collapse inside PETN crystal under dynamic compressive loading. The goal is to investigate the influence of the crystal orientation on the pore collapse by longitudinal waves. The rise in temperature due to the energy dissipation is calculated as

$$\Delta T = \int_0^t \frac{\alpha (\boldsymbol{\sigma} : \mathbf{d}^p)}{\rho C} dt \quad (19)$$

where α is the Taylor–Quinney coefficient, ρ the density and C the heat capacity, while $\boldsymbol{\sigma}$ is the stress tensor and $\mathbf{d}^p$ the plastic strain-rate tensor, calculated using the new anisotropic plastic potential.

4. Influence on the orientation of the PETN crystal on the rise in temperature during the dynamic collapse of a circular void.

To be able to predict the occurrence of hot spots that are local peaks in the fluctuation of the temperature field, it is imperative to correctly capture the influence of the crystal orientation on the plastic dissipation. Defect based mechanisms, such as pore collapse have been examined as possible causes of hot spots. Numerous experimental observations made on defect-free PETN and HMX single crystals show that initiation strongly depends on the crystalline orientation (Dick (1984), Dick et al. (2004)). In this section, we present an investigation on the influence of the PETN crystal orientation on the rise of the temperature during pore collapse. While the new model as well as the associated algorithms are developed for fully 3-D loadings, we will first examine the case of a void collapse under plane strain. A pore of diameter of 0.03 mm is located inside a PETN crystal specimen of 0.12 mm length and 0.1 mm width. The geometry of the specimen is shown in Figure 6(a). Due to the fact that the crystal axes may not necessarily align with the symmetry axes of the specimen, the whole specimen was meshed with 21,538 elements with reduced integration (Abaqus C3D8R). It is to be noted that in order to reduce the influence of the mesh on the shape of the pore takes during its collapse, a structured mesh was used. Thus, around the pore, the element size is smaller and the mesh is constructed such that it is ensured that no preferential direction or preferential shape of the pore will be induced by the mesh (see also Figure 6(c) showing “concentric” meshing around the pore).

The imposed boundary conditions are shown in Figure 6(a). The longitudinal velocity (i.e. along the $\mathbf{x}$ -axis) is imposed on the left side of the specimen and the prescribed time variation of the

velocity is shown in Figure 6(b). Note that the imposed velocity increases smoothly to a maximum velocity, V_{max} in an interval of $0.1\mu s$, then it is maintained constant. The results presented hereafter are for $V_{max} = 1000$ m/s.

FE simulations using the constitutive model (Eq.(7)) described previously in conjunction with the dynamic implicit solver were performed using the F.E software Abaqus/Standard. The new model has been implemented using a fully-implicit backward Euler method. Given that an implicit dynamic solver was used the equilibrium equations were solved for each increment. The time step was kept extremely small (between 10^{-9} and 10^{-8} s) in order to capture with high-fidelity the propagation of the elastic and plastic waves during the pore collapse/closure.

Simulations have been performed for 25 different crystal configurations in order to investigate the role of the crystal orientation on the rise of temperature during the dynamic collapse of a pore inside a PETN crystal. Only the results for a few crystal configurations are discussed in this section. A given crystal configuration is denoted by the crystalline directions aligned with the x and y -axis of the specimen shown in Figure 6(a). For example, crystal configuration $[100]$ - $[001]$ means that the x -axis and the y -axis of the specimen are aligned with the crystal direction $[100]$ and $[001]$, respectively, and the longitudinal compressive wave travels in the crystallographic plane of normal $[0\bar{1}0]$.

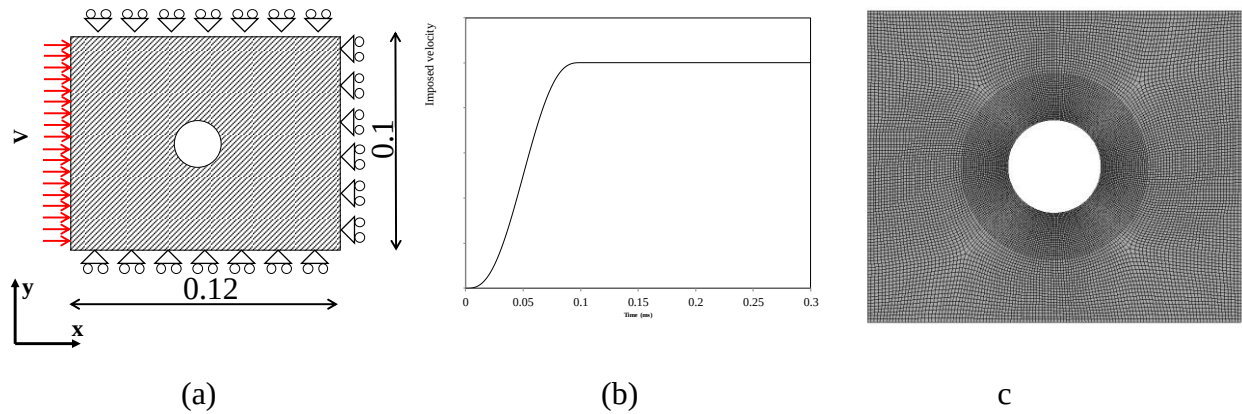


Figure 6. (a) Geometry of the specimen used in the FE simulations of the dynamic collapse of a pore inside a PETN crystal; (b) Imposed velocity on the specimen (c) F.E. mesh

Figure 7 shows, for $t=0.27\mu s$, the isocontours of the rise in temperature induced by the plastic dissipation during the pore collapse inside PETN crystals of different orientations with respect to

the loading axes (x-y). All the PETN crystals simulations shown in Figure 7 have their [100] axis aligned with the **x**-axis of the specimen (see also Figure 6), while the **y**-axis is along the [010], [001], [011] and [012] crystal axes, respectively (i.e. depending on the crystal configuration). Consequently in each case the wave propagates in a different crystallographic plane. Namely, the compressive wave travels along the crystalline plane of normal $\langle 001 \rangle$ (Figure 7(a)), $\langle 010 \rangle$ (Figure 7(b)), $\langle 0\bar{1}1 \rangle$ (Figure 7(c)) and $\langle 0\bar{2}1 \rangle$ (Figure 7(d)), respectively.

It is worth noting that the isocontours of the rise in temperature are strongly influenced by the crystal orientation, the size and position of the zone of maximum rise of temperature being totally different depending on the crystal orientation considered. Even if all the crystal configurations considered in Figure 7 have one common direction along the **x**-axis of the specimen, at the beginning of the pore collapse, the maximum rise of temperature varies by 38%, a temperature increase of 88.24 K being predicted for the [100]-[011] configuration (see Figure 7(c) with the longitudinal wave traveling in the plane of normal $\langle 0\bar{1}1 \rangle$) and of 122 K for the [101]-[001] configuration (see Figure 7(b) with the longitudinal wave traveling in the plane of normal $\langle 010 \rangle$). Moreover, the evolution of the shape of the pore differs depending on the crystal configuration (compare the [100]-[010] configuration (see Figure 7(a)) to the [100]-[001] configuration (see Figure 7(b))). For the same crystal configurations in Figure 8 are shown the isocontours at a time of 0.3 μ s, when the pore is close to full collapse. Note the important difference in the maximum rise in temperature between the crystal orientations, varying from a temperature increase of 244 K for the [100]-[010] configuration (see Figure 8(a)) to a temperature increase of 376 K for the [100]-[001] configuration (see Figure 8 (b)). Also note that the size and geometry of the zone for which the temperature increase is larger than 50 K strongly depends on the crystal configuration.

In conclusion, the results presented in Figure 7 and Figure 8 highlight the importance of accounting for the anisotropy of the energetic crystal for the prediction of the temperature increase during the dynamic collapse of a pore. Using the proposed yield criterion (7), it has been predicted that the temperature increase could change by more than 50% depending on the relative orientation between the crystallographic axes of the tetragonal crystal and the loading direction. Due to the fact that PETN crystals are strongly anisotropic, only an accurate model in conjunction with simulation will be able to correctly asses the role of the crystal orientation on the occurrence of hotspot during pore collapse.

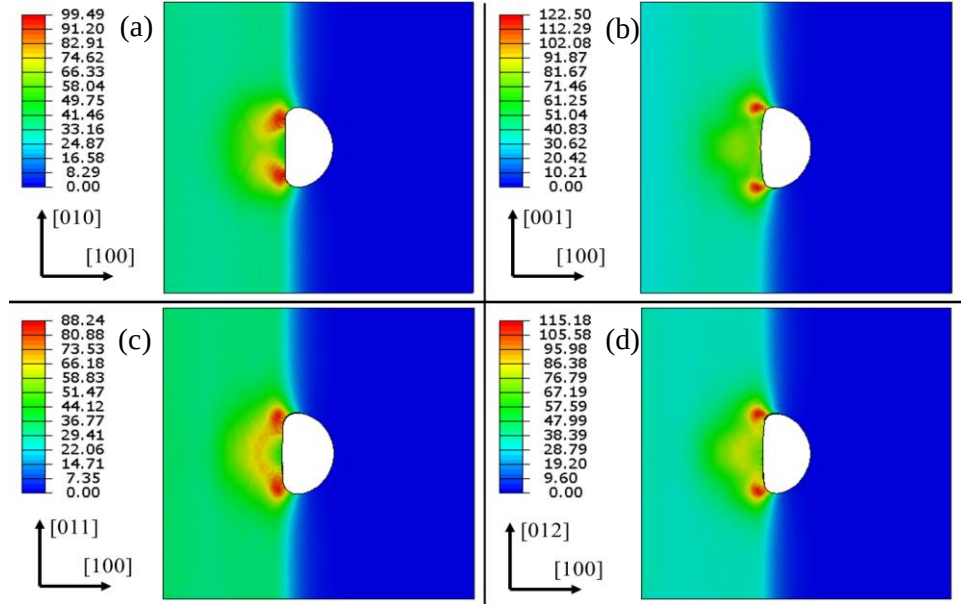


Figure 7. Isocontours of the rise in temperature induced by the plastic dissipation during a void collapse inside PETN crystals of different orientation at a time of $0.27 \mu\text{s}$. The x-loading axis is along the $[100]$ direction of each crystal, while the y-axis depends on the crystal configuration. The wave travels in the plane of normal: (a) $\langle 001 \rangle$; (b) $\langle 010 \rangle$; (c) $\langle 0\bar{1}1 \rangle$ and (d) $\langle 0\bar{2}1 \rangle$.

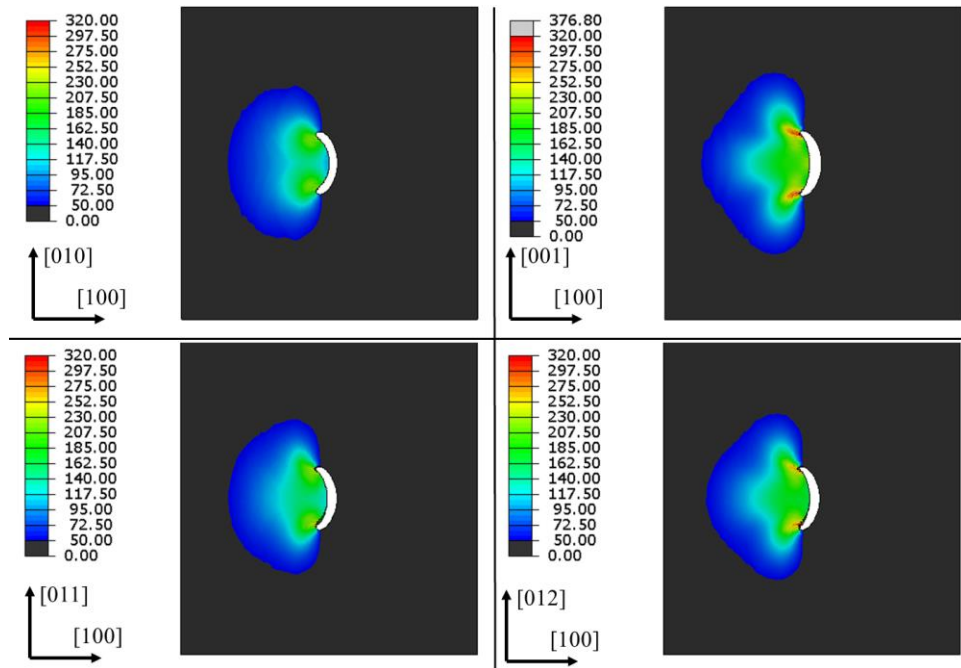


Figure 8. Isocontours of the rise of temperature induced by the plastic dissipation during a void collapse inside PETN crystals with different orientation at a time of $0.3 \mu\text{s}$. The x-loading axis is along the $[100]$ direction of each crystal, while the y-axis depends on the crystal configuration. The wave travels in the plane of normal: (a) $\langle 001 \rangle$; (b) $\langle 010 \rangle$; (c) $\langle 0\bar{1}1 \rangle$ and (d) $\langle 0\bar{2}1 \rangle$.

