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Interfacial effects on fracture nucleation and propagation in crystalline–amorphous energetic material systems

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ABSTRACT

Local failure modes, such as the nucleation and propagation of a pre-existing crack, have been investigated for energetic materials with a viscoelastic binder and crystalline grains subjected to dynamic thermal and mechanical loading conditions. A crystalline plasticity with dislocation density, finite viscoelasticity, dynamic fracture nucleation and propagation methods, and finite element methods were used to study crack nucleation and propagation due to dynamic thermal and mechanical loading conditions. The interrelated effects of dislocation densities, grain boundary (GB) misorientations, polymer binder relaxation, and interactions between crystal and binder were coupled to material thermal decomposition, adiabatic inelastic heating, viscous dissipation heating, and thermal conduction to analyze interfacial fracture behavior in RDX–estane systems. The predictions indicate that cracks propagated toward the binder and were arrested due to the viscous nature of the polymer binder and plasticity buildup. For low angle misorientations, the pre-existing crack propagated toward the binder with increasing crack tip speed until it reaches the binder, at which point the crack was arrested. For high angle misorientations, the crack propagated toward the binder and was arrested, adjacent to the binder, due to plastic deformation and lattice rotations. A secondary crack eventually nucleated and propagated to the interface, where it was arrested.

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1. Introduction

Energetic materials consist of a crystalline solid, encapsulated by a polymer binder [1]. Energetic crystals, at the molecular level, consist of carbon, hydrogen, nitrogen, and oxygen, which internally provide the energy required to sustain deflagration and detonation when the crystal is stimulated to a thermo-mechanically critical level. The defects internal to the crystal, defects in the polymer binder, and heterogeneous nature of energetic materials can localize energy within the aggregate, and upon reaching a critical level of thermo-mechanical stimulation, result in hot spot formation [1–13].

The heterogeneous crystalline-polymer nature and inherent defects can be further affected by complex dynamic loading conditions and inelastic deformations. Dynamic wave propagation and behavior can lead to local failure mechanisms, at the microstructural level, such as void coalescence, crack nucleation, and crack propagation [14–18]. Understanding the mechanisms by which local failure occurs in energetic materials, under dynamic loading conditions, is paramount, due to the material competition between dynamic crack nucleation, propagation, and plastic deformation.

Experimental work by Bouma et al. [15] has shown that energetic RDX crystals contain cracks and voids due to processing. Palmer and Field [16] showed experimentally that under compressive loading of HMX energetic crystals, twinning occurs, and this typically precedes crystal fracture. Sharma et al. [17] has shown that RDX energetic crystals undergo large scale nano-fracturing that breaks up crystals into nano-crystallites with sizes ranging from 20 to 500 nm for dynamic shock loading conditions. Modeling and experimental work by Bouma et al. [14] has also shown, for dynamically deformed energetic materials, that fracture and crystal debonding are major failure mechanisms. Smith and Thorpe [18] showed that fracture in the energetic material, Composition B, occurred by cracking in the RDX phase followed by cracking in the TNT matrix phase. Experimental characterization work by Voevodin and Zabinski [19] has also indicated that dynamic fracture of crystalline–amorphous composites occurs due to cracks nucleating in the crystalline phase, and then terminating at the crystalline–amorphous boundaries. Zhang et al. [20] also demonstrated that in a crystalline Cu and amorphous system that cracks nucleate and propagate in the crystalline phase and

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terminate at the amorphous phase boundary. Wang et al. [21] showed that fracture in a ductile crystalline–amorphous nanolaminate occurs by cracking in the crystalline region where cracks terminate at the amorphous phase boundary. Liu and Ravi-Chandar [22] showed that large amounts of stable crack growth occur before unstable crack growth occurs in highly filled polymeric materials.

Local failure in the heterogeneous crystalline–amorphous structure of energetic materials, the defects that span several spatial scales, and the dynamic thermo-mechanical loading conditions emphasize that a fundamental understanding of how local failure, at the interfaces in energetic materials, evolves is needed. Therefore, the objective of this investigation is to formulate a predictive framework that accounts for the interrelated microstructural effects of crystalline plasticity, polymer binder relaxation, crystalline–amorphous fracture, inherent microstructural defects and features, and dynamic loading conditions on dynamic crack nucleation and growth near the interfaces in energetic materials. A recently developed dislocation-density based crystalline plasticity [23] approach, which has been coupled to a finite viscoelasticity formulation, dynamic fracture formulation, and dynamic finite-element techniques will be used to understand local failure at RDX–estane interfaces. This paper is organized as follows: the dislocation-density based crystalline plasticity, finite viscoelasticity, and specialized dynamic finite-element formulations are outlined in Section 2, the coupling of thermo-mechanical effects is presented in Section 2.4 and the finite-element techniques are presented in Section 2.5. The representation of fracture surfaces and the fracture criterion is presented in Section 3. Results and discussion are presented in Section 4, and salient conclusions are presented in Section 5.

2. Constitutive formulations and thermo-mechanical coupling

In this section, a brief outline of the multiple-slip crystal plasticity rate-dependent constitutive formulation, the derivation of the evolution equations for the mobile and immobile dislocation-densities, which are coupled to the crystalline plasticity formulation, and the constitutive formulation for finite viscoelasticity are presented.

