A coupled phase field shear band model for Ductile-Brittle transition in notched plate impacts

Colin McAuliffe* Haim Waisman

*Department of Civil Engineering and Engineering Mechanics, Columbia University;
610 Seeley W. Mudd Building; 500 West 120th Street, Mail Code 4709; New York,
NY 10027*

Abstract

Well known experiments of projectile impacts on pre-notched plates have demonstrated a transition from brittle to ductile failure with increasing strain rate. At low rates cracks form at the notch tip and propagate at roughly 70 degrees counter clockwise from the loading direction. At high rates shear bands form and propagate in a downward curving path. This occurs because of the formation of shear bands, which occurs more readily at the higher velocities, prevents the development of the large principal strains needed to initiate a crack.

In this paper, we present a coupled model that is capable of capturing the failure transition. The finite deformation model consists of a thermoviscoplastic material with strain and strain rate hardening, thermal softening and diffusive regularization. Fracture is modeled with the phase field method, for which a novel modification is presented to account for degradation of the material due to inelastic working.

The numerical model including the discretization and linearization and monolithic scheme is presented and discussed in details. Numerical simulations of the notched plate impact problem studied by (Zhou et al., 1996b) are presented up to the point of shear band or fracture initiation, demonstrating the transition from brittle fracture under minor yielding to ductile failure by shear banding.

1 Introduction

Metals subjected to high strain rates may fail due to shear banding or fracture or a combination of both. Shear banding is a localization phenomenon where thermal softening leads to narrow zones of intense inelastic deformation (Wright, 2002). While a shear band typically precedes

* Corresponding author: cjm2176@columbia.edu (Colin McAuliffe)

fracture, it is also considered a failure mode in its own right, since the thermal softening leads to profound and rapid loss of load carrying capability, (Arriaga et al., 2015; Bai, 1982; Fressengeas and Molinari, 1987; Ling and Belytschko, 2009).

A ductile - brittle failure transition has been observed in the impact of notched plates by (Kalthoff, 2000; Kalthoff and Winkler, 1987; Zhou et al., 1996b). It was found that failure by shear banding occurred above a critical impact velocity, while brittle fracture resulted from lower impact velocities. Shear bands require significantly more energy to propagate than cracks do, and so this result means at some point, slightly increasing the impact velocity will cause the plate to dissipate a great deal more of the impact energy. Understanding the physics of this transition is extremely important for designing energy absorbing materials, where shear banding failure is clearly preferred. Of course, the rate of the impact loading is not under the control of the designer, but understanding the transition may provide insight into how to design systems at the component or material level which effectively dissipate energy under impact.

An early numerical study on the ductile - brittle transition modeled shear banding with a thermoviscoplastic model, and cleavage fracture by the attainment of a critical principal stress over a specified region (Needleman and Tvergaard, 1995). It was concluded that at higher impact velocities, the rapid formation of a shear band at the notch tip shielded the upper portion of the notch from developing the necessary principal strain to cause cleavage. Later work by the same authors (Needleman and Tvergaard, 2000) built upon this by accounting for ductile void growth and coalescence, with the same general trend observed regarding the mechanics of the transition. Additional studies on the effects of material parameters and notch tip geometry were studied by (Batra and Gummalla, 2000), and in (Li et al., 2002), meshfree methods were used to model the full shear band path instead of stopping shortly after shear band initiation.

In this paper the combined thermal softening shear banding and phase field fracture model developed in (McAuliffe and Waisman, 2015b) is employed to study the failure transition in notched plate impacts. The shear band model consists of an hyperelastic - viscoplastic, strain hardening, strain rate hardening, and thermally softening material. Thermal diffusion is accounted for, which weakly defines a length scale and regularizes the problem. This type of model and diffusive regularization have been studied in references (Batra and Lear, 2005; Batra, 1987; Batra and Chen, 2001; Batra and Kim, 1990, 1991; McAuliffe and Waisman, 2013, 2014; Wright and Walter, 1987). Fracture is accounted for with the phase field method, which is a regularized Griffith type (Griffith, 1921) fracture model based on energy minimization (Bourdin et al., 2008b; Francfort and Marigo, 1998b; Miehe et al., 2010b,d). The crack is approximated as a continuous entity, whose width is defined by a small process zone parameter. It is thus possible to approximate the fracture energy with a volume integral, which does not require a procedure for tracking the crack surface. It has been shown in (Bourdin et al., 2008b; Francfort and Marigo, 1998b) that in the limit as the process zone parameter tends to zero, the phase field approximation to the fracture energy converges to that of the discontinuous crack. Phase field models have been extended to account for dynamic brittle fracture in references (Borden et al., 2012; Bourdin et al., 2010), and inelasticity with phase field has been studied in (Borden, 2012; Crosby and Ghoniem, 2012; Duda et al., 2015).

Growth of cracks in the phase field models cited above is driven by the elastic free energy. As shown in the analysis by (Duda et al., 2015), once inelasticity is introduced, crack initiation in the phase field model may be delayed to very large strains depending on the value of the yield stress, the hardening modulus, and the critical fracture stress. This occurs because inelastic straining does not increase the elastic free energy, and thus the growth of the driving term for the crack is slower than it would be in the purely elastic case. An additional source term for crack growth due to the evolution of inelastic internal variables was introduced in (McAuliffe and Waisman, 2015b), meaning that some portion of the inelastic work will contribute to the growth and propagation of fracture surfaces.

The model is presented and discretized in the following section, and a monolithic solution procedure is outlined for its numerical solution. Numerical studies are conducted for the notched plate impact problem from (Zhou et al., 1996b), over a range of impact velocities, and the transition from fracture to shear banding behavior is observed. This work builds upon the work of (McAuliffe and Waisman, 2015b) where the theoretical foundations of the model used here were developed, but experimental validation was limited. An important feature considered here that was not considered in the numerical simulations of (McAuliffe and Waisman, 2015b) is the role that hyperelasticity plays in tendency of a material to fail by shear banding or fracture. In the context of the present model, the hyperelastic law used here increases the tendency to shear band (McAuliffe and Waisman, 2015a), while simultaneously decreasing the tendency to fracture (see the appendix). The simulated transition velocity matches well with experiments, demonstrating the predictive capability of the modeling framework.

2 Strong Form of the Governing Equations

The basic kinematic quantities and inelastic constitutive relations that are used in this work are defined in this section.

2.1 Kinematics

A multiplicative decomposition of the deformation gradient $\mathbf{F}$ is assumed (see also Figure 1) so that

$$F_{iA} = F_{ia}^e F_{aq}^t F_{qA}^p \quad (1)$$

Where elastic deformations are included in $\mathbf{F}^e$, thermal deformations in $\mathbf{F}^t$ and irreversible, inelastic deformations are in $\mathbf{F}^p$. The determinant of the deformation gradient describes the local volume change, and is often called the Jacobian

$$J = \det(\mathbf{F}) = \det(\mathbf{F}^e) \det(\mathbf{F}^t) \det(\mathbf{F}^p) = J^e J^t J^p \quad (2)$$

In this work, isochoric metal plasticity is assumed so that $J^p = 1$. With the multiplicative split,

the velocity gradient $\mathbf{l}$, which is defined as

$$l_{ij} = \dot{F}_{iA} F_{Aj}^{-1} \quad (3)$$

can thus be expanded as

$$l_{ij} = \dot{F}_{ia}^e F_{aj}^{e,-1} + F_{ia}^e \dot{F}_{aq}^t F_{qb}^{t,-1} F_{bj}^{e,-1} + F_{ia}^e F_{aq}^t \dot{F}_{qA}^p F_{Ar}^{p,-1} F_{rb}^{t,-1} F_{bj}^{e,-1} \quad (4)$$