Additional simulations have been performed for other crystal orientations. In Figure 9 are plotted the isocontours of the rise of temperature during pore collapse inside a PETN crystal oriented in the configuration $[100]$ - $[010]$ (compressive wave traveling in the plane of normal $\langle 001 \rangle$); $[001]$ - $[100]$ (plane of normal $\langle 010 \rangle$); $[001]$ - $[110]$ (plane of normal $\langle \bar{1}10 \rangle$) and $[110]$ - $[001]$ (plane of normal $\langle 1\bar{1}0 \rangle$), respectively at a time of $0.28 \mu\text{s}$. Among these four configurations, the maximum rise of temperature varies between 175 K to 271 K, thus a variation of 60% in the prediction of the maximum temperature due to the pore collapse. Furthermore, the strong influence of the crystal orientation on the rise of temperature could be illustrated by comparing the configurations $[100]$ - $[010]$ (see Figure 9(a)) and $[001]$ - $[100]$ (see Figure 9(b)), i.e. one configuration obtained from the other by a rotation of $\pi/2$ along the normal to the specimen $\mathbf{x}$ (i.e. for these two cases, the compressive waves are traveling on 2 planes that are normal to each other). Note that a simple rotation of $\pi/2$ of the in the plane in which the compressive wave is travelling could lead to a change in the temperature increase associated to energy dissipation of almost 100K. Also, at a time of $0.28 \mu\text{s}$, note that for the two configurations the shape of the pore is different (compare Figure 9(a) to Figure 9(b)).

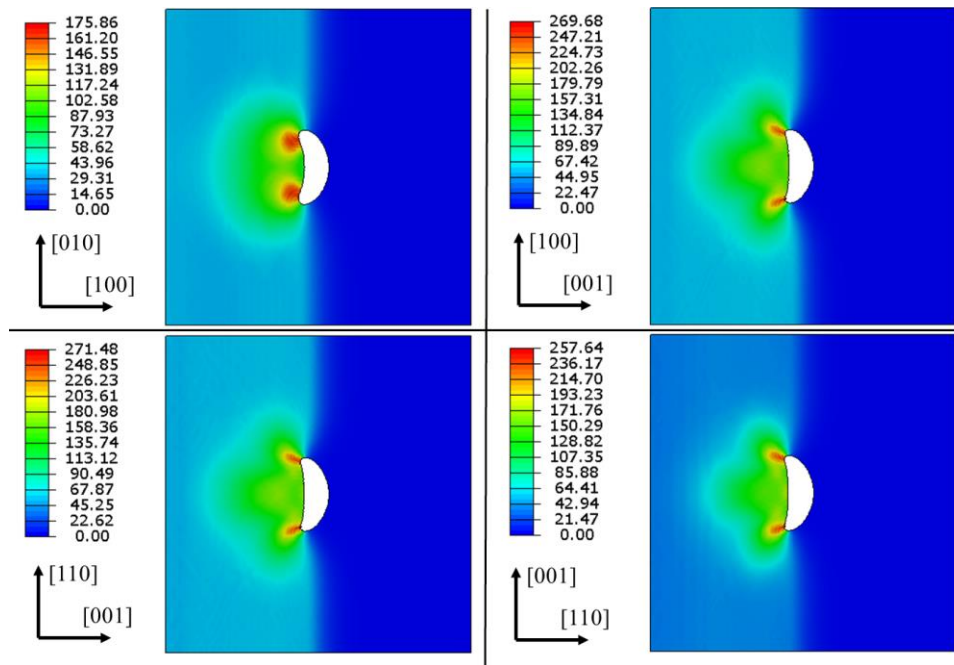


Figure 9. Isocontours of the rise of temperature induced by the plastic dissipation during a void collapse inside PETN crystals with different orientation at a time of $0.28 \mu\text{s}$. The orientation of the PETN are $[100]$ - $[010]$; $[001]$ - $[100]$; $[001]$ - $[110]$ and $[110]$ - $[001]$, respectively.

Finally, to further illustrate the importance of the crystal orientation on the plastic dissipation, it is shown in Figure 10 the isocontours of the temperature rise during the pore collapse inside a PETN crystal oriented in the configuration $[100]$ - $[031]$ (plane of normal $\langle 0\bar{1}3 \rangle$); $[001]$ - $[130]$ (plane of normal $\langle \bar{3}10 \rangle$); $[110]$ - $[\bar{1}\bar{1}2]$ (plane of normal $\langle 1\bar{1}\bar{1} \rangle$) and $[111]$ - $[\bar{1}0\bar{1}]$ (plane of normal $\langle \bar{1}2\bar{1} \rangle$), respectively. It is worth noting that there exist crystal configurations for which the rise of temperature is very local and not symmetric with respect to the x -axis (see configuration $[111]$ - $[\bar{1}0\bar{1}]$ in Figure 10(d)).

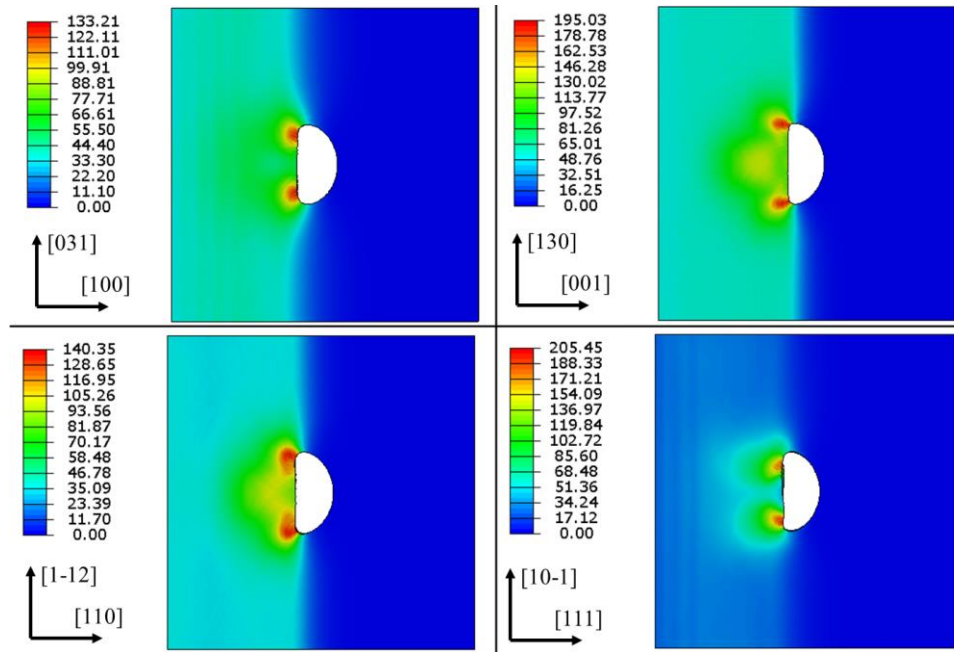


Figure 10. Isocontours of the rise of temperature induced by the plastic dissipation during a void collapse inside PETN crystals with different orientation at a time of $0.27 \mu s$. The orientation of the PETN are : (a) $[100]$ - $[031]$ (plane of normal $\langle 0\bar{1}3 \rangle$); (b) $[001]$ - $[130]$ (plane of normal $\langle \bar{3}10 \rangle$); (c) $[110]$ - $[\bar{1}\bar{1}2]$ (plane of normal $\langle 1\bar{1}\bar{1} \rangle$) and (d) $[111]$ - $[\bar{1}0\bar{1}]$ (plane of normal $\langle \bar{1}2\bar{1} \rangle$).

The simulations of the dynamic collapse of a pore inside a single PETN crystal illustrate the importance of the consideration of the anisotropy of the plastic behavior of the energetic crystal. In summary the new yield criterion (7) for the PETN crystal is to accounting for the effect of the crystal orientation on the rise of the temperature when the crystal is subjected to high strain-rate loading. The temperature rise, the location of the maximum temperature, geometry of the pore, isocontours of temperature depend on the orientation of the PETN crystal.

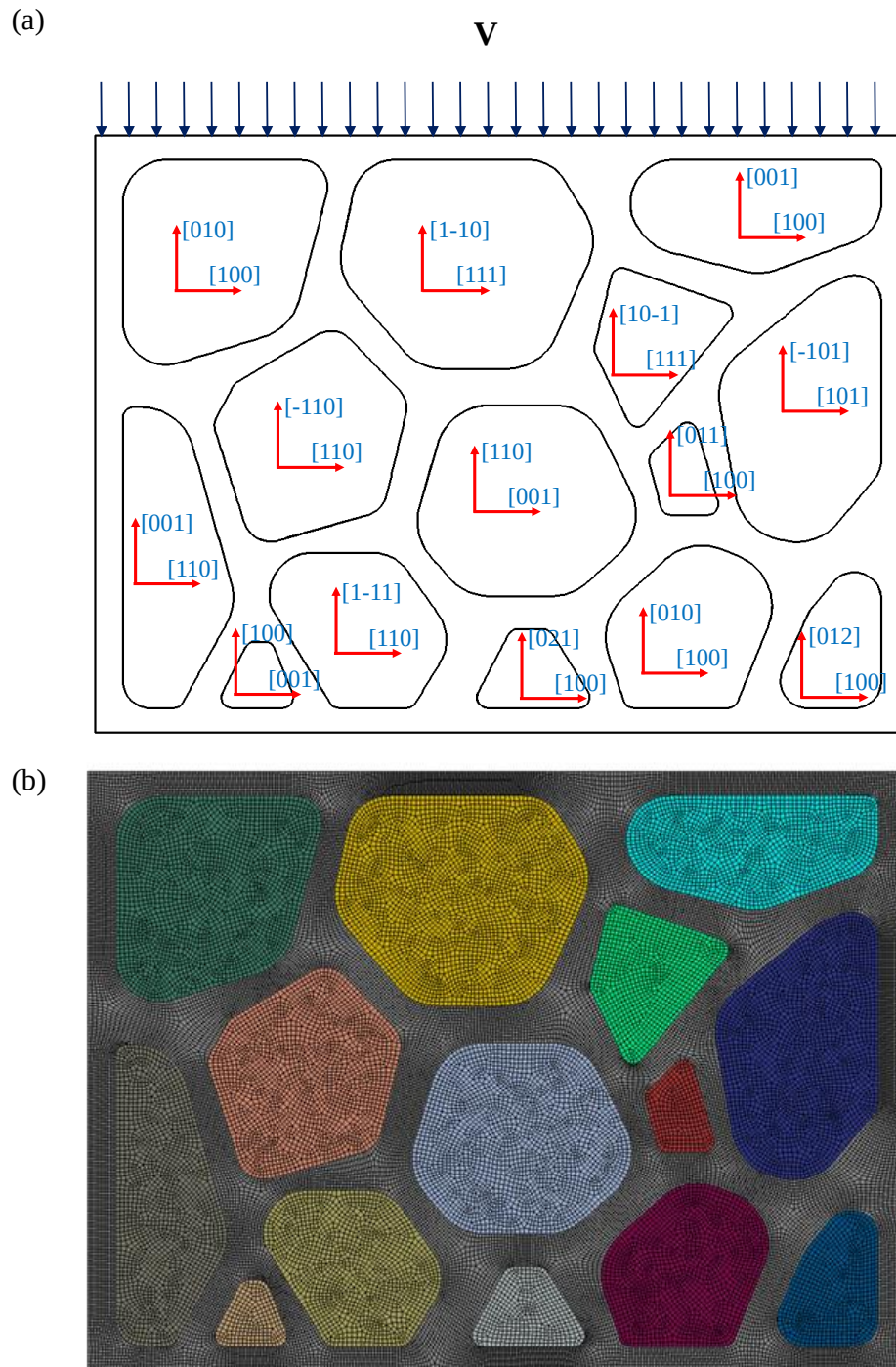


Figure 11. Mesoscale simulation of a PBX (75% PETN and 25% Sylgard 182) subjected to an uniaxial compressive wave. The PBX is made of 14 PETN crystals surrounded by a Sylgard 182 matrix. (a) Orientation of each PETN crystals (b) F.E. mesh

5. Development of a numerical framework allowing the simulation of the mechanical behavior at the mesoscale.

As seen previously, the developed yield criterion for the energetic crystal allow investigating the influence of the crystallinity on the rise in temperature induced by energy dissipation during the dynamic collapse/closure of a pore. Energetic materials are complex systems composed of explosive crystals surrounded by a polymer binder and as well as metallic particles inside the energetic systems. Consequently, their mechanical strength depends on the specificities of the deformation of its constituents. Therefore, a meso-scale approach could lead to improving the understanding of the role of each constituent on the initiation, either partial or global, of the energetic system. In this section, we present results concerning meso-scale modeling of energetic systems consisting of dozens of energetic crystals surrounded by a polymer.

