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Micro-RVE modeling of mechanistic response in porous intermetallics subject to weak and moderate impact loading

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ABSTRACT

In this article we propose macroscopic (continuum) simulation schemes to predict response of porous heterogeneous material systems subjected to weak and moderate impact velocities. The proposed simulation model includes (1) an equation of state for porous solids that describes the evolution of porosity in the material as a function of shock pressure and, (2) a macroscopic rate dependent plasticity model for the porous composite that accounts for the deviatoric strength of the material at weak to moderate shock strengths. In addition, the numerical scheme employs cold-mixture theory to predict shock response of porous intermetallics. The material model is validated using gas-gun impact experiments on Ni/Al Intermolecular Reactive Composite (IRC) at 70% TMD. The proposed model is also used to understand the effect of microstructure on the material response predictions.

1. Introduction

Intermolecular Reactive Composites (IRCs) are a class of high energy density, structural materials that are capable of self-sustained exothermic reactions when subjected to thermal or mechanical initiation. A unique feature of these systems is the ability to undergo *gasless solid-state* reactions with little to no melting of the bulk material at threshold initiation energies (Reeves et al., 2010; Mukasyan et al., 2011; Manukyan et al., 2012). Due to this property, these materials are also called solid state reactive composites (SSRCs). Manukyan et al. (2012) observed that at impact velocities close to its threshold values (i.e., the minimum impact velocity required to initiate reactions), mechanically activated Ni/Al IRC powder compacts ignite through chemical reactions that occur on a time-scale much longer (on the order of milli-seconds) than the time required to mechanically equilibrate the material system (on the order of micro-seconds). While in recent years there has been a sustained effort to characterize these materials, there has been an evolving need to develop macroscopic models for energetic composites that are amenable to large scale computations. In this work, we propose a generalized continuum framework to model porous, heterogeneous materials that can be used to predict the deformed configuration and the localized stress-fields in the material as it undergoes impact assisted deformation. We envision that the proposed mechanistic model can be subsequently coupled with a suitable reaction model to predict initiation and propagation of chemistry in energetic materials. It has been noted that the distinct properties of porous IRCs are due to (a) spatial heterogeneity (i.e., multiple solid phases and pores) that helps localize energy through pore collapse and plastic deformation of grains to initiate reaction, and (b) an optimized material nano and microstructure with decreased inter-diffusional lengths that is key to sustaining reactions follow-

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ing initiation. In the following paragraphs a review of the methods that has been proposed to model many facets of deformation in porous, heterogenous materials are discussed.

Mechanistically, porous materials are divergent in the manner in which shock energy is distributed and localized within the material relative to their dense (non-porous) counterparts. Porosity in the energetic material acts to localize shock energy into "hot-spots" within the bulk material that could induce a chemical reaction. In particular, shock compression in discrete particle systems undergo the following stages of densification as a function of increasing shock pressure (a) particle rearrangement (b) void collapse and particle deformation, and finally (c) bulk compression of the material system. Due to the complexities involved in modeling fine-scale physics of porous materials, computational schemes such as Eulerian hydrocodes (Benson et al., 1997; Eakins and Thadhani, 2007), discrete particle modeling and direct numerical simulation (Kumar et al., 1999; Barua et al., 2012) are popular choices in studying these materials. While these modeling techniques explicitly resolve the heterogeneities, common disadvantages include (a) the inability to study non-trivial boundary conditions and (b) the computational difficulty in scaling to larger system sizes and time-scales. The alternative is multi-scale modeling of these systems in a macroscopic setting in which the problem studied could be scaled to study longer time-scales (on the order of thermal equilibration of the system) and larger system sizes (on the order of sample sizes). However, the challenges involved in describing the physics of these materials in a macroscopic setting are significantly harder as discussed below.