This can be viewed as an additive split of the velocity gradient, where the first term on the right hand side of (4) is the elastic part of $\mathbf{l}$, the second term is the thermal part and the third is the inelastic part, i.e.

$$l_{ij}^e = \dot{F}_{ia}^e F_{aj}^{e,-1} \quad (5)$$

$$l_{ij}^t = F_{ia}^e \dot{F}_{aq}^t F_{qb}^{t,-1} F_{bj}^{e,-1} \quad (6)$$

$$l_{ij}^p = F_{ia}^e F_{aq}^t \dot{F}_{qA}^p F_{Ar}^{p,-1} F_{rb}^{t,-1} F_{bj}^{e,-1} \quad (7)$$

Isotropic thermal expansion is considered, allowing for simplification of the thermal and inelastic velocity gradients in equations (6) and (7). The thermal deformation gradient and its time derivative are

$$F_{iq}^t = \aleph(T) \delta_{iq} \quad (8)$$

$$\dot{F}_{iq}^t = \frac{\partial \aleph}{\partial T} \dot{T} \delta_{iq} \quad (9)$$

Where $\aleph(T)$ is the thermal stretch (Lubarda, 2004). Then the quantity $\dot{F}_{aq}^t F_{qb}^{t,-1} = \alpha \dot{T} \delta_{ab}$ where the coefficient of thermal expansion is given by $\alpha = \frac{1}{\aleph} \frac{\partial \aleph}{\partial T}$. The thermal and plastic velocity gradients are now

$$l_{ij}^t = \alpha \dot{T} \delta_{ij} \quad (10)$$

$$l_{ij}^p = F_{iq}^e \dot{F}_{qA}^p F_{Ar}^{p,-1} F_{rj}^{e,-1} \quad (11)$$

and the total deformation gradient becomes

$$F_{iA} = \aleph F_{iq}^e F_{qA}^p \quad (12)$$

The symmetric part of the velocity gradient is known as the rate of deformation $\mathbf{d}$, namely

$$d_{ij} = \text{sym}(l_{ij}) = \frac{1}{2} (l_{ij} + l_{ji}) \quad (13)$$

This can also be decomposed additively into elastic, thermal, and plastic parts as follows

$$d_{ij}^e = \frac{1}{2} \left(\dot{F}_{ia}^e F_{aj}^{e,-1} + \dot{F}_{ja}^e F_{ai}^{e,-1} \right) \quad (14)$$

$$d_{ij}^t = \alpha \dot{T} \delta_{ij} \quad (15)$$

$$d_{ij}^p = \frac{1}{2} \left(F_{iq}^e \hat{l}_{qr}^p F_{rj}^{e,-1} + F_{jq}^e \hat{l}_{qr}^p F_{ri}^{e,-1} \right) \quad (16)$$

where the plastic velocity gradient with respect to the intermediate configuration $\hat{\mathbf{l}}^p$ is given by

$$\hat{l}_{qr}^p = \dot{F}_{qA}^p F_{Ar}^{p,-1} \quad (17)$$

This tensor will be fully specified later, where the inelastic constitutive relations are defined. Once specified, the elastic rate of deformation $\mathbf{d}^e$ can be defined in terms of the total, thermal and plastic rates of deformation as follows

$$d_{ij}^e = d_{ij} - d_{ij}^p - d_{ij}^t \quad (18)$$

For the hyperelastic material law used in the following sections, the primary kinematic quantity is the elastic left Cauchy Green tensor $\mathbf{b}^e$. This is

$$b_{ij}^e = F_{iq}^e F_{jq}^e \quad (19)$$

The elastic deformation gradient can be found by solving (12) and is given by

$$F_{iq}^e = \frac{1}{\aleph} F_{iA} F_{Aq}^{p,-1} \quad (20)$$

Substituting this into (19) along with the definition of the thermal deformation gradient given by (8) gives

$$b_{ij}^e = F_{iA} C_{AB}^{tp,-1} F_{jB} \quad (21)$$

where

$$C_{AB}^{tp,-1} = \frac{1}{\aleph^2} F_{Aq}^{p,-1} F_{Bq}^{p,-1} \quad (22)$$

This is the inverse of the thermal-plastic right Cauchy Green tensor.

It can be shown, that the rate equation for $\mathbf{b}^e$, which is needed to incrementally update this tensor in the numerical implementation, can be written as (McAuliffe and Waisman, 2015a)

$$-\frac{1}{2} \mathcal{L}_v b_{il}^e = \left(d_{ik}^p + d_{ik}^t \right) b_{kl}^e \quad (23)$$

Lastly, since the hyperelastic model is based on the logarithms of the principal stretches, a spectral decomposition of $\mathbf{b}^e$ is required. This is

$$\mathbf{b}^e = \sum_{A=1}^3 \epsilon_A^e{}^2 p_A \otimes p_A \quad (24)$$

Where the eigenvalues of $\mathbf{b}^e$ are the squares of the principal stretches ϵ_A^e , and p_A are the eigenvectors of $\mathbf{b}^e$. The left elastic stretch tensor $\mathbf{v}^e$ is then

$$\mathbf{v}^e = \sum_{A=1}^3 \epsilon_A^e p_A \otimes p_A \quad (25)$$

and the logarithmic elastic $\mathbf{v}^e$ strain is

$$\mathbf{v}^e = \ln(\mathbf{v}^e) = \sum_{A=1}^3 \ln(\epsilon_A^e) p_A \otimes p_A \quad (26)$$

Since $J^e = \epsilon_1^e \epsilon_2^e \epsilon_3^e$ then we can write

$$\ln(J^e) = \ln(\epsilon_1^e \epsilon_2^e \epsilon_3^e) \quad (27)$$

$$= \ln(\epsilon_1^e) + \ln(\epsilon_2^e) + \ln(\epsilon_3^e) \quad (28)$$

$$= v_{kk}^e \quad (29)$$

and therefore, the logarithm of the elastic Jacobian is the trace of the logarithmic elastic strain.

2.2 Elastic Constitutive Relations

A hyperelastic constitutive law based on the logarithms of the stretch is employed. This has been shown to be a reasonable law up to moderate elastic stretches for metals and polymers (Anand, 1979), and has been used in numerical computations for elastoplasticity by (Auricchio and Taylor, 1999; Caminero et al., 2011; Weber and Anand, 1990). The elastic part of the free energy is

$$\psi^e = \frac{\lambda}{2} v_{kk}^{e,2} + \mu v_{ij}^e v_{ij}^e \quad (30)$$

Where λ and μ are Lamé's parameters. The Kirchhoff stress is then given by

$$\tau_{ij} = \lambda v_{kk}^e \delta_{ij} + 2\mu v_{ij}^e \quad (31)$$

Conceptually, this law may be thought of as a generalization of linear elasticity to the finite deformation regime, with $\mathbf{v}^e$ replacing the elastic small strain tensor.