Let us consider a PBX aggregate composed of 14 PETN crystals surrounded by a polymer binder subjected to a uniaxial compressive loading induced by the velocity V (see Figure 11) with no lateral displacement on the side of the specimen. The PBX mass composition is 75% PETN ($\rho = 1770 \text{ kg/m}^3$) and 25% Sylgard 182 ($\rho = 1000 \text{ kg/m}^3$). Each crystal has a different shape, size and crystal orientation with respect to the loading axis (see Figure 11). The specific orientation of the crystal is given in Figure 11(a). The plastic behavior of PETN crystal is described by the yield criterion (6) and the Sylgard 182 polymer binder is assumed to be linear elastic ($E = 10 \text{ MPa}$, $\nu = 0.48$). As shown in Figure 11(b), the PBX aggregate is meshed with 43471 hexahedral elements with reduced integration (Abaqus C3D8R). The interaction between the energetic crystals and the polymer binder are assumed to follow the Coulomb friction law with a friction coefficient of 0.7. Furthermore, normal decohesion between the binder and the energetic crystal is considered when the contact normal stress is larger than 0.2 MPa, which is the tear strength of Sylgard 182. The PBX is subjected to an uniaxial compressive wave through the imposed velocity V applied at the upper surface. The applied velocity reaches 1000m/s at a time $T = 0.1 \mu\text{s}$ and is kept constant for $t \in [T, T + 0.4\mu\text{s}]$.

In Figure 12 is shown the rise in temperature (in K) at several times as the compressive wave travel through the energetic aggregate. Note that at a time $t = 3.4 \mu\text{s}$, the compressive wave has reached the bottom surface of the energetic aggregate. It is worth noting that the rise in temperature inside

the energetic aggregate and inside each energetic crystal is not homogenous. For locations that are far enough from the contact boundaries between the polymer binder and the energetic crystals, the rise in temperature is mainly influenced by the relative orientation of the energetic crystal with respect to the loading wave. As an example, the evolution with time of the rise in temperature away from the boundary of each of the 3 energetic crystals located close to the upper surface of the aggregate is shown in Figure 13.

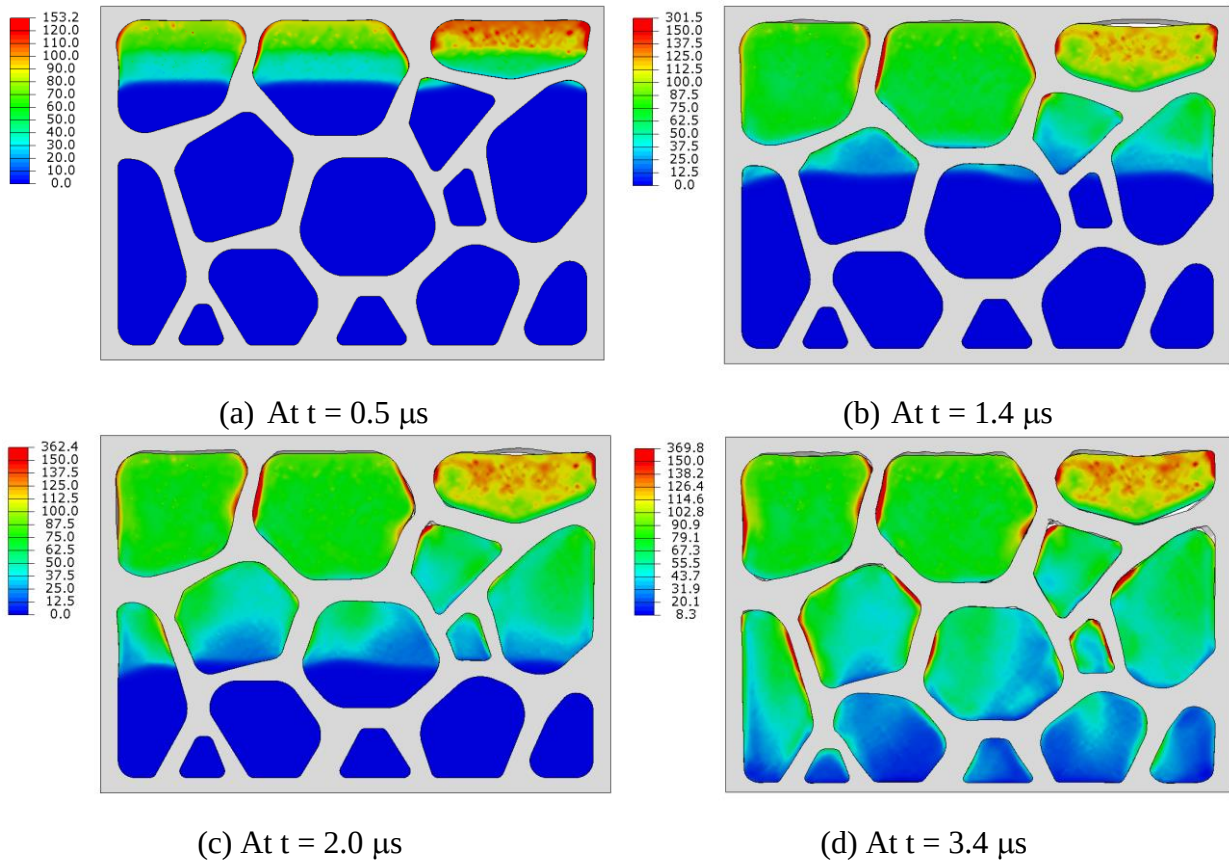


Figure 12. Rise in temperature inside a PBX made of 14 PETN crystal surrounded by a Sylgard182 matrix (in gray) at different time: (a) $t = 0.5 \mu\text{s}$; (b) $t = 1.4 \mu\text{s}$; (c) $t = 2.0 \mu\text{s}$ and (d) $t = 3.4 \mu\text{s}$

The rise in temperature experienced by the grains (1) and (2) is very close, being 71K and 75 K, respectively. However, for the grain (3) which has its [001] direction aligned with the loading direction (see Figure 11(a)), the rise in temperature is about 118 K, which is about 60% larger than the grains (1) and (2). The interaction between the polymer matrix and the energetic crystal also causes rise in temperature. It can be seen in Figure 12 that in each grain the most increase in

temperature in each grain is observed at the boundary of the grain. However, this phenomenon leads to a very local rise in temperature which depends on the orientation of the polymer-crystal boundary with respect to the loading direction. If this boundary is oriented such to facilitate shearing, the rise in temperature will be more important (see Figure 12). It is to be noted that the overall rise in temperature of the crystal is dictated by the plastic dissipation inside the crystal. In other words, the rise in temperature in most of the crystal is mainly influenced by its (see Figure 13 and comparison between crystal (2) and (3)). It is also worth noting that the mesoscale simulation enables the modeling of the decohesion between the energetic crystal and the polymer matrix (see the “opening” space between the matrix and the crystal in Figure 12).

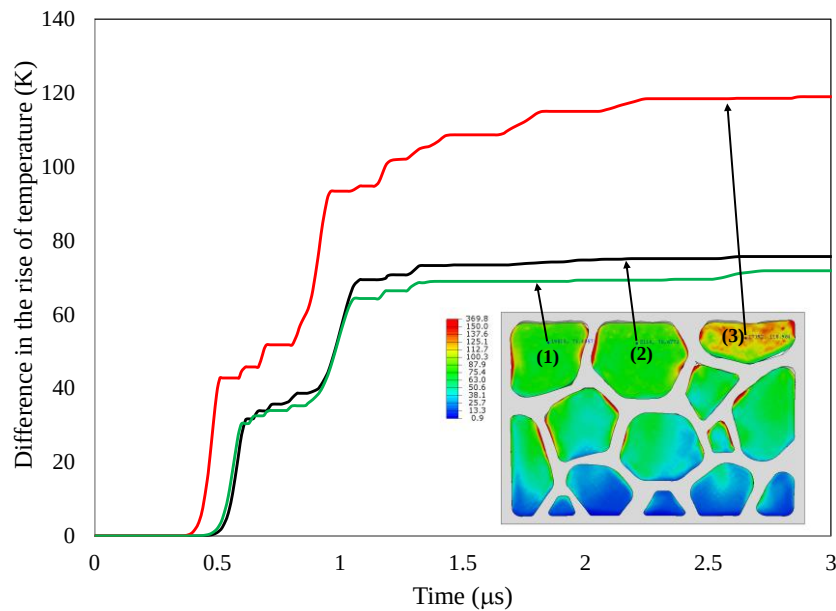


Figure 13. Rise in temperature inside several PETN crystals with different orientation with respect to the compressive wave (see Figure 11(a)). Note that the crystal orientation influences the rise in temperature inside an energetic crystal.

Examination of Figure 12 and Figure 13 enables to assess the rise in temperature inside the PBX as the compressive wave travels through the aggregate. When the compressive wave reaches the bottom surface, the wave is reflected. As this reflected wave travels back through the aggregate, the PETN crystal experience a secondary loading which causes further change in temperature. A comparison of the rise in temperature field at $t=3.4\mu\text{s}$, i.e. a time before the wave reflects at the bottom surface (Figure 12(d)) and at $t=5.4\mu\text{s}$ when the reflected wave has passed through the

aggregate (see Figure 14) shows that this secondary loading produces a non-negligible in terms of rise in temperature.

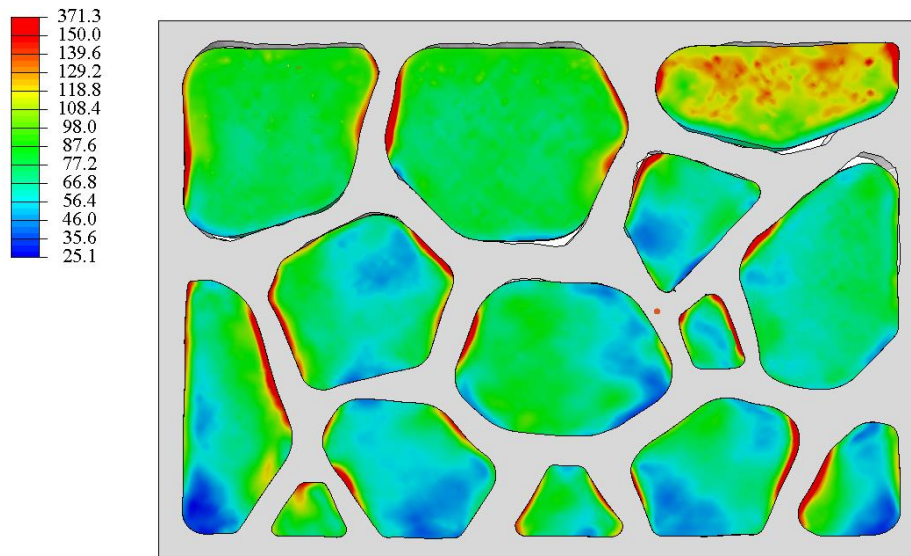


Figure 14. Rise in temperature inside a PBX made of 14 PETN crystal surrounded by a Sylgard182 matrix (in gray) as the reflected wave travel back through the aggregate ($t = 5.4 \mu\text{s}$)

6. Development of a mechanical framework for high-fidelity simulation of high-strain deformation of energetic materials

The development of the computational framework that enables the description of the mechanical response of an energetic aggregate material is a key accomplishment of this research effort. It is well accepted that the prediction of the mechanical behavior of aggregates of energetics crystals under impact loadings is a formidable challenge. An explosive aggregate is composed of millions of energetics crystals with different orientations. Even when the explosive aggregate is composed of randomly oriented energetics crystals and as such its overall/global mechanical behavior can be assumed isotropic, the crystals that compose the aggregate experience different loadings. Therefore, the main challenge associated with simulating the mechanical behavior of energetics materials is to have a model simple enough to enable large scale simulations of the given engineering application and at the same time, the numerical framework and the model be able to describe with accuracy local fields. Specifically, the local plastic dissipation in each crystal need to be monitored in order to determine the maximum rise in temperature.