2.1. Multiple-slip dislocation-density based crystal plasticity formulation

The dislocation-density based crystal plasticity constitutive framework used in this study is based on the formulation developed by Zikry [24], Ashmawi and Zikry [25], and Shanthraj and Zikry [26], and a brief outline will be presented here. It is assumed that the velocity gradient is decomposed into a symmetric deformation rate tensor D_{ij} and an anti-symmetric spin tensor W_{ij}. The tensors D_{ij} and W_{ij} can then be additively decomposed into elastic and inelastic components as

$$D_{ij} = D^{*}_{ij} + D^{P}_{ij}, \text{ and } W_{ij} = W^{*}_{ij} + W^{P}_{ij}, \tag{1a-b}$$

The inelastic parts are defined in terms of the crystallographic slip-rates as

$$D^{P}_{ij} = \sum_{\alpha} P^{(\alpha)}_{ij} \dot{\gamma}^{(\alpha)}, \text{ and } W^{P}_{ij} = \sum_{\alpha} \omega^{(\alpha)}_{ij} \dot{\gamma}^{(\alpha)}. \tag{2a-b}$$

where α is summed over all slip-systems, and $P^{(\alpha)}_{ij}$ and $\omega^{(\alpha)}_{ij}$ are the symmetric and anti-symmetric parts of the Schmid tensor in the current configuration respectively. The objective stress rate is given by

$$\sigma^{\Delta}_{ij} = L_{ijkl}(D_{kl} - D^{p}_{kl}) - W^{p}_{ik}\sigma_{kj} - W^{p}_{jk}\sigma_{ki}, \tag{3}$$

where L_{ijkl} is the elastic modulus fourth-order tensor of the crystal.

A power law correlation can be used to describe the rate-dependent deformation for each slip system as

$$\dot{\gamma}^{(\alpha)} = \dot{\gamma}^{(\alpha)}_{ref} \left[\frac{\tau^{(\alpha)}}{\tau^{(\alpha)}_{ref}}\right] \left[\frac{\tau^{(\alpha)}}{\tau^{(\alpha)}_{ref}}\right]^{\frac{1}{m}-1}, \tag{4}$$

where $\tau^{(\alpha)}$ is the resolved shear stress on slip system α, $\dot{\gamma}^{(\alpha)}_{ref}$ is the reference shear strain-rate which corresponds to a reference shear stress $\tau^{(\alpha)}_{ref}$, m is the rate sensitivity parameter. The reference stress, $\tau^{(\alpha)}_{ref}$, is a modification of [27], which relates the reference stress to the immobile dislocation-density ρ_{im} as

$$\tau^{(\alpha)}_{ref} = \left(\tau^{(\alpha)}_{y} + G\sum_{\beta=1}^{nss} b^{(\beta)} \sqrt{a_{\alpha\beta}\rho^{(\beta)}_{im}}\right)\left(\frac{T}{T_0}\right)^{-\xi}, \tag{5}$$

where $\tau^{(\alpha)}_{y}$ is slip system $\alpha's$ static yield stress, G is the shear modulus, $b^{(\beta)}$ is the magnitude of the Burgers vector, nss is the number of total slip systems, and $a_{\alpha\beta}$ are Taylor coefficients which are functions of the interaction strengths between slip systems [28]. T is the temperature, T_0 is the reference temperature, and ξ is the thermal softening exponent.

2.2. Mobile and immobile dislocation density evolution equations

From the derivations of Zikry and Kao [29] it can be assumed that for a given material deformation state, the total dislocation-density, $\rho^{(\alpha)}$, can be additively decomposed into an immobile dislocation-density, $\rho^{(\alpha)}_{im}$, and a mobile, $\rho^{(\alpha)}_{m}$. Additionally, the immobile and mobile dislocation-density rates can be coupled through the destruction and formation of junctions, where the stored immobile dislocations act as obstacles for advancing mobile dislocations. Therefore, the immobile and mobile dislocation density evolutionary nature is taken as

$$\frac{d\rho^{\alpha}_{m}}{dt} = |\dot{\gamma}^{(\alpha)}|\left(\left(\frac{g^{\alpha}_{sour}}{b^{2}}\right)\left(\frac{\rho^{\alpha}_{im}}{\rho^{\alpha}_{m}}\right) - \left(g^{\alpha}_{mnter-}\right)\left(\rho^{\alpha}_{m}\right) - \left(\frac{g^{\alpha}_{immob-}}{b}\right)\sqrt{\rho^{\alpha}_{im}}\right), \tag{6}$$

$$\frac{d\rho^{\alpha}_{im}}{dt} = |\dot{\gamma}^{(\alpha)}|\left(\left(g^{\alpha}_{mnter+}\right)\left(\rho^{\alpha}_{m}\right) + \left(\frac{g^{\alpha}_{immob+}}{b}\right)\sqrt{\rho^{\alpha}_{im}} - \left(g^{\alpha}_{recov}\right)\left(\rho^{\alpha}_{im}\right)\right), \tag{7}$$

where g_{sour} is a coefficient relating to the increase in the mobile dislocation-densities due to dislocation sources, g_{mnter} is a coefficient associated with the pinning of mobile dislocations due to forest intersections, dislocation interactions, or cross-slip around obstacles, g_{recov} is a coefficient pertaining to the annihilation and rearranging of immobile dislocations, and g_{immob} is a coefficient associated with the immobilization of mobile dislocations.

To couple the equations for the evolution of immobile and mobile dislocation densities to the crystalline plasticity constitutive formulation, the non-dimensional coefficients in Eqs. (6) and (7) are evaluated as a function of the microstructural inelastic deformation and crystallographic orientations, by considering the generation, interaction and recovery of dislocation densities as detailed by Shanthraj and Zikry [23]. These equations are given in Table 1, where f_0 and ϕ are geometry parameters, H_0 is the reference activation enthalpy, ρ_s is the saturation density, and the average junction length, l_c, is

$$l_c = \frac{1}{\sum_{\beta}\sqrt{\rho^{(\beta)}_{im}}}. \tag{8}$$

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