Increases in the phase field parameter c will lead to degradation of the material's ability to store elastic energy, and thus bear force. To account for cracking in tension only, we introduce a

splitting of the elastic free energy as follows

$$\psi^e = W^- + m(c) W^+ \quad (32)$$

$$W^- = \frac{\lambda}{2} \langle v_{kk}^e \rangle_-^2 + \mu v_{ij}^{e,-} v_{ij}^{e,-} \quad (33)$$

$$W^+ = \frac{\lambda}{2} \langle v_{kk}^e \rangle_+^2 + \mu v_{ij}^{e,+} v_{ij}^{e,+} \quad (34)$$

The tensile and compressive parts of $\mathbf{v}^e$ are defined by

$$\mathbf{v}^{e,-} = \sum_{A=1}^3 \langle \ln(\epsilon_A^e) \rangle_- p_A \otimes p_A \quad (35)$$

$$\mathbf{v}^{e,+} = \sum_{A=1}^3 \langle \ln(\epsilon_A^e) \rangle_+ p_A \otimes p_A \quad (36)$$

The positive and negative Macauley brackets are defined by

$$\langle x \rangle_+ = \begin{cases} 0, & \text{if } x \leq 0 \\ x, & \text{if } x > 0 \end{cases} \quad (37)$$

and

$$\langle x \rangle_- = \begin{cases} x, & \text{if } x \leq 0 \\ 0, & \text{if } x > 0 \end{cases} \quad (38)$$

Accounting for material degradation due to cracking, the Kirchhoff stress is then given by

$$\tau_{ij} = \tau_{ij}^- + m(c) \tau_{ij}^+ \quad (39)$$

$$\tau_{ij}^- = \lambda \langle v_{kk}^e \rangle_- \delta_{ij} + 2\mu v_{ij}^{e,-} \quad (40)$$

$$\tau_{ij}^+ = \lambda \langle v_{kk}^e \rangle_+ \delta_{ij} + 2\mu v_{ij}^{e,+} \quad (41)$$

The small strain counterpart of this splitting of the free energy based on the principal strains has been used to model fracture in elastic materials by (Borden, 2012; Miehe et al., 2010b,d), and for elastic-plastic materials by (Duda et al., 2015). This hyperelastic law is convenient since it is a straightforward generalization of the linearized theory and lends itself easily to the principal strain based split used for small deformations. Other hyperelastic models for metals, such as the neo-Hookean model, could also be used with this type of splitting after being recast in terms of the principal stretches. An important difference between the linear elastic form and the logarithmic form used here is that the log form will have a slower rate of increase of the free energy as the strain increases, resulting in a weaker driving term for fracture for a given amount of deformation than the linear elastic case. See the appendix for more details. The consequences of this effect of hyperelasticity on fracture have been studied in molecular dynamics simulations by (Buehler and Gao, 2006; Buehler et al., 2003). Further discussion of the use of the phase field method for hyperelastic materials with application to rubber elasticity may be found in (Miehe and Schänzel, 2014).

2.3 Inelastic Constitutive Relations

The equivalent plastic strain $\bar{\gamma}^p$ evolves according to the following equation

$$\dot{\bar{\gamma}}^p = \sqrt{\frac{2}{3} d_{ij}^p d_{ij}^p} \quad (42)$$

To specify $\mathbf{l}^p$ and hence $\mathbf{d}^p$, first the symmetric part of $\hat{\mathbf{l}}^p$ is denoted by $\hat{\mathbf{d}}^p$ and defined as (Lubarda, 2004; Miehe, 1994; Simo and Miehe, 1992)

$$\hat{d}_{qr}^p = \frac{1}{2} (\hat{l}_{qr}^p + \hat{l}_{rq}^p) = g(\bar{\sigma}, T, \bar{\gamma}^p) \hat{n}_{qs} C_{sr}^e \quad (43)$$

Where $g(\bar{\sigma}, T, \bar{\gamma}^p)$ is a constitutive function with units of strain rate and $\hat{n}_{qs}$ is the direction of plastic flow with respect to the intermediate configuration. The kinematic decomposition given by (1) only defines the intermediate configuration up to a rigid body rotation. However, rigid body rotations on the intermediate configuration have no effect upon the elastic constitutive laws used here. Thus the antisymmetric part of $\hat{\mathbf{l}}^p$ can be chosen arbitrarily, as long as all other constitutive equations are consistent with this choice (Dafalias, 1998). For convenience, the so called spinless configuration is chosen so that $\hat{l}_{qr}^p = \hat{l}_{rq}^p$, and thus plugging (43) into (11) gives

$$l_{ij}^p = g(\bar{\sigma}, T, \bar{\gamma}^p) F_{iq}^e \hat{n}_{qs} C_{sr}^e F_{rj}^{e,-1} \quad (44)$$

$$= g(\bar{\sigma}, T, \bar{\gamma}^p) n_{ij} \quad (45)$$

Where the plastic flow direction with respect to the current configuration is $n_{ij} = \hat{n}_{qr} F_{iq}^e F_{jr}^e$ is defined as

$$n_{ij} = \frac{3s_{ij}}{2\bar{\sigma}} \quad (46)$$

where $s_{ij} = \sigma_{ij} - \frac{1}{3}\sigma_{kk}\delta_{ij}$ is the deviatoric Cauchy stress and $\bar{\sigma} = \sqrt{\frac{3}{2}s_{ij}s_{ij}}$ is the effective Cauchy stress. Since $\mathbf{n}$ is symmetric, then $\hat{\mathbf{l}}^p = \hat{\mathbf{d}}^p$ and

$$d_{ij}^p = g(\bar{\sigma}, T, \bar{\gamma}^p) n_{ij} \quad (47)$$

Using (46) and (45) in (42) gives

$$\dot{\bar{\gamma}}^p = g(\bar{\sigma}, T, \bar{\gamma}^p) \quad (48)$$

and thus the constitutive function $g(\bar{\sigma}, T, \bar{\gamma}^p)$ gives the equivalent plastic strain rate as a function of stress, temperature and equivalent plastic strain. The particular form of $g(\bar{\sigma}, T, \bar{\gamma}^p)$ used in this work is phenomenological, and has the form

$$g(\bar{\sigma}, T, \bar{\gamma}^p) = \dot{\gamma}_0 \left[\frac{\bar{\sigma}}{\sigma_0 (1 + \bar{\gamma}^p/\gamma_0)^n} r(T) \right]^m \quad (49)$$

where the thermal softening function $r(T)$ is given by

$$r(T) = \max[r^{exp}(T), r^{tanh}(T)] \quad (50)$$

$$r^{exp}(T) = 1 - \delta \left[\exp\left(\frac{T - T_0}{k}\right) - 1 \right] \quad (51)$$

$$r^{tanh}(T) = 1 - \tanh[k_{ab}(T - T_0)] \quad (52)$$

$$k_{ab} = \frac{\ln(2)}{k \left[\ln\left(\frac{1+\delta}{\delta}\right) (1 + \delta) - 1 \right]} \quad (53)$$

The exponential form r^{exp} was introduced by (Zhou et al., 1996a) for modeling c300 steel. However, this model was criticized by (Areias and Belytschko, 2006, 2007), who pointed out that $r^{exp} = 0$ at temperatures well below the material's melting point. Further, beyond this critical temperature, r^{exp} becomes negative, and thus does not represent a physically reasonable material response. As an alternative, these authors suggested the hyperbolic tangent form r^{tanh} , which approaches zero asymptotically. While this form alleviates the aforementioned deficiencies of r^{exp} , we have found that r^{tanh} leads to too much loss of strength at low temperatures. Therefore, we use a composite of the two where r^{exp} is used at low temperature and r^{tanh} is used at high temperatures. Phenomenological models with qualitatively similar behavior may be found in (Bodner and Partom, 1975; Johnson and Cook, 1985; Khan and Huang, 1992; Khan and Liang, 1999; Zerilli and Armstrong, 1987).