In this research effort, a numerical framework for the description of the thermo-mechanical behavior of an energetic aggregate which accounts for the specificities of the behavior of constituent crystallites has been developed. In this framework, the stress $\boldsymbol{\sigma}$ of the aggregate, expressed in the coordinate system associated to the loading is given by the relation

$$\boldsymbol{\sigma} = \frac{1}{N} \sum_{i=1}^N \mathbf{R}_i^T \boldsymbol{\sigma}_i^{loc} \mathbf{R}_i \quad (20)$$

with N being the number of grains considered in the aggregate, $\boldsymbol{\sigma}_i^{loc}$ the local stress tensor for the given grain i , expressed in the coordinate system associated with the crystallographic axes, that is defined with respect to the loading frame by the rotation matrix $\mathbf{R}_i$. The local stress tensor $\boldsymbol{\sigma}_i^{loc}$ of the grain i is calculated by solving the following system of governing equations:

$$\left\{ \begin{array}{l} \mathbf{d}_i = \mathbf{d}_i^e + \mathbf{d}_i^p \\ \dot{\boldsymbol{\sigma}}_i^{loc} = \mathbf{C}^e : \mathbf{d}_i^e \\ f(\dot{\boldsymbol{\sigma}}_i^{loc}, \bar{\boldsymbol{\varepsilon}}^p) = \varphi(\dot{\boldsymbol{\sigma}}_i^{loc}) - Y(\bar{\boldsymbol{\varepsilon}}^p, \dot{\bar{\boldsymbol{\varepsilon}}}_i) \leq 0 \\ \mathbf{d}_i^p = \dot{\lambda} \frac{\partial \varphi}{\partial \boldsymbol{\sigma}_i^{loc}} \\ \dot{\bar{\boldsymbol{\varepsilon}}}_i^p = \dot{\lambda} \end{array} \right. \quad (21)$$

The Eq. (21)₁ expresses that the local strain-rate tensor $\mathbf{d}_i$ is decomposed into an elastic part, $\mathbf{d}_i^e$, and a plastic part, $\mathbf{d}_i^p$. For the tetragonal crystal, Linear elastic and anisotropic behavior governed by Hooke's law is considered, with $\mathbf{C}^e$ (Eq. (21)₂) denoting the elastic fourth-order tensor, which is expressed in Voigt notation in the coordinates associated with the crystallographic axes by the matrix:

$$\mathbf{C}^e = \begin{bmatrix} C_{11} & C_{12} & C_{13} & 0 & 0 & 0 \\ C_{12} & C_{11} & C_{13} & 0 & 0 & 0 \\ C_{13} & C_{13} & C_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{55} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{55} \end{bmatrix} \quad (22)$$

with $C_{11} = 17.12$ GPa, $C_{33} = 12.18$ GPa, $C_{12} = 6.06$ GPa, $C_{13} = 7.98$ GPa, $C_{55} = 5.03$ GPa and $C_{44} = 3.81$ GPa (see Hooks et al. (2015)). The yield surface for the energetic crystal is expressed in the form:

$$f(\dot{\boldsymbol{\sigma}}_i^{loc}, \bar{\boldsymbol{\varepsilon}}^p) = \varphi(\dot{\boldsymbol{\sigma}}_i^{loc}) - Y(\bar{\boldsymbol{\varepsilon}}^p, \dot{\bar{\boldsymbol{\varepsilon}}}_i) \quad (23)$$

where φ is the new anisotropic yield criterion developed (see Eq.(6) of Section 2) that accounts for the specific symmetries of the energetic crystal, and $Y(\bar{\boldsymbol{\varepsilon}}^p, \dot{\bar{\boldsymbol{\varepsilon}}}_i)$ is the hardening law of the energetic crystal that depends on the local equivalent plastic strain $\bar{\boldsymbol{\varepsilon}}^p$ and the local strain-rate $\dot{\bar{\boldsymbol{\varepsilon}}}_i$. Assuming associated plasticity, the local plastic strain-rate tensor is obtained with the flow rule

$$\mathbf{d}_i^p = \dot{\lambda} \frac{\partial \varphi}{\partial \boldsymbol{\sigma}_i^{loc}} \quad (24)$$

with $\dot{\lambda}$ the plastic multiplier. The average temperature inside the energetic aggregate made of PETN crystals is determined as

$$T_{avg} = \frac{1}{N} \sum_{i=1}^N \int_0^t \frac{\alpha(\sigma_i^{loc} : \mathbf{d}_i^p)}{\rho C} dt \quad (25)$$

While the maximum temperature inside the energetic aggregate is defined as

$$T_{max} = \max_{i=1..N} \int_0^t \frac{\alpha(\sigma_i^{loc} : \mathbf{d}_i^p)}{\rho C} dt \quad (26)$$

(see also Eq.(19)).

A fully-implicit backward Euler method is used for the integration of the set of elastic-plastic governing equations given by the system of Eq. (21). In addition to a very good accuracy, the backward Euler method was shown to be unconditionally stable with respect to the size of the strain increment.

It is to be noted that the developed numerical framework (see Eqs.(20)-(26)) is able to capture with accuracy the local plastic behavior within the energetic crystal, the evolution of all components of the plastic strain tensor, the plastic energy as a function of the loading history and the evolution of the temperature field. Indeed, for the given strain path imposed macroscopically, the loading history of each grain is accounted for. Because the history of plastic deformation is monitored in each energetic crystal, it is possible to determine accurately the evolution of the local temperature field and the rise in temperature due to the energy dissipation and to monitor the occurrence of hot spots during dynamic events.

In the following are presented illustrations of the predictive capabilities of this new computational framework that accounts for the specificities of the tetragonal crystals in both elastic and plastic regimes. First, FE simulation of a Taylor impact test of a cylinder (length of 50 mm and diameter of 10 mm) of an energetic aggregate is presented. For this purpose, 19456 reduced integration elements have been used to mesh one quarter of the Taylor impact specimen. For each element, 250 randomly oriented PETN crystal are considered ($N = 250$ in Eq.(20)). In total the stress history and local rise of temperature for 4.8 million of PETN crystals are monitored for this Taylor impact

simulations. In terms of computation time, the Taylor impact simulation requires a calculation time of about 13 hours on 6 cores (desktop computer i7-4770 CPU – 16 GB RAM).

Figure 15 shows the maximum local rise of temperature (see Eq. (26)) for a Taylor impact of a PETN aggregate at an impact velocity of 150 m/s. Obviously the maximum temperature increase occurs close to the impact surface. Furthermore, as discussed previously, it is very important to know which orientation of the crystal undergoes the maximum rise of temperature. Unlike the case when the stress state does not evolve during the event (e.g. always uniaxial compression), in this application, the crystal orientation that experiences the maximum rise will totally depend on the local stress path (i.e. the evolution of the stress state experienced by the given PETN crystal). The numerical framework allows to identify the critical orientation. As an example, Figure 16 shows the orientations of the PETN crystals that underwent the maximum plastic dissipation and temperature rise at several locations inside the Taylor impact specimen. It is worth noting that the “critical” orientation varies depending in the location on the specimen. For the Taylor impact simulation shown in Figure 15, there are 6 different orientations that can be seen as critical. It is worth noting the strong influence of the relative orientation of the **c**-axis of the tetragonal structure with respect to the impact direction. This influence can be explained based on the anisotropy in yield stresses in compression according to the new single crystal criterion which is shown in Figure 5.

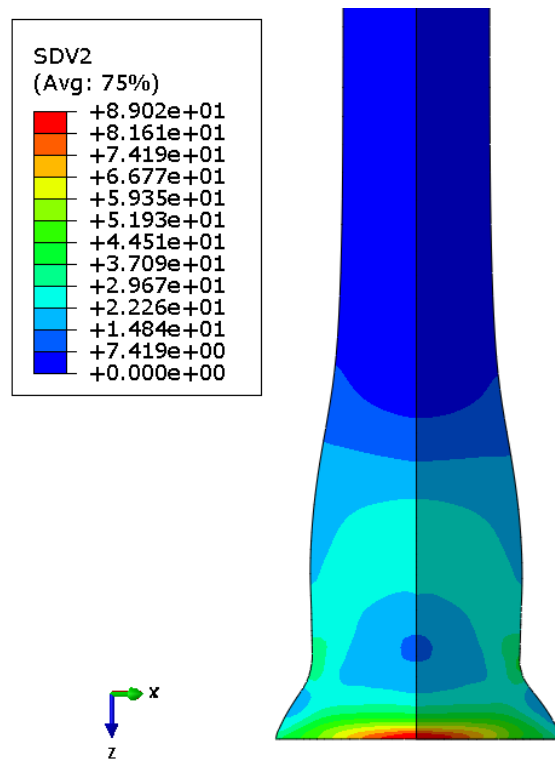


Figure 15. Isocontours of the maximum local rise of temperature per element (250 tetragonal crystals with different orientations per element) (see Eq. (26)) in a Taylor impact simulation of a PETN aggregate. Impact velocity of 150m/s.

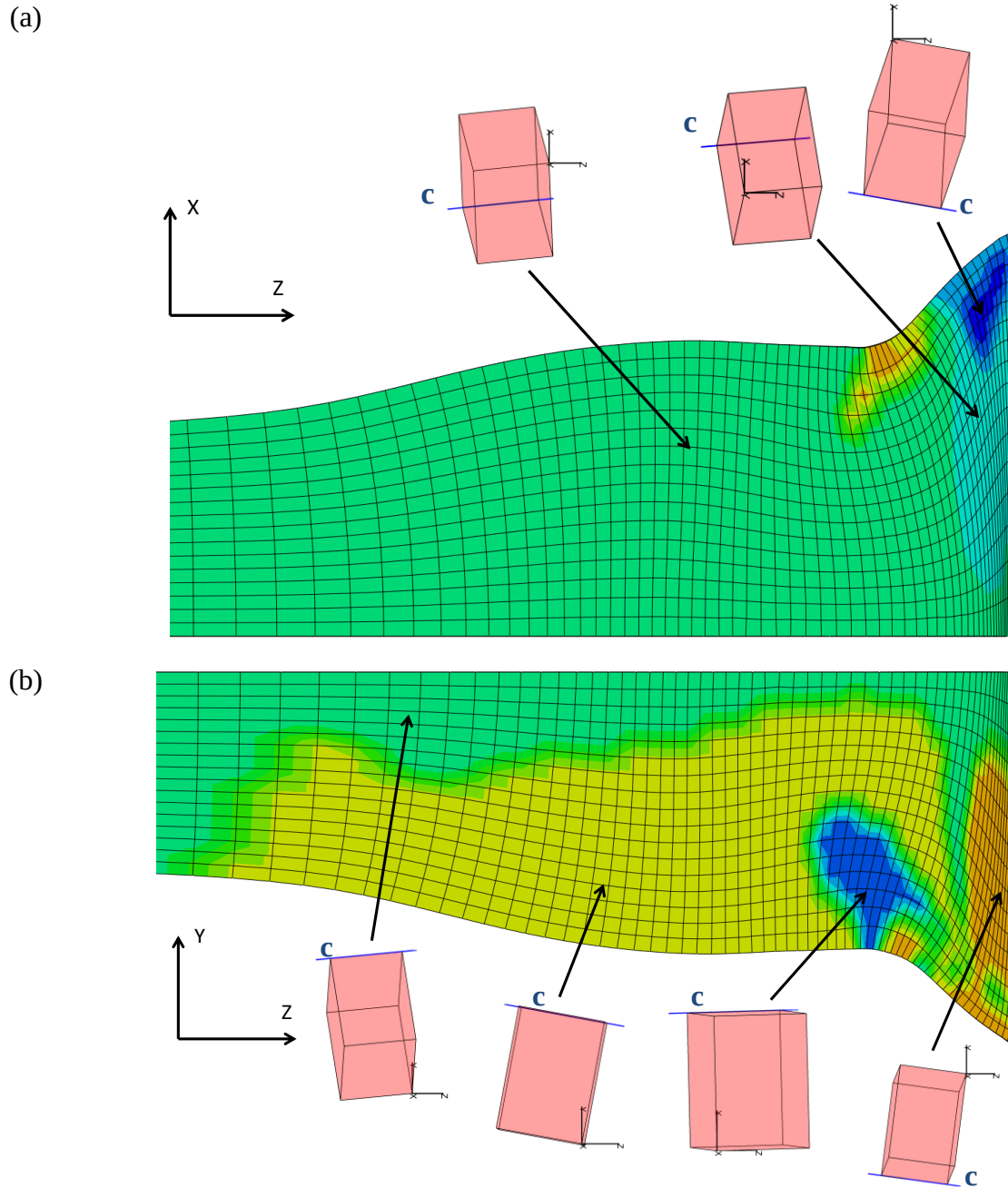


Figure 16. Critical PETN crystal orientations that underwent the maximum rise of temperature depending on their location in a Taylor impact simulation with an initial velocity of 150 m/s. It is noted that the critical orientation are different in the (x,z) plane (a) and the (y,z) plane (b). The blue arrow of the tetragonal crystal lattice represents the orientation of the c-axis

5.1 Simulation of the dynamic compaction of energetic aggregates

As seen in the previous section, depending on the loading and the crystal orientation, the rise of temperature induced by the plastic dissipation could be totally different. This is demonstrated thru simulation of the dynamic compression of an aggregate composed of 250 crystals, randomly oriented.

Simulations are conducted using the numerical framework and the Abaqus user routine described in previous section (See Eqs.(20)-(24) in Section 5). The geometry of the specimen is shown in Figure 17. One quarter of the specimen has been meshed using 4000 reduced integration elements. Stress history and local rise of temperature for 1.0 million of PETN crystals have been monitored during the FE simulation. It is worth noting that for this geometry and 1.0 million of energetic crystal, the average size of a PETN crystal is about 20 μm .