Shock modeling of solids has been an active area of research since World War II. It has been noted that weak to moderate shock waves widely differ in behavior relative to strong shocks[1] (Germain and Lee, 1973; Wallace, 1980). At moderate shock strengths (i.e. at shock strengths lower than the dynamic yield strength of the material), the deviatoric strength of the solid plays an important part in shock response. It manifests as the classic elastic–plastic two wave structure in the shock response of ductile materials (Germain and Lee, 1973). However, wave propagation in discrete systems differ widely from their dense counterparts. Menikoff (2001) uses direct numerical simulation on powder beds subject to piston driven boundary conditions to study the influence of increasing shock strength on the mechanistic behavior of the powder bed. As expected, the material response at various shock strengths was observed to be strongly correlated to the discreteness of the material system. For weak shock strengths, material porosity does not decrease significantly behind the shock wave and the material system retains its discreteness which leads to attenuated shock waves with the transmitted waves being mostly dispersive.[2] In this phase, the material deforms largely due to particle rearrangement behind the compaction wave with sparse regions of the system beginning to interlock. For moderate input energies widespread particle interlocking leads to particle deformation which, depending on its character leads to material fracture and/or plastic deformation. In this regime, the material exhibits a stress bridging behavior along with a clearly defined two part elastic–plastic wave structure very similar to that in a fully dense material. Further increases in input energy result in a singular shock driven through the system in which dynamic compaction of the material occurs directly behind the shock wave. While it is intractable to include all features of the discrete system in a macroscopic continuum setting, it is still feasible to incorporate the effective behavior of the discrete system into the constitutive model with the choice of an appropriate equation of state (EOS).

Historically, the Mie-Gruneisen EOS (McQueen and Marsh, 1991; Meyers, 1994) has been extensively used to model shock response of solids. Simons and Legner (1982) derived a shock Hugoniot for porous solids in terms of cold pressure, cold energy and density of the porous material. The construction of the EOS follows the isochoric approach (McQueen and Marsh, 1991; Dijken and De Hosson, 1994), wherein the Gruneisen parameter is used to relate the deformation states in a dense solid (with a known pressure) to its porous counterpart (unknown pressure) to derive the shock EOS. The alternate choice to shock modeling in porous materials is the isobaric approach (Wu and Jing, 1996; Mostert and Viljoen, 1999) in which the specific enthalpy is used to derive the shock EOS in the porous solid. Dai et al. (2008) summarizes for nano-sized iron powder compacts either approach showed decreasing accuracy in predicting shock Hugoniot with increasing porosity. In general, either EOS is unable to predict shock Hugoniots for nano-sized powders with large porosities. In modeling multi-component mixtures, McQueen and Marsh (1991) proposed cold-mixture theories to determine shock pressure however in this approach the Gruneisen parameter is considered to be linearly dependent on specific volume, which may not true for all cases (Vocadlo et al., 2000). Zhang et al. (2011) derives shock EOS for porous intermetallic mixtures using a combination of the isobaric and isochoric approaches in addition to a non-linear relation between Gruneisen parameter and specific volume. Reding (2009) suggests as part of a multi-scale modeling strategy, two iterative techniques to determine shock pressure in multi-component porous energetic materials.

As discussed above, the discrete-system dynamics is characterized by its porosity at weak to moderate impact velocities. The empirical $p-\alpha$[3] model suggested by Herrmann (1969) is a widely used approach in compaction modeling of porous materials. The $p-\lambda$[4] model (Grady et al., 2000) is a generalization of $p-\alpha$ to treat mixtures with multiple-phases (such as void space filled with air/moisture). Micromechanics based RVE approaches have also been suggested to model pore collapse. Carroll and Holt (1972) derive static and dynamic pore collapse relations for an elastic-perfectly plastic spherical RVE model undergoing axi-symetric reduction in volume under the influence of an external pressure field. Tong and Ravichandran (1993) extended the Caroll and Holt model to study the effect of microinertia related to dynamic pore collapse in rate dependent viscoplastic

[1] In this paper, strong shocks refer to the pressure singularity that travels with velocity much larger than the bulk velocity of the solid material.
[2] It should be noted that in this scenario, the *shock* wave is primarily a dispersed pressure wave.
[3] α is the inverse solid volume fraction of the porous material.
[4] λ is the fraction of each phase in a multi-phase mixture.