2.4 Governing Equations

In this section the strong form of the governing equations are presented and described briefly. Full details of the derivation of these equations may be found in (McAuliffe and Waisman, 2015b). First, the momentum balance is given by

$$\rho_0 \ddot{u}_i = \tau_{ij,j} \quad (54)$$

where ρ_0 is the initial density of the material, u_i are the displacements and $\boldsymbol{\tau}$ is the Kirchhoff stress tensor defined as $J\boldsymbol{\sigma}$. Body forces are not considered in this work. The energy balance is

$$\rho_0 \bar{c} \dot{T} = \kappa J T_{,jj} + \chi \bar{\tau} g(\bar{\sigma}, T, \bar{\gamma}^p) \quad (55)$$

Where the specific heat is $\bar{c}$, the thermal conductivity is κ , and the Taylor Quinney fraction, which determines the fraction of inelastic work converted to heat, is χ . The inelastic work per unit undeformed volume is given by $\bar{\tau} g(\bar{\sigma}, T, \bar{\gamma}^p)$, where the effective Kirchhoff stress is $\bar{\tau} = J\bar{\sigma}$. The governing equation for the evolution of the phase field parameter c , which may be interpreted as a microforce balance equation is

$$c = 4l_0^2 c_{,II} - \frac{2l_0}{\mathcal{G}_c} \frac{\partial m}{\partial c} (W^+ + P^+) \quad (56)$$

W^+ was defined previously in (34), and represents the contribution of the elastic free energy to fracture. The term P^+ accounts for damage resulting from inelastic work and was introduced in (McAuliffe and Waisman, 2015b). One possible definition for P^+ is

$$P^+ = \int_0^t (1 - \chi) \bar{\sigma} g(\bar{\sigma}, T, \bar{\gamma}^p) dt' \quad (57)$$

Thus, some portion of the total inelastic work determined by the value of χ will be converted to heat while the remainder generate and propagate fracture surfaces. This partition is in general dependent on several factors such as strain, strain rate, and temperature. However, as an approximation, we assume χ is constant, resulting in a constant partition of the inelastic work into heat and damage, resulting in P^+ being related to the accumulated inelastic work.

The full set of coupled shear band and phase field equations that define the strong form to be solved becomes

$$\text{Conservation of Macro Momentum:} \quad \rho_0 \ddot{u}_i = \tau_{ij,j} \quad (58)$$

$$\text{Conservation of Energy:} \quad \rho_0 \hat{c} \dot{T} = \kappa J T_{,jj} + \chi \bar{\tau} g(\bar{\sigma}, T, \bar{\gamma}^p) \quad (59)$$

$$\text{Conservation of Micro Momentum:} \quad c = 4l_0^2 c_{,II} - \frac{2l_0}{\mathcal{G}_c} \frac{\partial m}{\partial c} (W^+ + P^+) \quad (60)$$

$$\text{Elastic Constitutive Equation:} \quad \tau_{ij} = \tau_{ij}^- + m(c) \tau_{ij}^+ \quad (61)$$

$$\text{Inelastic Constitutive Equation:} \quad \dot{\bar{\gamma}}^p = g(\bar{\sigma}, T, \bar{\gamma}^p) \quad (62)$$

$$\text{Flow Rule:} \quad \mathcal{L}_v b_{il}^e = -2 \left(d_{ik}^p + d_{ik}^t \right) b_{kl}^e \quad (63)$$

with the boundary conditions

$$\begin{aligned} u &= \bar{u} \quad \text{on } \Gamma^u \\ T &= \bar{T} \quad \text{on } \Gamma^T \\ n_i \sigma_{ij} &= \bar{t}_j \quad \text{on } \Gamma^t \\ n_i q_i &= \bar{q} \quad \text{on } \Gamma^q \end{aligned} \quad (64)$$

and initial conditions for an undamaged and unloaded initial state

$$u_i(t=0) = u_i^0 \quad (65)$$

$$T(t=0) = T^0 \quad (66)$$

$$c(t=0) = 0 \quad (67)$$

$$\tau_{ij}(t=0) = 0 \quad (68)$$

$$\bar{\gamma}^p(t=0) = 0 \quad (69)$$

$$b_{ij}^e(t=0) = \delta_{ij} \quad (70)$$

3 The Numerical Formulation

In this section we detail the discretization and linearization of weak form residual equations that arise from the strong form set (58)-(63), the choice of shape functions and the monolithic solver employed.

3.1 The Discrete Model

3.1.1 The Discrete Residual

The weak form is obtained by multiplying the macro-momentum equation, micro-momentum equation, energy equation, elastic constitutive equation, and inelastic constitutive relation by the weight functions w^u , w^c , w^T , w^σ , and $w^{\bar{\gamma}^p}$ respectively, and integrating over the problem domain in the initial configuration. This defines the weak form of the residual $\mathbf{R} = \begin{bmatrix} R^u & R^c & R^T & R^\sigma & R^{\bar{\gamma}^p} \end{bmatrix}^T$ where

$$R^u = \int_{\Omega_0} [w_i^u \rho_0 \ddot{u}_i + w_{i,j}^u \tau_{ij}] d\Omega_0 - \int_{\Gamma_0^T} w_i^u \bar{T}_i d\Gamma_0^T = 0 \quad (71)$$

$$R^c = \int_{\Omega_0} w^c \left[c + \frac{2l_0}{\mathcal{G}_c} \frac{\partial m}{\partial c} (W^+ + P^+) \right] + 4l_0^2 w_{,I}^c c_{,I} d\Omega_0 = 0 \quad (72)$$

$$R^T = \int_{\Omega_0} \left\{ w^T [\rho_0 \dot{\bar{c}}T - \chi \bar{\tau} g(\bar{\sigma}, T, \bar{\gamma}^p)] + \kappa J w_{,j}^T T_{,j} \right\} d\Omega_0 - \int_{\Gamma_0^q} \kappa w^T \bar{q} d\Gamma_0^q = 0 \quad (73)$$

$$R^\sigma = \int_{\Omega_0} w_{ij}^\sigma [\tau_{ij} - \tau_{ij}^- - m(c) \tau_{ij}^+] d\Omega_0 = 0 \quad (74)$$

$$R^{\bar{\gamma}^p} = \int_{\Omega_0} w^{\bar{\gamma}^p} [\dot{\gamma}^p - g(\bar{\sigma}, T, \bar{\gamma}^p)] d\Omega_0 = 0 \quad (75)$$

Note that integration by parts has been used where appropriate. Also bold letters are used indicate a matrix or a vector and a bold face uppercase $\mathbf{T}$ indicates the transpose operation, not to be confused with plain uppercase T which indicates temperature. This weak form contains spatial derivatives of displacement, phase field, and temperature, and therefore these three fields must be approximated by C^0 functions. On the other hand, spatial derivatives of the equivalent plastic strain and the stresses do not appear and thus C^{-1} functions will suffice. Thus, with these minimum continuity requirements in mind, we seek to find $u \in S_u, c \in S_c, T \in S_T, \sigma \in C^{-1}$, and $\bar{\gamma}^p \in C^{-1}$ such that at any time t

$$R = 0, \quad \forall w^u \in S_u^0, \quad \forall w^c \in S_c^0, \quad \forall w^{\bar{\gamma}^p} \in S_T^0, \quad \forall w^\sigma \in C^{-1}, \quad \forall w^{\gamma^p} \in C^{-1} \quad (76)$$

Where

$$S_u = \{u(X, t) | u \in C^0, u = \bar{u} \text{ on } \Gamma^u\} \quad S_u^0 = \{w^u(X) | w^u \in C^0, w^u = 0 \text{ on } \Gamma^u\} \quad (77)$$

$$S_c = \{c(X, t) | c \in C^0\} \quad S_u^0 = \{w^c(X) | w^c \in C^0\} \quad (78)$$

$$S_T = \{T(X, t) | T \in C^0, T = \bar{T} \text{ on } \Gamma^T\} \quad S_T^0 = \{w^T(X) | w^T \in C^0, w^T = 0 \text{ on } \Gamma^T\} \quad (79)$$

The weak form is discretized in time using Newmark's method for the momentum equation with integration parameters $\mathcal{B}$ and $\mathcal{G}$.