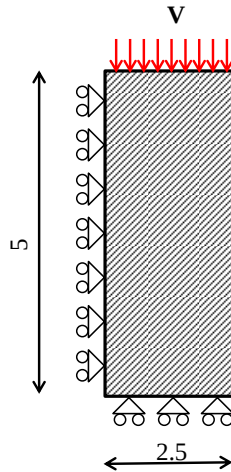


Figure 17. Geometry of the specimen used for the dynamic compression simulation of the pressed energetic aggregate. Dimensions are in mm.

For an applied velocity $V=1000\text{m/s}$, in Figure 18 are shown the maximum local rise of temperature for the dynamic compression of a PETN aggregate and the local difference in the rise of temperature between all the crystals considered (250 crystal per element) inside the energetic aggregate, i.e. $(\text{Max}T-\text{Min}T)/\text{Min}T$. For this applied loading, it can be seen that among the 250 crystal orientations that compose the energetic aggregate, the temperature difference could be of 50%. Furthermore, as seen previously, it is very important to know which orientation of the crystal undergoes the maximum rise of temperature. As an example, Figure 19 shows the rise of

temperature for two particular crystal orientations that are present in the PETN energetic aggregate at 1mm, 4mm and respectively 6mm from the top surface of the specimen. It is worth noting that this numerical framework enables large-scale simulations of dynamics events by predicting the overall mechanical behavior of the energetic aggregate, while also monitoring the local field (plastic dissipation, local rise in temperature) at the grain level for each grain that compose the aggregate.

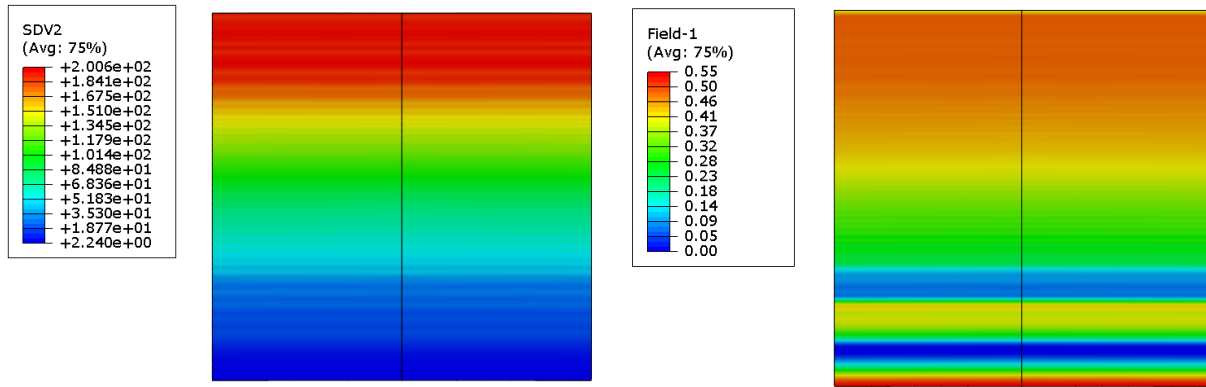


Figure 18. (a) Isocontours of the maximum local rise of temperature per element under dynamic compression of a PETN aggregate. (b) Difference in rise of temperature inside the energetic aggregate (i.e. $(MaxT-MinT)/MinT$). Applied longitudinal velocity of 1000m/s.

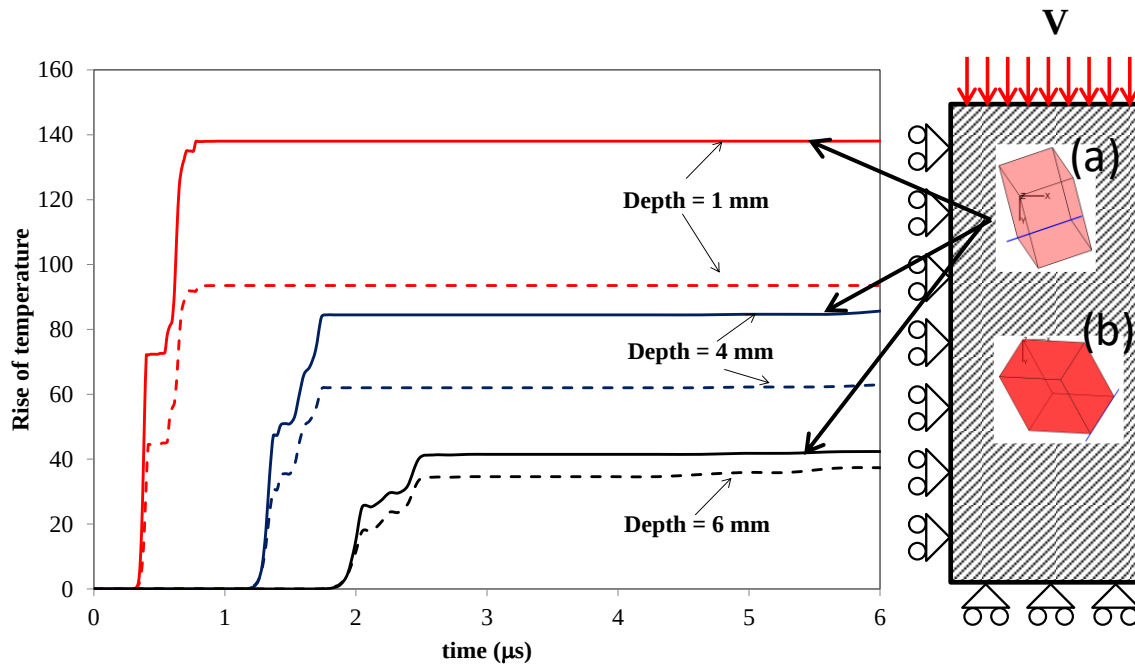


Figure 19. Evolution of the rise of temperature for two orientations that are present in the energetic aggregate at location of 1mm, 4 mm and 6 mm, respectively from the top surface of the specimen. Orientation (a) is represented by solid line, while orientation (b) by dashed line

Additionally, dynamic compression simulation have been performed for different axial velocity V ranging from 100 m/s to 1500 m/s. Figure 20 shows the average temperature (initial temperature of 275 K) inside the energetic aggregate at a time $t = 1 \mu\text{s}$ for several tests. Note that the average temperature inside the energetic aggregate (see Eq. (25)) varies from about 280 K for a velocity of 200m/s to about 540 K for a velocity of 1500m/s. It is worth noting that the average temperature almost doubles when the applied velocity increases from 200m/s to 1500m/s. In Figure 21 are shown the isocontours of the maximum local temperature (see Eq. (26)).

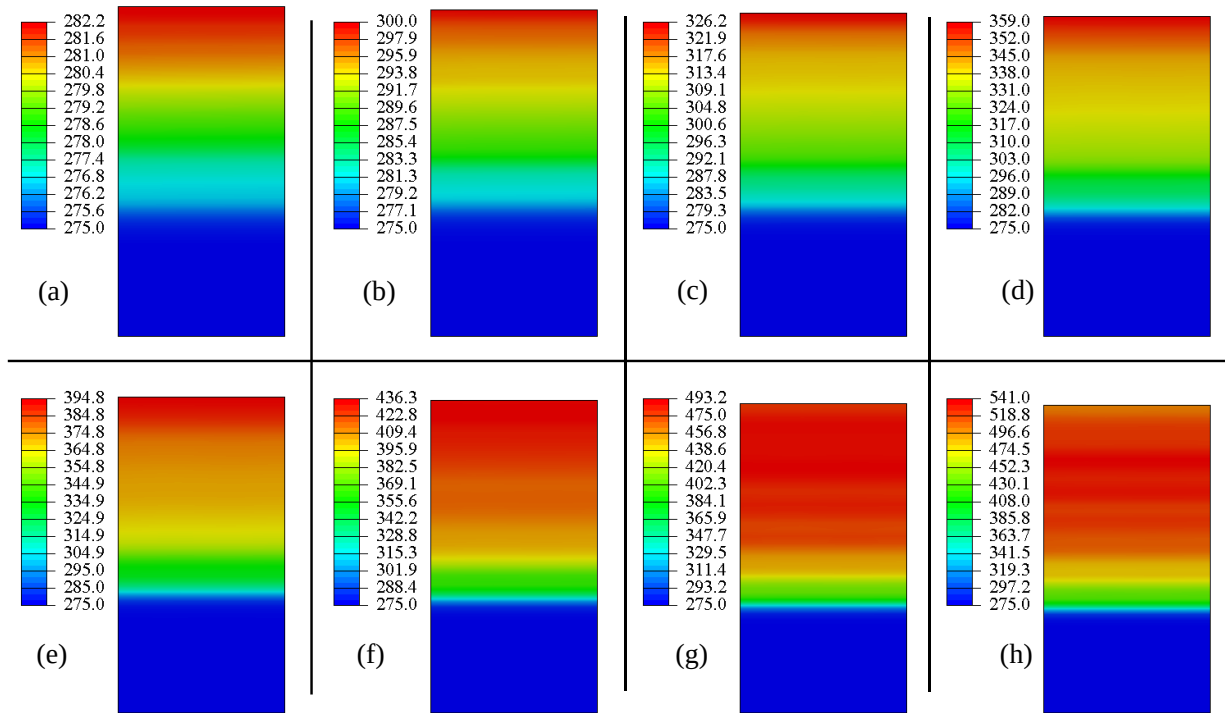


Figure 20. Average temperature inside the energetic aggregate subjected to uniaxial dynamic compression at different axial velocity (a) 200m/s; (b) 400 m/s (c) 600m/s; (d) 800m/s; (e) 1000m/s; (f) 1200 m/s; (g) 1400m/s and (h) = 1500 m/s

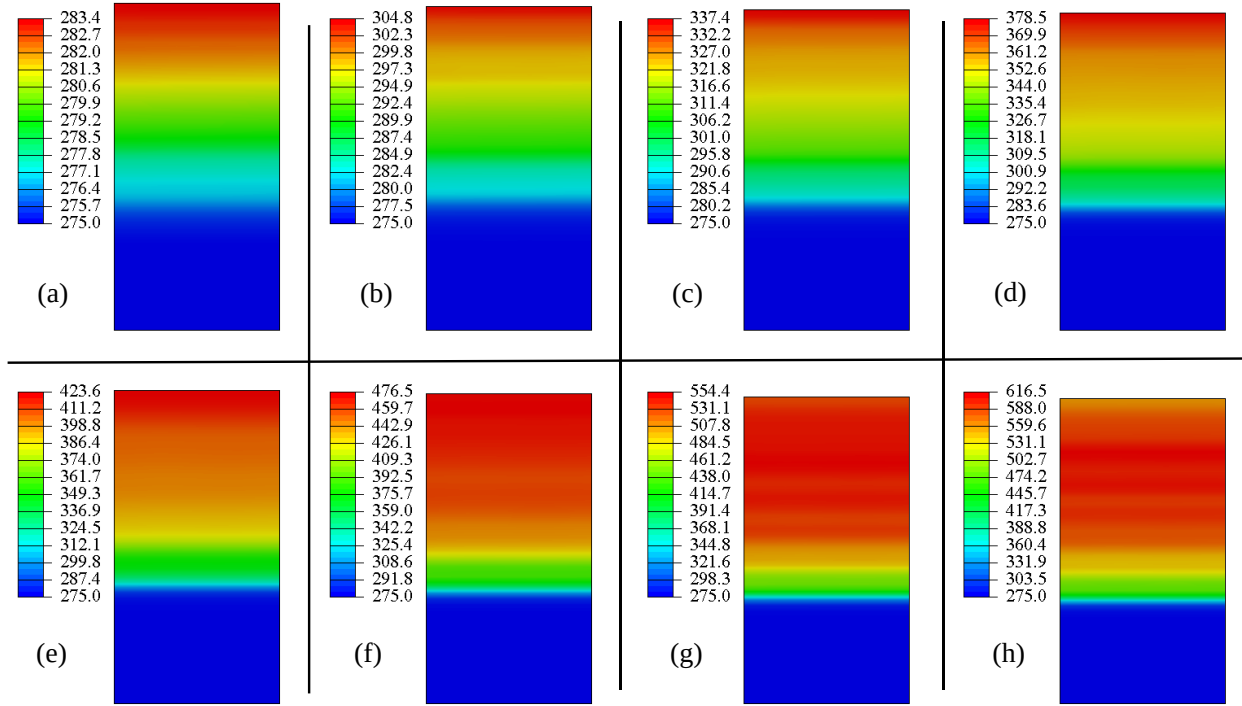


Figure 21. Maximum temperature inside the energetic aggregate subjected to uniaxial dynamic compression at different axial velocity (a) 200m/s; (b) 400 m/s (c) 600m/s; (d) 800m/s; (e) 1000m/s; (f) 1200 m/s; (g) 1400m/s and (h) = 1500 m/s

The maximum temperature varies between 283 K for an applied velocity of 200 m/s to 616 K for a velocity of 1500m/s. It is worth noting that the difference between the average temperature and the maximum temperature increases with the velocity. For a low applied velocity, e.g. $V=200\text{m/s}$, the difference is rather small (around 1%) while for a applied large velocity $V=1500\text{m/s}$, the difference is significant (around 15%). From the dynamic compression simulations, it is also possible to get insights concerning the temperature increase as a function of the shock pressure. While an axial velocity of 200m/s generate a pressure of around 1 GPa, for an axial velocity of 1500m/s, the pressure is around 9.2 GPa. In Figure 22 is shown the evolution of the temperature increase with respect to the loading pressure for the same energetic aggregate made of randomly oriented PETN crystals. Both the average temperature (see Eq. (25)) and the maximum temperature (see Eq. (26)) are displayed in Figure 22. It is worth noting that as the pressure increases, the difference between the average temperature and the maximum temperature also increases. A difference of 30% in temperature increase between the average temperature and the maximum temperature is observed.