The backward Euler method is used for the remaining equations. The trapezoidal rule has not been used because for certain regimes of mesh size and time step for diffusion problems, this method can result in oscillations in the temperature field, which is undesirable for this problem due to the nonlinear coupling of temperature to other fields.

The time discrete residual at time $n+1$ is then ${}_{n+1}\mathbf{R} = \left[{}_{n+1}R^u \quad {}_{n+1}R^c \quad {}_{n+1}R^T \quad {}_{n+1}R^\sigma \quad {}_{n+1}R^{\bar{\gamma}^p} \right]^T$. Note, for the rest of this paper, quantities to the right of an equal sign shall be assumed to be evaluated at time step $n+1$ unless otherwise noted by a left subscript.

The time stepping procedure results in the following semi discrete residuals

$$R^u = \int_{\Omega_0} \left[w_i^u \frac{\rho_0}{\beta \Delta t^2} [u_i - \tilde{u}_i] + w_{i,j}^u \tau_{ij} \right] d\Omega_0 - \int_{\Gamma_0^T} w_i^u \bar{T}_i d\Gamma_0^T \quad (80)$$

$$R^c = \int_{\Omega_0} w^c \left[c + \frac{2l_0}{\mathcal{G}_c} \frac{\partial m}{\partial c} (W^+ + P^+) \right] + 4l_0^2 w_{,I}^c c_{,I} d\Omega_0 \quad (81)$$

$$R^T = \int_{\Omega_0} w^T \left[\frac{\rho_0 \hat{c}}{\Delta t} (T - {}_n T) - \chi \bar{\tau} g(\bar{\sigma}, T, \bar{\gamma}^p) + \kappa J w_{,j}^T T_{,j} \right] d\Omega_0 \quad (82)$$

$$- \int_{\Gamma_0^Q} \kappa w^T \bar{Q} d\Gamma_0^Q$$

$$R^\sigma = \int_{\Omega_0} w_{ij}^\sigma [\tau_{ij} - \tau_{ij}^- - m(c) \tau_{ij}^+] d\Omega_0 \quad (83)$$

$$R^{\bar{\gamma}^p} = \int_{\Omega_0} w^{\bar{\gamma}^p} \left[\frac{1}{\Delta t} (\bar{\gamma}^p - {}_n \bar{\gamma}^p) - g(\bar{\sigma}, T, \bar{\gamma}^p) \right] d\Omega_0 \quad (84)$$

Where $\bar{T}_i$ and $\bar{Q}$ are the prescribed traction and heat flux on the reference configuration. The momentum equation uses a second order time stepping procedure where

$$\tilde{u}_i = {}_n u_i + \Delta t \quad {}_n v_i + \frac{\Delta t^2}{2} (1 - 2\mathcal{B}) \quad {}_n a_i \quad (85)$$

$\mathbf{b}^e$ is stored as a history variable and is updated with the backward Euler method. Details may

be found in (McAuliffe and Waisman, 2015a), and the final result is

$$b_{ij}^e = \theta \left[\tilde{b}_{ij}^e - \frac{2}{3} \theta \Delta t g(\bar{\sigma}, T, \bar{\gamma}^p) n_{ij} \tilde{b}_{kk}^e \right] \quad (86)$$

where the thermal expansion contribution is captured by $\theta = \frac{1}{1+2\Delta t \alpha_{n+1} \bar{T}}$. Secondly, $\tilde{\mathbf{b}}^e$ is ${}_n \mathbf{b}^e$ at time step n , pushed to the current configuration at time step $n+1$ by the incremental deformation gradient $f_{ij} = F_{iA} {}_n F_{Aj}^{-1}$, i.e.

$$\tilde{b}_{ij}^e = f_{jl} f_{ik} {}_n b_{kl}^e \quad (87)$$

For a single element, let the Galerkin approximation be

$$u_i = N_{i\alpha}^u \hat{u}_\alpha \quad w_i^u = N_{i\alpha}^u \hat{w}_\alpha^u \quad (88)$$

$$c = N_\alpha^c \hat{c}_\alpha \quad w^c = N_\alpha^c \hat{w}_\alpha^c \quad (89)$$

$$T = N_\alpha^T \hat{T}_\alpha \quad w^T = N_\alpha^T \hat{w}_\alpha^T \quad (90)$$

$$\sigma_{ij} = N_{ij\alpha}^\sigma \hat{\sigma}_\alpha \quad w_{ij}^\sigma = N_{ij\alpha}^\sigma \hat{w}_\alpha^\sigma \quad (91)$$

$$\bar{\gamma}^p = N_\alpha^{\bar{\gamma}^p} \hat{\gamma}_\alpha^p \quad w^{\bar{\gamma}^p} = N_\alpha^{\bar{\gamma}^p} \hat{w}_\alpha^{\bar{\gamma}^p} \quad (92)$$

Where $\mathbf{N}$ is a tensor containing the appropriate shape functions. Note the number of indices for $\mathbf{N}$ depends on whether the field is a scalar, vector, or tensor. The subscript α is always associated with the number of degrees of freedom, the range of which depends on the field in question and its associated shape functions. The hatted field variables are to be understood as vectors of degrees of freedom belonging to one element. Substitution of the Galerkin approximation into the time discrete residual, Eqs. (80)- (84), leads to the fully discrete residual, which forms a set of coupled nonlinear algebraic equations:

$$\hat{\mathbf{R}}_\alpha^u = \mathbf{M}_{\alpha\beta}^u (\hat{u}_\beta - \tilde{u}_\beta) + \mathbf{f}_\beta^{u \text{ int}} - \mathbf{f}_\beta^{u \text{ ext}} = 0 \quad (93)$$

$$\hat{\mathbf{R}}_\alpha^c = \mathbf{M}_{\alpha\beta}^c \hat{c}_\beta + \mathbf{f}_\beta^{c \text{ int}} = 0 \quad (94)$$

$$\hat{\mathbf{R}}_\alpha^T = \mathbf{M}_{\alpha\beta}^T (\hat{T}_\beta - {}_n \hat{T}_\beta) + (\mathbf{f}_\beta^{T \text{ int}} - \mathbf{f}_\beta^{T \text{ ext}}) = 0 \quad (95)$$

$$\hat{\mathbf{R}}_\alpha^\sigma = \mathbf{M}_{\alpha\beta}^\sigma \hat{\sigma}_\beta + \mathbf{f}_\beta^\sigma = 0 \quad (96)$$

$$\hat{\mathbf{R}}_\alpha^{\bar{\gamma}^p} = \mathbf{M}_{\alpha\beta}^{\bar{\gamma}^p} (\hat{\gamma}_\beta^p - {}_n \hat{\gamma}_\beta^p) + \mathbf{f}_\beta^{\bar{\gamma}^p} = 0 \quad (97)$$

All matrices $\mathbf{M}$ are mass matrices. Linearization of (93) - (97) is presented in the next section.