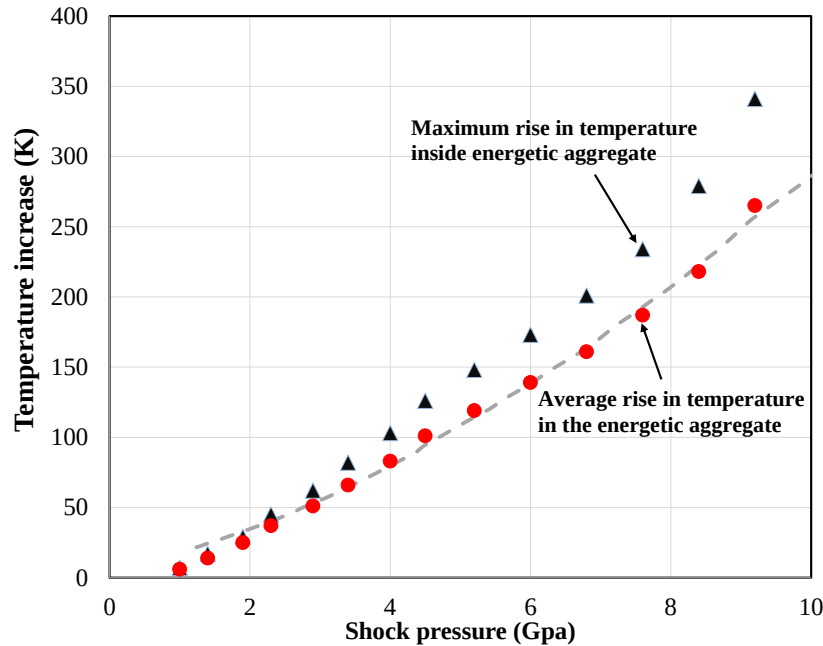


Figure 22. Temperature increase (in K) as a function of the shock pressure (in GPa) for an energetic aggregate made of PETN crystals randomly oriented. The predicted average temperature (red circle) and the maximum temperature (black triangle) are shown in comparison with the curve obtained by Stirpe et al. (1970) for a PETN aggregate with $\rho = 1770 \text{ kg/m}^3$.

Furthermore, in Figure 22 is also plotted the evolution of the temperature increase as a function of the pressure obtained by Stirpe et al. (1970) for a PETN energetic aggregate of density $\rho = 1770 \text{ kg/m}^3$. A good agreement is obtained between the Stirpe et al. (1970) results and the prediction of the average temperature increase obtained using the model described by Eqs.(20)-(24).

5.2 Simulation of impact loading: interaction between the casing material and the energetic aggregate.

To further assess the predictive capabilities of the new numerical framework for energetic aggregate with the constituent crystals obeying the newly developed model for tetragonal crystal, simulation of impact events accounting for the interaction of the energetic aggregate and the casing material have been performed.

The casing material is considered to be a high-strength martensitic steel. The experimental data show that for this martensitic steel is isotropic but display tension-compression asymmetry with the yield stress in uniaxial compression is larger than in uniaxial tension (see Kleiser et al. (2017)

and Bartlett (2018)). Modeling of the plastic behavior of this martensitic steel is done with the Cazacu et al. (2006) isotropic yield criterion that accounts for the tension-compression asymmetry. According to this yield criterion, the equivalent stress is

$$\bar{\sigma} = \frac{3}{\sqrt{2(3k^2 - 2k + 3)}} \left[(|s_1| - ks_1)^2 + (|s_2| - ks_2)^2 + (|s_3| - ks_3)^2 \right]^{1/2} \quad (27)$$

where s_i , $i = 1 \dots 3$ are the principal values of the stress deviator, k is a parameter. For this martensitic steel, $k = -0.15$. The hardening law for the martensitic steel is described by a Johnson-Cook hardening law (see Johnson and Cook, 1983 which account for strain-rate effects, i.e

$$\bar{\sigma} = \left(A + B \left(\bar{\varepsilon}^p \right)^n \right) \left(1 + C \ln \frac{\dot{\bar{\varepsilon}}}{\dot{\bar{\varepsilon}}_0} \right) \quad (28)$$

where A , B , C and n are material parameters, $\dot{\bar{\varepsilon}}_0$ a reference strain-rate, $\dot{\bar{\varepsilon}}$ the strain-rate and $\bar{\varepsilon}^p$ is the equivalent plastic strain associated to $\bar{\sigma}$ using the work equivalence principle. For the martensitic steel, we have $A = 1716$ MPa, $B = 756$ MPa, $C = 0.0128$, $n = 0.321$ and $\dot{\bar{\varepsilon}}_0 = 0.0005$.

For more details about the modeling of the plastic behavior of metallic materials, the reader is referred to Cazacu, Revil-Baudard and Chandola (2019) and Cazacu and Revil-Baudard (2020).

A schematic of the specimen geometry is shown in Figure 23. The specimen has a casing made of the high strength steel. The four cavities inside the casing are partially filled with an energetic aggregate made of randomly oriented PETN crystals. The back surface of the energetic aggregate is in contact with a component made of high strength steel, that can slide inside the casing. The total length of the specimen is 47 mm and the external radius is of 6 mm. The length of the energetic aggregate filling is 24.6 mm. The total mass of the specimen is about 28g. In the simulation, the contact between the energetic aggregate and the high strength steel is considered frictionless. Only one fourth of the specimen is mesh with 18900 C3D8R elements (hexahedral element with reduce integration) for the high strength steel and 56780 C3D8R elements for the energetic aggregate, for which the microstructure is described by 250 randomly distributed crystal orientations per finite element. It is worth noting that more than 14 million of PETN crystals are considered in this simulation, the average size of a PETN crystal being around 20 μm . The history of plastic deformation is monitored in each energetic crystal, therefore it is possible to determine accurately

the evolution of the local temperature field and the rise in temperature due to plastic dissipation for each crystal constituting the energetic aggregate.

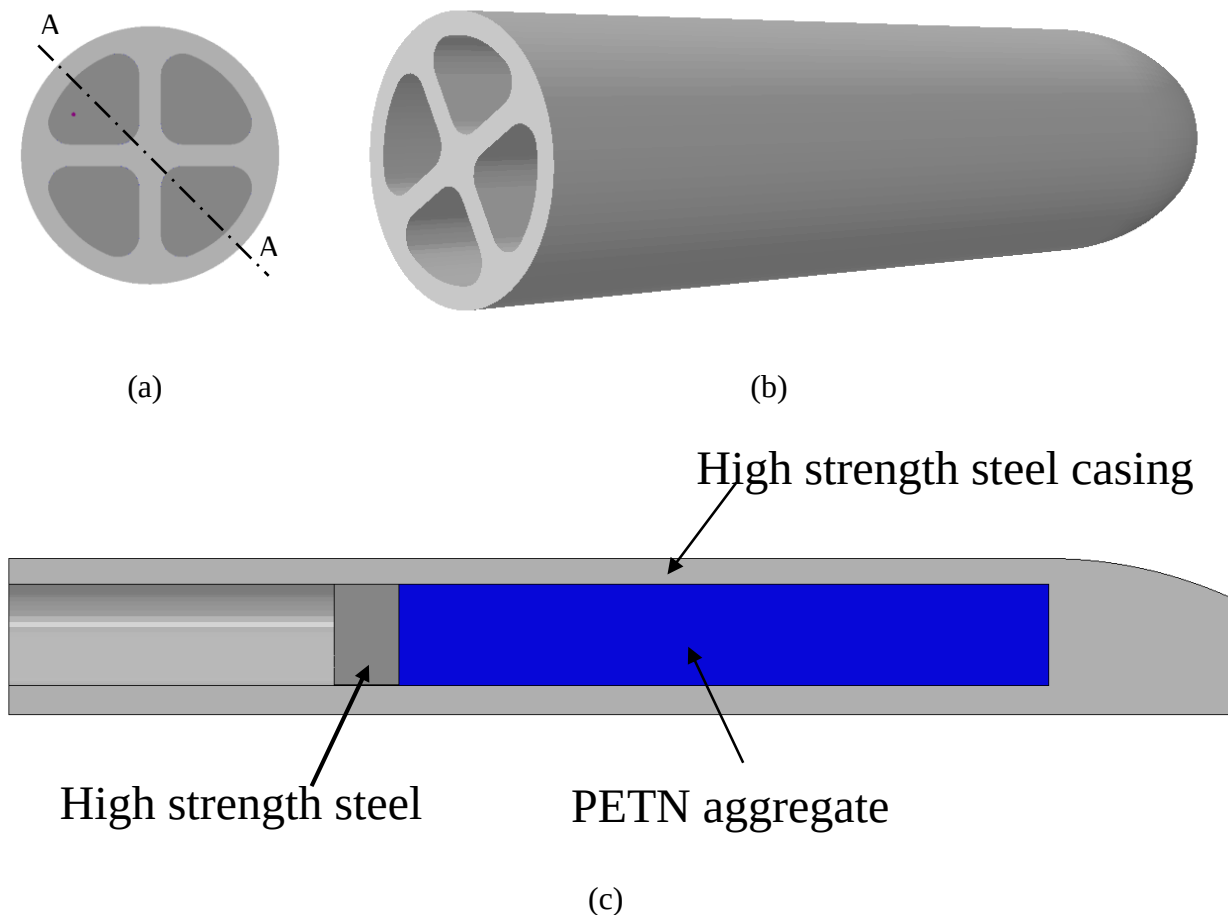


Figure 23. Geometry of the specimen containing the energetic aggregate made of PETN crystals inside a casing made of high strength steel. (a) back view, (b) isometric view (c) cut view along the AA plane (only one half is shown)

Simulation of the impact of the specimen against a rigid anvil has been performed for an impact velocity of 350m/s. Due to the high contrast in mechanical properties between the high strength steel and the energetic aggregate, the wave propagation in the two materials is very different. Figure 24 shows the evolution of the pressure wave (i.e. $p = -1/3tr(\boldsymbol{\sigma})$) in the high-strength steel and in the energetic aggregate for locations at a distance of 0.5 mm from the front boundary between the high strength steel and the energetic aggregate (see the insert in Figure 24 for the locations considered). It is worth noting that at this boundary, most of the pressure wave is reflected

back in the high strength steel, the compressive pressure peak being of 3.35 GPa in the high strength steel and only of 1 GPa in the energetic aggregate. Furthermore, due to the fact that most of the wave is reflected at the boundary, a tensile pressure wave of about 2.3 GPa travels back in the high strength steel (see Figure 24).

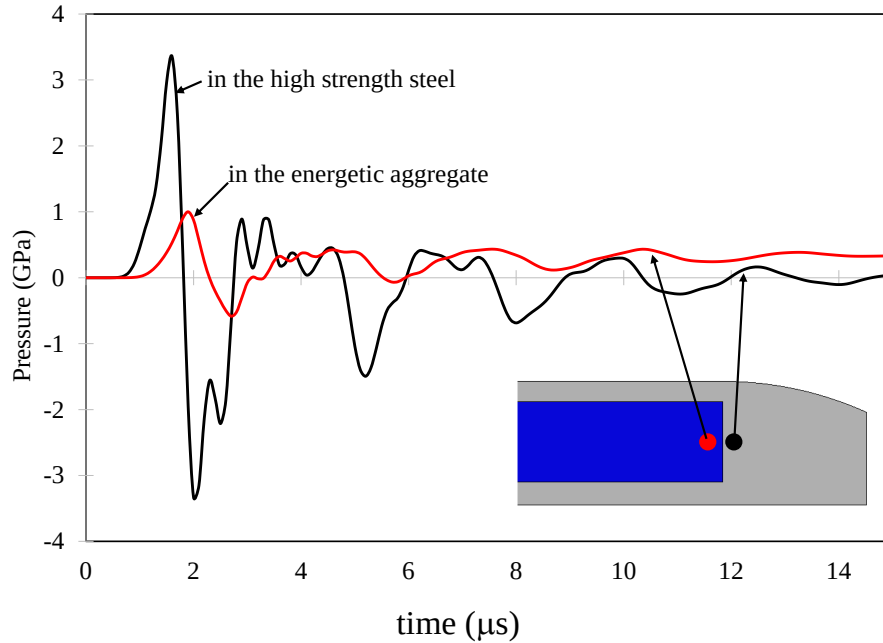


Figure 24. Evolution of the pressure (i.e. $p = -1/3tr(\sigma)$) in the high-strength steel and the energetic aggregate for locations at a distance of 0.5 mm from the front boundary between the high strength steel (black point) and the energetic aggregate (red).