3.1.2 Consistent Linearization

A consistent linearization of the PDE system can be obtained in one of two ways. The first is by differentiating the time discrete (but spatially continuous) residual (80) - (84), and substituting the Galerkin approximation into the result. The second method is to differentiate the fully discrete residual (93) - (97). In this study, the former method is used, however, either method could

be used to linearize the system without the need for numerical differentiation. The linearized system can be written in a partitioned form, at nonlinear iteration k and time step $n+1$, as

$$\begin{bmatrix} J_i^{uu} & J_i^{uc} & J_i^{uT} & J_{ij}^{u\sigma} & J_i^{u\bar{\gamma}^p} \\ J_i^{cu} & J^{cc} & J^{cT} & J_{ij}^{c\sigma} & J^{c\bar{\gamma}^p} \\ J_i^{Tu} & J^{Tc} & J^{TT} & J_{ij}^{T\sigma} & J^{T\bar{\gamma}^p} \\ J_i^{\sigma u} & J^{\sigma c} & J^{\sigma T} & J_{ij}^{\sigma\sigma} & J^{\sigma\bar{\gamma}^p} \\ J_i^{\bar{\gamma}^p u} & J^{\bar{\gamma}^p c} & J^{\bar{\gamma}^p T} & J_{ij}^{\bar{\gamma}^p\sigma} & J^{\bar{\gamma}^p\bar{\gamma}^p} \end{bmatrix}^k \begin{bmatrix} \delta u_i \\ \delta c \\ \delta T \\ \delta \sigma_{ij} \\ \delta \bar{\gamma}^p \end{bmatrix} + \begin{bmatrix} R^u \\ R^c \\ R^T \\ R^\sigma \\ R^{\bar{\gamma}^p} \end{bmatrix}^k = \mathbf{0} \quad (98)$$

The Galerkin approximation of the Newton correction is also needed. This is

$$\delta u_i = N_{i\alpha}^u \delta \hat{u}_\alpha \quad \delta c = N_\alpha^c \delta \hat{c}_\alpha \quad \delta T = N_\alpha^T \delta \hat{T}_\alpha \quad \delta \sigma_{ij} = N_{ij\alpha}^\sigma \delta \hat{\sigma}_\alpha \quad \delta \bar{\gamma}^p = N_\alpha^{\bar{\gamma}^p} \delta \hat{\gamma}_\alpha^p \quad (99)$$

The product of the Jacobian $\mathbf{J}$ and the Newton correction $\delta \mathbf{p}$ is the first variation of $\mathbf{R}$ in the direction of $\delta \mathbf{p}$, where $\mathbf{p} = [u_i \ c \ T \ \sigma_{ij} \ \bar{\gamma}^p]^T$. This is also known as the Gateaux derivative and is defined as

$$\mathbf{J} \delta \mathbf{p} = \delta \mathbf{R} [\mathbf{p}^k] = \lim_{\epsilon \rightarrow 0} \frac{1}{\epsilon} \left(\mathbf{R} [\mathbf{p}^k + \epsilon \delta \mathbf{p}] - \mathbf{R} [\mathbf{p}^k] \right) = \frac{d}{d\epsilon} \mathbf{R} [\mathbf{p}^k + \epsilon \delta \mathbf{p}] \Big|_{\epsilon=0} \quad (100)$$

This derivative can be computed analytically without numerical differentiation in blocks, and subsequently the Galerkin approximation can be introduced, leading to the fully discrete Jacobian. The resulting fully discrete linearized system is then

$$\begin{bmatrix} \mathbf{M}_{\alpha\beta}^u + \mathbf{L}_{\alpha\beta}^u & \mathbf{0} & \mathbf{0} & \mathbf{K}_{\alpha\beta}^u & \mathbf{0} \\ \mathbf{W}_{\alpha\beta}^{cu} & \mathbf{M}_{\alpha\beta}^c + \mathbf{K}_{\alpha\beta}^c + \mathbf{C}_{\alpha\beta}^c & \mathbf{G}_{\alpha\beta}^{cT} & \mathbf{G}_{\alpha\beta}^{c\sigma} & \mathbf{G}_{\alpha\beta}^{c\bar{\gamma}^p} \\ \mathbf{L}_{\alpha\beta}^T & \mathbf{0} & \mathbf{M}_{\alpha\beta}^T + \mathbf{K}_{\alpha\beta}^T + \mathbf{G}_{\alpha\beta}^{TT} & \mathbf{G}_{\alpha\beta}^{T\sigma} & \mathbf{G}_{\alpha\beta}^{T\bar{\gamma}^p} \\ \mathbf{H}_{\alpha\beta}^\sigma + \mathbf{L}_{\alpha\beta}^\sigma & \mathbf{C}_{\alpha\beta}^{\sigma c} & \mathbf{G}_{\alpha\beta}^{\sigma T} & \mathbf{M}_{\alpha\beta}^\sigma + \mathbf{S}_{\alpha\beta}^\sigma + \mathbf{G}_{\alpha\beta}^{\sigma\sigma} & \mathbf{G}_{\alpha\beta}^{\sigma\bar{\gamma}^p} \\ \mathbf{0} & \mathbf{0} & \mathbf{G}_{\alpha\beta}^{\bar{\gamma}^p\sigma} & \mathbf{G}_{\alpha\beta}^{\bar{\gamma}^p T} & \mathbf{M}_{\alpha\beta}^{\bar{\gamma}^p} + \mathbf{G}_{\alpha\beta}^{\bar{\gamma}^p\bar{\gamma}^p} \end{bmatrix}^k \begin{bmatrix} \delta \hat{u}_\beta \\ \delta \hat{c}_\beta \\ \delta \hat{T}_\beta \\ \delta \hat{\sigma}_\beta \\ \delta \hat{\gamma}_\beta^p \end{bmatrix} + \begin{bmatrix} \mathbf{R}_\alpha^u \\ \mathbf{R}_\alpha^c \\ \mathbf{R}_\alpha^T \\ \mathbf{R}_\alpha^\sigma \\ \mathbf{R}_\alpha^{\bar{\gamma}^p} \end{bmatrix}^k = \mathbf{0} \quad (101)$$

$\mathbf{M}$ denotes mass matrices, $\mathbf{K}$ stiffness matrices arising from linear material behavior such as the Laplacian terms in the energy and micro-momentum equations, $\mathbf{G}$ matrices arising from the derivatives of the flow law $g(\bar{\sigma}, T, \bar{\gamma}^p)$. Note that $g(\bar{\sigma}, T, \bar{\gamma}^p)$ appears not only in the inelastic constitutive relations and the heating term in the energy equation, but also in P^+ and, due to the dependence of $\mathbf{b}^e$ on $g(\bar{\sigma}, T, \bar{\gamma}^p)$, in the elasticity equation and in W^+ . $\mathbf{L}$ matrices arising from nonlinear geometric behavior which arise due to the dependence of the deformation gradient, its inverse, and its determinant on the displacement, $\mathbf{C}$ arise from derivatives of the degradation function $m(c)$. $\mathbf{W}$ matrices are due to linearizing W^+ with respect to displacement. Lastly, $\mathbf{H}$ is due to linearizing the hyperelastic material law defining the stress. The structure of the Jacobian reflects the strongly coupled nature of the system of PDEs, and does not reveal any clear way to simplify or reduce the system by eliminating any of the five fields in $\mathbf{p}$. Note that the Jacobian is not symmetric.