It is worth investigating the importance of accounting for the crystallinity of the PETN material in the evolution of the temperature field during impact events. For this purpose, the prediction of the temperature increase according to the model given by Eqs. (20)-(24) in conjunction with the new yield criterion for energetic crystal (Eq. (7)) is compared to the predictions obtained assuming that the crystallinity of PETN crystal can be neglected (i.e. the PETN material is assumed to be isotropic). These comparisons will enable the assessment of the role of the crystallinity on the temperature increase during an impact event. In Figure 25 are shown the isocontours of the maximum temperature field ((see Eq. (26)) at a time $t = 15 \mu s$ after impact. If the crystallinity of the PETN crystal is accounted for, the maximum temperature in the energetic aggregate is about 420 K (or a temperature increase of 145 K) while if the crystallinity is neglected, the temperature is about 360K (or a temperature increase of 85 K), which is a difference of 16 % in the maximum

temperature (or a difference of 80% in temperature increase). Figure 25 highlight the importance of accounting for the crystallinity of the PETN material.

Comparisons between the predictions using the two models corresponding to at a time $t = 20 \mu\text{s}$ and $t = 30 \mu\text{s}$ after impact, are shown in Figure 26 and Figure 27, respectively. It is worth noting that irrespective of the time from impact, the difference in the maximum temperature predicted with the anisotropic model and the von Mises criterion is significant. Furthermore, this difference in the predicted maximum temperature between the isotropic and anisotropic model that accounts for the crystallinity due to the accounting of the crystallinity is seen in the whole domain. Note also the large zone of high temperature increase predicted with the anisotropic model.

To further investigate the importance of accounting for the crystallinity of the PETN crystal on the temperature increase during an impact event, in Figure 28 are compared the evolution of the maximum temperature with time, at several distance d from the boundary surface between the high strength steel and the energetic aggregate, namely $d=0.5$, 1.8 and 5 mm . The difference in temperature is about 106 K (58 % difference in temperature increase), 91K (65 % difference in temperature increase) and 68 K (71 % difference in temperature increase) for $d = 0.5 \text{ mm}$, 1.8 mm and 5 mm , respectively.

These simulations highlight the strong role of the crystallinity of the energetic crystal on the rise in temperature associated to energy dissipation. The proposed model for the energetic aggregate given by Eqs. (20)-(24) in which the crystals plastic behavior is described by the newly developed yield criterion for tetragonal crystals (Eq. (7)) allows to account for the role of the crystallinity on the temperature increase, and therefore leads to a better description of the temperature field inside the energetic aggregate during dynamic events.

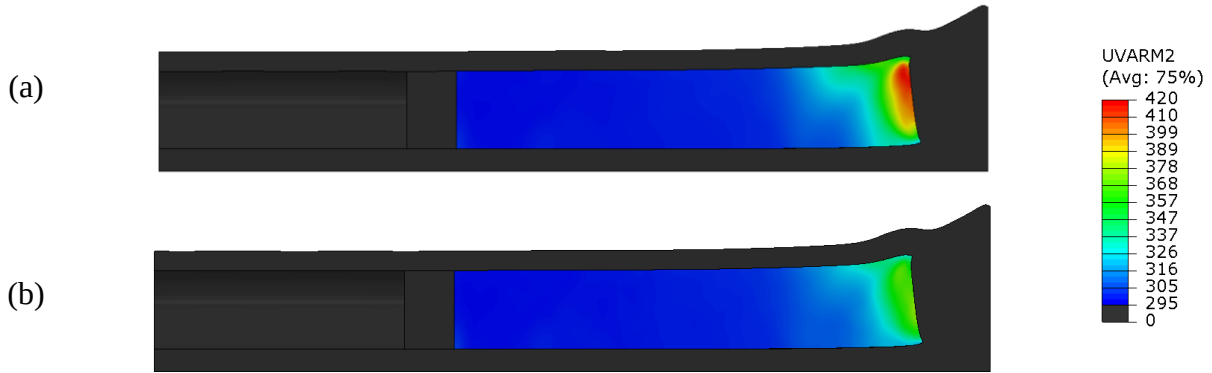


Figure 25. Isocontours of the maximum temperature inside the energetic aggregate made of randomly oriented PETN crystals at a time $t = 15 \mu s$ after impact (a) model accounting for the crystallinity of PETN crystal (i.e. using the developed model (7) at the crystal level) (b) neglecting the crystallinity of PETN crystal (i.e. the PETN crystal is assumed to be isotropic)

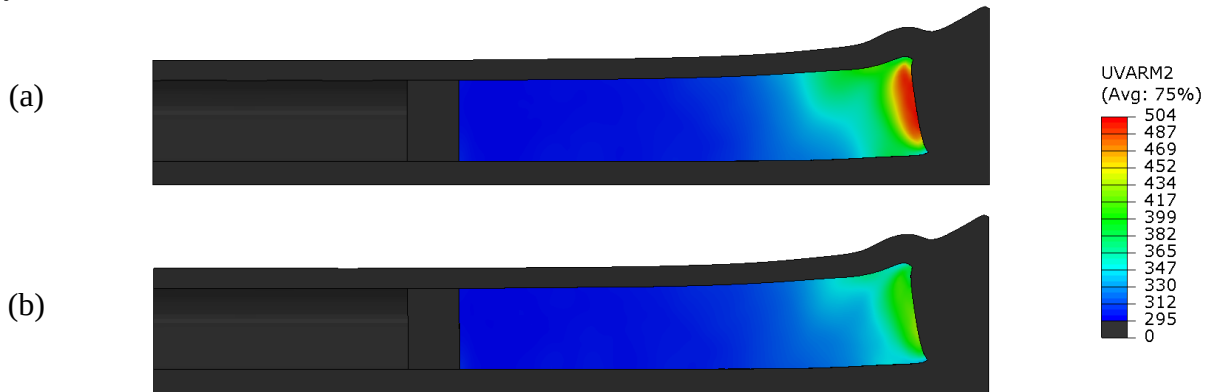


Figure 26. Isocontours of the maximum temperature inside the energetic aggregate made of randomly oriented PETN crystals at a time $t = 20 \mu s$ after impact (a) model accounting for the crystallinity of PETN crystal (i.e. using the developed model (7) at the crystal level) (b) neglecting the crystallinity of PETN crystal (i.e. the PETN crystal is assumed to be isotropic)

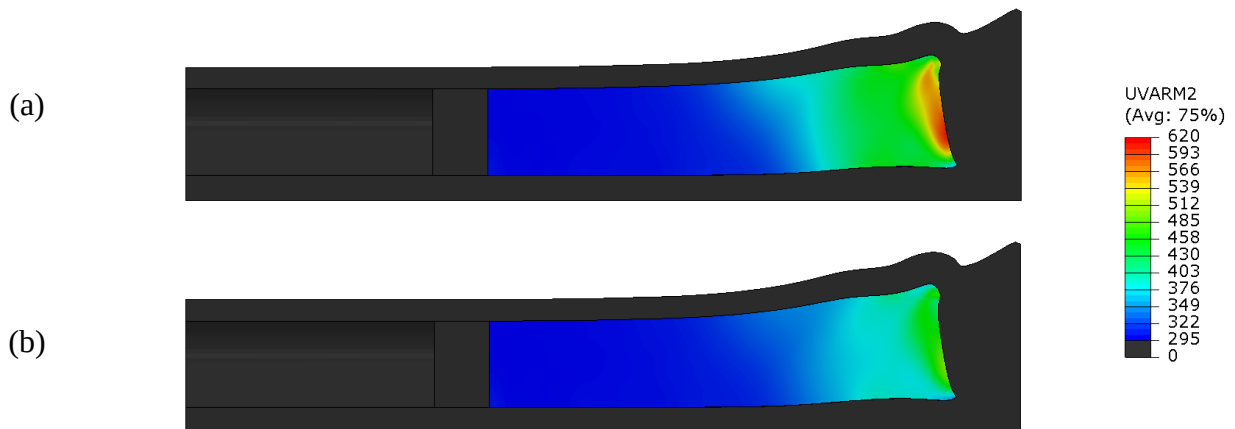
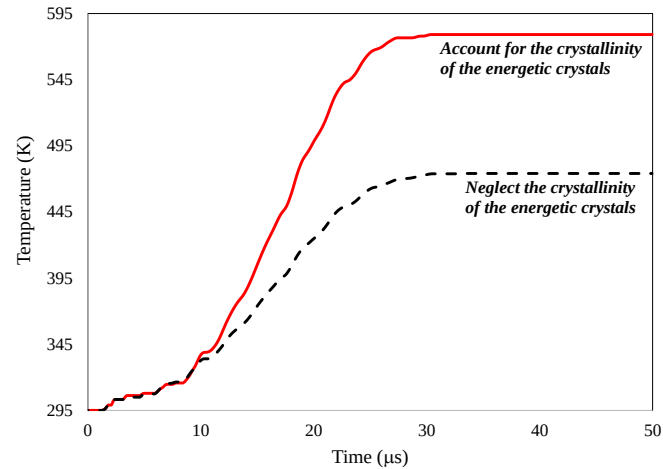
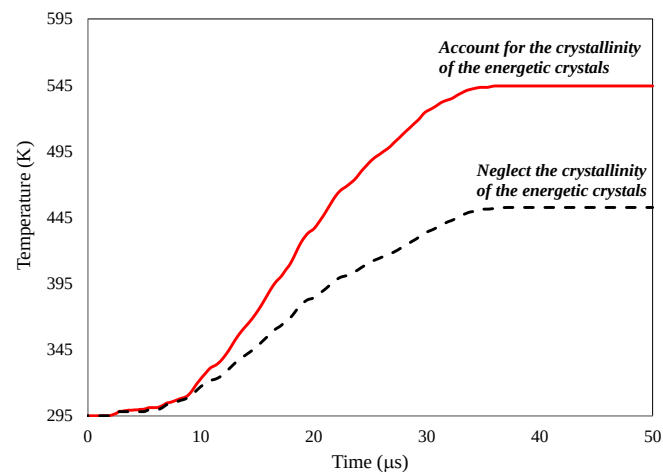


Figure 27. Isocontours of the maximum temperature inside the energetic aggregate made of randomly oriented PETN crystals at a time $t = 30 \mu s$ after impact (a) model accounting for the crystallinity of PETN crystal (i.e. using the developed model (7) at the crystal level) (b) neglecting the crystallinity of PETN crystal (i.e. the PETN crystal is assumed to be isotropic)

(a) at 0.5 mm



(b) at 1.8 mm



(c) at 5 mm

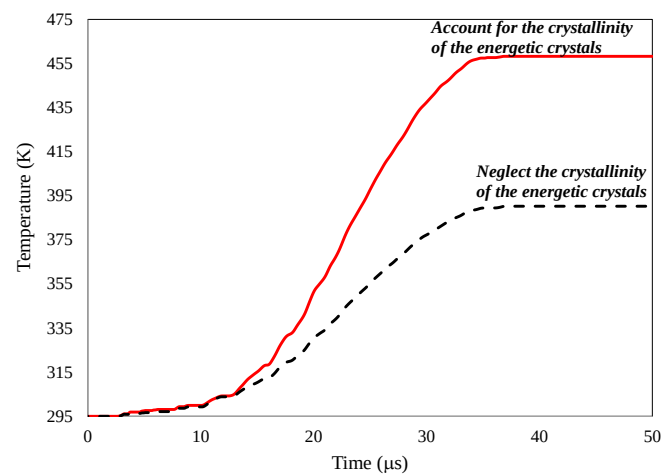


Figure 28. Comparison of the evolution of the maximum temperature at different position inside the energetic aggregate $d=0.5$ (a), 1.8 (b) and 5 (c) mm from the boundary surface with the high strength steel depending on the fact that the crystallinity of the PETN crystal is accounted for in the prediction or not.

Another advantage/benefit of the developed numerical framework is that it can be used for any distribution of the PETN crystals in the aggregate. Thus one can use it to predict the response of an energetic aggregate in which the crystals are no longer randomly oriented, but have a preferential orientation due to the processing of the energetic aggregate. This could be the case for a pressed aggregate, since there is reorientation/realignment of the crystals during pressing. To demonstrate this capability of the new numerical framework, a simulation of an impact event is performed. The specimen geometry is shown in Figure 29. The microstructure of the energetic aggregate is described by 50 different crystal orientations per finite element, and the crystals follow a specific texture map, i.e. the crystals orientation are not randomly distributed but primarily having their c-axis along the impact axis (see the [001] and [111] pole figures in Figure 29). It is worth noting that 2.21 million of PETN crystals are considered in this FE simulation.