3.2 Shape Functions

The preceding formulation has been presented as a general mixed formulation which permits the use of a monolithic thermo-mechanical solver. Choice of shape functions should be made carefully taking into consideration the continuity requirements in equations (77) and (79), and the Babuška-Brezzi conditions (Babuška, 1971; Brezzi, 1974). Additionally, careful choice of shape functions can be used to develop a locking free formulation, an important feature for simulating large, nearly incompressible deformations, as is the case with shear bands. The simplest choice is identical interpolation to an irreducible element, but retains the fully monolithic thermo-mechanical solver. For a four node quad this is done by choosing bilinear shape functions for u , c , and T , and the following shape functions for equivalent plastic strain and each stress component

$$N_i(\xi_1^j, \xi_2^j) = \delta_{ij} \quad i, j = 1, 2, 3, 4 \quad (102)$$

Where ξ_1, ξ_2 are the isoparametric coordinates, and (ξ_1^j, ξ_2^j) are the typical gauss quadrature points. Note that in this case the history variables are sampled at the gauss points. Thus in the linearized system (101), the Newton corrections for stresses and equivalent plastic strains $\delta\hat{\sigma}$ and $\delta\hat{\gamma}^p$ are vectors containing stress and equivalent plastic strains at the gauss points. However, in contrast with typical implementations of a four noded quad, where history variables are updated locally on the gauss points, here the updates are done on the global level by solving for all gauss points at once. For more details of this type of interpolation in the context of plasticity, see (Comi and Perego, 1995)

Note that a local constitutive update at the gauss points requires either freezing of some combination of the fields u , c , and T , or freezing the terms involving spacial derivatives, for example the thermal diffusion term. Therefore, there is no guarantee that utilizing a nonlinear solution procedure at the gauss points to update the constitutive variables will accelerate the convergence of system. On the other hand, simultaneously updating the constitutive variables with the rest of the system, as is done in (101) leads to fast convergence.

The global linear system (101) can be efficiently solved by taking advantage of the structure of the jacobian, which arises from the shape functions (102). To outline the procedure, first the system is partitioned into four blocks, where the C^0 and C^{-1} fields are collected together so that the original linear system

$$\begin{bmatrix} J_i^{uu} & J_i^{uc} & J_i^{uT} & J_{ij}^{u\sigma} & J_{ij}^{u\bar{\gamma}^p} \\ J_i^{cu} & J_i^{cc} & J_i^{cT} & J_{ij}^{c\sigma} & J_{ij}^{c\bar{\gamma}^p} \\ J_i^{Tu} & J_i^{Tc} & J_i^{TT} & J_{ij}^{T\sigma} & J_{ij}^{T\bar{\gamma}^p} \\ \hline J_i^{\sigma u} & J_i^{\sigma c} & J_i^{\sigma T} & J_{ij}^{\sigma\sigma} & J_{ij}^{\sigma\bar{\gamma}^p} \\ J_i^{\bar{\gamma}^p u} & J_i^{\bar{\gamma}^p c} & J_i^{\bar{\gamma}^p T} & J_{ij}^{\bar{\gamma}^p\sigma} & J_{ij}^{\bar{\gamma}^p\bar{\gamma}^p} \end{bmatrix} \begin{bmatrix} \delta u_i \\ \delta c \\ \delta T \\ \delta\sigma_{ij} \\ \delta\bar{\gamma}^p \end{bmatrix} = - \begin{bmatrix} R^u \\ R^c \\ R^T \\ R^\sigma \\ R^{\bar{\gamma}^p} \end{bmatrix} \quad (103)$$

Becomes

$$\begin{bmatrix} \mathbf{J}_{11} & \mathbf{J}_{12} \\ \mathbf{J}_{21} & \mathbf{J}_{22} \end{bmatrix} \begin{bmatrix} \delta \mathbf{x}_1 \\ \delta \mathbf{x}_2 \end{bmatrix} = - \begin{bmatrix} \mathbf{R}_1 \\ \mathbf{R}_2 \end{bmatrix} \quad (104)$$

This linear system can be solved exactly using the Schur complement approach by solving two linear systems as follows

$$\mathbf{S} \delta \mathbf{x}_1 = - \left(\mathbf{R}_1 - \mathbf{J}_{12} \mathbf{J}_{22}^{-1} \mathbf{R}_2 \right) \quad (105)$$

$$\mathbf{J}_{22} \delta \mathbf{x}_2 = - \mathbf{R}_2 - \mathbf{J}_{21} \delta \mathbf{x}_1 \quad (106)$$

where the Schur complement is defined as

$$\mathbf{S} = \mathbf{J}_{11} - \mathbf{J}_{12} \mathbf{J}_{22}^{-1} \mathbf{J}_{21} \quad (107)$$

Operations involving the inverse of $\mathbf{J}_{22}$ can be done on the element level, where these local contributions are assembled into global matrices or vectors. Thus, the procedure becomes to first assemble the following vectors and matrices

$$\mathbf{S} = \mathcal{A} \left(\mathbf{J}_{11}^e - \mathbf{J}_{12}^e \mathbf{J}_{22}^{e,-1} \mathbf{J}_{21}^e \right) \quad (108)$$

$$\mathbf{R}_1^{mod} = \mathcal{A} \left(\mathbf{R}_1^e - \mathbf{J}_{12}^e \mathbf{J}_{22}^{e,-1} \mathbf{R}_2^e \right) \quad (109)$$

$$\mathbf{J}_{21}^{mod} = \mathcal{A} \left(\mathbf{J}_{22}^{e,-1} \mathbf{J}_{21}^e \right) \quad (110)$$

$$\mathbf{R}_2^{mod} = \mathcal{A} \left(\mathbf{J}_{22}^{e,-1} \mathbf{R}_2^e \right) \quad (111)$$

Where $\mathcal{A}$ is the finite element assembly operator and the superscript e indicates that the matrix is the contribution from a single element. This requires one LU factorization of $\mathbf{J}_{22}^e$ per element, but since this matrix is small and dense, the operations can be performed efficiently with the heavily optimized LAPACK library.

The system is then solved in two steps

$$\mathbf{S} \delta \mathbf{x}_1 = - \mathbf{R}_1^{mod} \quad (112)$$

$$\delta \mathbf{x}_2 = - \mathbf{R}_2^{mod} - \mathbf{J}_{21}^{mod} \delta \mathbf{x}_1 \quad (113)$$

Iterative solvers for the phase-field shear-band model can also be developed, which is an ongoing work. This can lead to very efficient and robust preconditioners as has been developed in (Berger-Vergiat et al., 2015)

4 Numerical Study of Notched Plate Impacts

The above formulation has been used to study impacts on the notched plate problem studied by (Zhou et al., 1996a,b), the problem geometry of this problem may be found in figure 2. Computations were done in the finite element code FEAP version 8.3 (Taylor, 2011), and the results were post processed using Paraview (Henderson, 2012) and Matplotlib (Hunter, 2007). PETSc version 3.4 (Balay et al., 1997, 2014a,b) was used to assemble and solve the global equation system where the sparse direct linear solver UMFPACK (Davis, 2004) was the particular solver chosen. The material parameters were chosen as representative of structural steel, see Table 2. Runs with five different velocities are applied to the plate, from 10 m/s to 30 m/s by increments of 5 m/s . In each run, the applied velocity is ramped from 0 to the final value linearly over $0.5\mu s$.

The formulation described in the previous sections requires a rather fine mesh in the shear band or crack path to be effective. In general, the crack and shear band paths are not known a priori, and therefore some sort of adaptive method is likely needed to keep computational costs reasonable for many practical situations. For the simulations here, we fully refine the area around the notch tip, which is adequate for modeling the initiation of failure, as well as a small amount of shear band or crack propagation.

Surface plot of $\bar{\gamma}^p$ and c for each applied velocity are shown in figures 3 and 4, and the characteristics of the failure mode are summarized in table 1.