Simulation of the specimen composed of the casing material and the PETN aggregate was performed for an impact velocity of 300 m/s. The isocontours of the maximum local rise of temperature (see Eq.(26)) (each element contains 50 tetragonal crystals with different orientations) is shown in Figure 30 (b). Note also that the casing material undergoes large deformation close to the impact surface. The history of plastic deformation is monitored in each energetic crystal, therefore it is possible to determine accurately the evolution of the local temperature field and the rise in temperature due to plastic dissipation for each crystal constituting the energetic aggregate. The maximum and minimum rise of temperature inside the PETN aggregate for a particular element close to the impact surface are plotted in Figure 30 (a). The difference between the maximum and minimum rise of temperature between the 50 crystal orientations in this element is around 200K. Note that the local rise in temperature inside an PETN aggregate is strongly dependent on the crystal orientation.

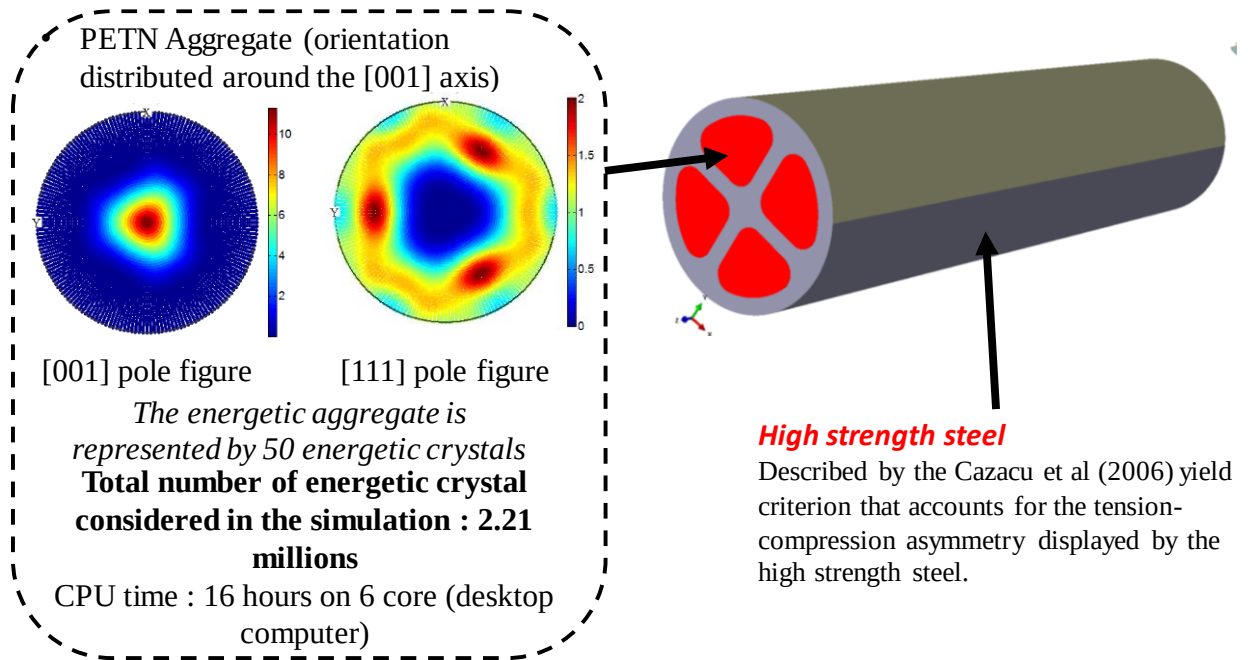


Figure 29. Simulation of an impact of a specimen made of a high strength steel (casing material (gray)) and PETN aggregate (filing material, red)). 2.21 million of PETN crystal has been considered in this simulation.

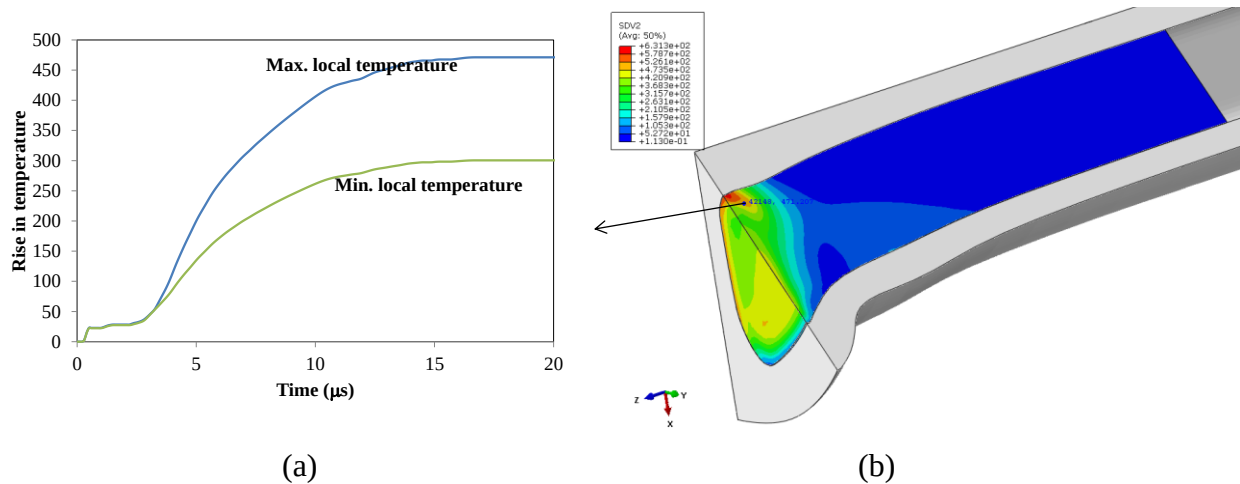


Figure 30. (a) Evolution of the maximum local rise in temperature and the minimum local rise in temperature among the 50 crystal orientations located in an element located closed to the impact surface (represented by the arrow in Fig.29 (b)); (b) Isocontours of the maximum local rise of temperature per element (each element contains 50 tetragonal crystals with different orientations) for an impact simulation of a PETN aggregate. Impact velocity of 300m/s.

6. Conclusion

During this research effort, a new yield criterion for tetragonal energetic crystal has been developed. The newly developed yield criterion account for the specific symmetries of the PETN crystal. The single crystal parameter can be identified analytically based on four uniaxial tests and on the crystalline structure geometry (the c/a ratio) and has been applied to a PETN crystal. It is worth noting the very good agreement between the model predictions and the data for uniaxial compression. The new yield criterion predict that the maximal yield stress ratio is 1.85 along [001], i.e. along the c -axis, while the lowest predicted yield stress is 0.78 along an orientation closed to [506]. Therefore, for the PETN single crystal, the maximal variation in yield stress in uniaxial compression is about 134%. *In uniaxial compression, the single crystal model predict that the local rise of temperature can vary by 134% depending on the orientation of the PETN single crystal.*

The new PETN crystal model has been implemented into the Finite Element framework. Simulation of dynamic collapse of a pore inside an energetic crystal under plane strain loading condition have been performed for different orientations of the PETN crystal. These simulations illustrate the importance of the consideration of the anisotropy of the plastic behavior of energetic crystal. The new proposed yield criterion for the PETN crystal allows accounting for the crystal orientation on the rise of the temperature when submitting to high strain-rate loading. Difference in temperature rise, location of the maximum temperature, geometry of the pore, isocontours of the temperature will be dependent of the orientation of the PETN crystal. It has been shown that ***during the dynamic pore collapse inside a PETN crystal, the rise of temperature induced by the plastic dissipation can varies by at least 60% depending on the orientation of the crystal.***

Energetic materials are complex systems composed of explosive crystals surrounded by a polymer binder and as well as metallic particles inside the energetic systems. Consequently, their mechanical strength depends on the specificities of the deformation of its constituents. Therefore, a meso-scale approach has been developed to improving the understanding of the role of each component on the initiation, either partial or global, of the energetic systems. Meso-scale modeling of energetic systems accounting for dozens of energetic crystals surrounded by a polymer binder has been performed with the newly developed yield criterion for PETN crystals.

A multi-scale numerical framework has also been developed to perform large scale simulation of high rate loading of energetic aggregate. This numerical framework enables large-scale simulations of dynamics events by predicting the overall mechanical behavior of the energetic aggregate, while also monitoring the local field (plastic dissipation, local rise in temperature) at the grain level. The performance of the new framework has been demonstrated with F.E. simulation of dynamic compression of pressed PETN aggregates composed of millions of PETN tetragonal crystals. The evolution of the temperature increase with respect to the loading pressure for an energetic aggregate made of randomly oriented PETN crystals has been established. It is worth noting that as the pressure increases, the difference between the average temperature and the maximum temperature inside the energetic aggregate also increases. A difference of 30% in temperature increase between the average temperature and the maximum temperature has been predicted.

Finally, this new numerical framework associated with the newly developed yield criterion for the PETN energetic crystal has been extended to account for the interaction between the casing material and the energetic aggregate during the impact event. These simulations highlight the strong role of the crystallinity of energetic crystal in the rise in temperature due to energy dissipation. If we made use of the proposed model for energetic aggregate given by Eqs. (20)-(24) that exploit the newly developed yield criterion for energetic crystal (Eq. (7)) allows to account for the role of the crystallinity on the temperature increase, the maximum temperature increase is about 60% larger than the one predicted while neglecting the crystallinity of the PETN crystals that composed the energetic aggregate.

Appendix : Research dissemination as part this research grant

Book

Cazacu O. and Revil-Baudard B. 2020, “Plasticity of Metallic Materials: modeling and applications”, Elsevier, ISBN 9780128179840.

Research papers:

Cazacu, O., Chandola, N., Revil-Baudard, B., Frodal, B.H., Børvik, T. and Hopperstad, O.S., 2020. Modeling the effect of notch geometry on the deformation of a strongly anisotropic aluminum alloy. *European Journal of Mechanics-A/Solids*, p.104004.

Revil-Baudard, B. (2021). Numerical investigation into the dynamic behavior of sands. *Mechanics Research Communications*, 103664.

Revil-Baudard, B. A new constitutive model for tetragonal energetic single crystal. *Journal of the Mechanics and Physics of Solids* (submitted)

Revil-Baudard, B. and Cazacu O. Role of the crystallinity on the thermos-mechanical behavior of energetic aggregates under impact. *J. of Impact Engineering*. (submitted)

Conference participations:

B. Revil-Baudard, Dynamic behavior of cohesionless granular materials. ASME 2019 International Mechanical Engineering Congress & Exposition, Salt Lake City, UT, 10-15 November, 2019.

B Revil-Baudard, Forming of Materials With Cubic Crystal Structure, 23rd International Conference on Material Forming (ESAFORM 2020), Postdam, Germany, Mai 2020

B. Revil-Baudard, New multiscale model for energetic crystals and applications to simulation of dynamic events, Congress & Exposition, Salt Lake City, UT, 10-15 November, 2020.

B Revil-Baudard, Numerical investigation revealing key factors associated with instabilities in granular materials during impact, XXV International Union of Theoretical and Applied Mechanics (ICTAM), Milano, Italy. 23-28 August 2021,

Organizer of Symposia

Co-chair “Symposium on Plasticity, Damage, and Fracture”, ASME 2019 International Mechanical Engineering Congress & Exposition, Salt Lake City, UT, 8-14 November, 2019.

Co-chair “Symposium on Plasticity, Damage, and Fracture of metallic materials”, ASME 2020 International Mechanical Engineering Congress & Exposition, Portland, OR, 8-14 November, 2020.

Co-chair “Symposium on Plasticity, Damage, and Fracture”, ASME 2021 International Mechanical Engineering Congress & Exposition, November 1 – 5, 2021

Others activities:

- **Implementation of a model for pressure dependent cohesion-less materials to be transition into the EPIC F.E. code. (2019-2020)**

This research grant has also partially supported the development of F.E. implementation algorithms and user subroutine (VUMAT) to facilitate the transition to DoD codes, especially EPIC, of an advanced constitutive model for pressure dependent cohesion-less material.

Specifically, F.E. implementation algorithms for the numerical integration of the elasto-plastic model of Lade (1977) for a cohesion-less material has been developed in a Lagrangian framework in the commercial code Abaqus. The implementation of the models has been verified in Abaqus-Vumat format at UF-REEF and then transferred to SWRI in EPIC-VUMAT format in order for the EPIC's users to exploit this model. It is worth mentioning that a transition protocol for constitutive models implementation have already been successfully established between the PI's at UF-REEF and EPIC's development team at SWRI.

The code in EPIC-VUMAT format with an attached documentation that includes 1) the formulation of the model, 2) the method to determine constants from laboratory test data, 3) a set of constants determined from laboratory test data in the literature, 4) results of verification computations for a single-element problem and a multi-element problem, have been transitioned to the EPIC's development team at SWRI.

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