At 10 m/s , there is no failure since there is neither enough thermal softening for shear band formation nor tensile stress for crack formation. For 15 m/s and 20 m/s , failure is by fracture, but at 20 m/s there is significant shear localization while there is none at 15 m/s . Finally, at 25 m/s and 30 m/s , shear bands form with very mild amounts of damage accumulation. Essentially, each of the two failure modes are in competition, and whichever one becomes unstable first will dominate. This is the primary motivation for consideration of the hyperelastic law used here, that was not considered in the simulations in (McAuliffe and Waisman, 2015b). In order to accurately model the transition, the two phenomena need to be accurately modeled individually. Since hyperelastic effects clearly play a role in both fracture and shear banding, it is important that they be considered. The dominance of one mode vs the other can be observed in Figure 5, where the maximum value of the c is plotted against the maximum value of the temperature at the notch tip. Fast temperature growth is accompanied by relatively slow damage accumulation. On the other hand, the flat portions of the green and red curves, which represent the formation of an unstable crack, are accompanied by almost no temperature growth whatsoever. This figure shows that the formulation is capable of capturing the failure transition within a single model.

It is instructive to examine the various energy quantities in the system. Since the plate is mostly elastic and undamaged everywhere except the notch tip, we consider a portion of the domain Θ , over which the energy quantities will be integrated. See figure 6. At time 0, this subdomain is given by a circle centered at (0.0508 m , 0.11315 m) with radius of 0.001016 m , which includes the notch tip and the surrounding material. Throughout the simulation, Θ deforms with the

mesh. The subdomain integrated stress power $\dot{\mathcal{M}}$ is defined by

$$\dot{\mathcal{M}} = \int_{\Theta} \sigma_{ij} d_{ij} d\Theta \quad (114)$$

where Θ is the deformed notch tip subdomain. This power quantity can be split with the additive decomposition of $\mathbf{d}$ into elastic, inelastic and thermal contributions as follows

$$\dot{\mathcal{M}}^e = \int_{\Theta} \sigma_{ij} d_{ij}^e d\Theta \quad (115)$$

$$\dot{\mathcal{M}}^p = \int_{\Theta} \sigma_{ij} d_{ij}^p d\Theta \quad (116)$$

$$\dot{\mathcal{M}}^t = \int_{\Theta} \sigma_{ij} d_{ij}^t d\Theta \quad (117)$$

Integrating the power in time gives the total mechanical work $\mathcal{M}$, which is again split into elastic, inelastic and thermal parts $\mathcal{M}^e$, $\mathcal{M}^p$, and $\mathcal{M}^t$ respectively. Note, that $\mathcal{M}^e$ is simply the elastic part of the free energy, and $\mathcal{M}^p$ represents the irreversible work that the material dissipates by deforming inelastically. The phase field approximation to the fracture energy, which represents the energy change in the system due to growth of c , is defined as (Bourdin et al., 2008a; Francfort and Marigo, 1998a; Miehe et al., 2010a,c)

$$\mathcal{S} = \int_{\Theta} \mathcal{G}_c \left[\frac{c^2}{4l_0} + l_0 c_{,I} c_{,I} \right] d\Theta \quad (118)$$

The integrand of this expression is the work done by the internal micro force K and its conjugate variable c , as well as the work done by the micro traction H_I and its conjugate variable $c_{,I}$. (McAuliffe and Waisman, 2015b) Therefore, while $\mathcal{M}$ is the work done by the macro stresses, $\mathcal{S}$ may be interpreted as the work done by the micro forces, i.e.

$$\mathcal{S} = \int_{\Theta} Kc + H_I c_{,I} d\Theta \quad (119)$$

This work is irreversible, since we have enforced the condition $\dot{c} > 0$. Thus, the total irreversible part of the work is due the inelasticity and fracture, i.e. $\mathcal{M}^p + \mathcal{S}$, while $\mathcal{M}^e$ and $\mathcal{M}^t$ are reversible. The irreversible and reversible parts of the work are shown in figure 7, where it is found that the most significant contributions to the mechanical work are due to irreversible sources. Breaking down the irreversible sources of work in figure 8 shows that the majority of the dissipated work is due to inelasticity. In fact, unless a crack forms and becomes unstable, the surface energy is insignificant.

For the cases where the failure is by fracture, there is some buildup of plastic deformation at the notch tip, but once initiated, the crack propagates with negligible inelastic deformation at roughly 77.7° . This is demonstrated in Figure 9, which shows the phase field and equivalent plastic strain distributions along the crack path at several different times. Further, Figure 10 shows that after initiation, the elastic deformation is dominated by a single tensile stretch.

From this we can surmise that, excepting the inelastic deformation that occurs at the notch pre initiation, the cracks propagate in a brittle, mode I fashion.

5 Conclusion

The formulation developed in (McAuliffe and Waisman, 2015b) was used to simulate notched plate impact experiments at several impact velocities. The model consists of thermo-visco-hyperelastic-plastic model coupled to the phase field method for fracture. This work builds upon (McAuliffe and Waisman, 2015b), where the simulations conducted did not consider finite deformations and hyperelastic effects. The hyperelastic model considered here increases the tendency for shear banding while decreasing the tendency for fracture. Since the two failure modes are in competition, in the sense that the first mode to become unstable will dominate the behavior, accurate prediction of the failure transition relies on accurate modeling of each mode. The transition of the initial failure at the notch from brittle fracture to ductile shear band failure occurs between impact velocities of 20 and 25 m/s , which is in line with experimental observations.

Floats

Fig. 1. Multiplicative Split of F per equation (1)

Fig. 2. Single notched plat problem

Table 1
Summary of results

Applied Velocity m/s	Failure Mode	Shear Localization	Max c	Max $\bar{\gamma}^p$
10	None	None	0.30889	0.21172
15	Fracture	None	1.0	0.31179
20	Fracture	Mild	1.0	1.1308
25	Shear Band	Intense	0.28682	1.8325
30	Shear Band	Intense	0.28093	2.0027

Table 2
Material Properties and Parameters

Property Name	Symbol	Value	Unit
Young's Modulus	E	200E9	Pa
Poisson's Ratio	ν	0.3	-
Mass Density	ρ	7830	$\frac{kg}{m^3}$
Specific Heat	c	448	$\frac{J}{kgK}$
Taylor - Quinney Coefficient	χ	0.9	-
Thermal Conductivity	κ	50.0	$\frac{W}{mK}$
Thermal Expansion Coefficient	α	11.0E-6	$\frac{1}{K}$
Reference Strain Rate	$\dot{\gamma}_0$	0.001	$\frac{1}{s}$
Rate Sensitivity Parameter	m	70	-
Yield Stress	σ_0	2000E6	Pa
Yield Strain	γ_0	0.01	-
Strain Hardening Exponent	n	0.01	-
Reference Temperature	T_0	293	K
Thermal Softening Parameter	δ	0.8	-
Thermal Softening Parameter	k	500	K
Phase field process zone parameter	l_0	5.0e-5	m
Critical energy release rate	$\mathcal{G}_c$	2.2E4	$\frac{J}{m^2}$

(a) Phase Field, $v_0 = 10$ m/s

(b) Equivalent Plastic Strain, $v_0 = 10$ m/s

(c) Phase Field, $v_0 = 15$ m/s

(d) Equivalent Plastic Strain, $v_0 = 15$ m/s

Fig. 3. Surface plots of phase field parameter and equivalent plastic strain, showing no failure at an applied impact velocity of $v_0 = 10$ m/s. With an increase of the impact velocity to $v_0 = 15$ m/s, fracture at approximately 77° is observed without any shear band localization.

(a) Phase Field, $v_0 = 20$ m/s

(b) Equivalent Plastic Strain, $v_0 = 20$ m/s

(c) Phase Field, $v_0 = 25$ m/s

(d) Equivalent Plastic Strain, $v_0 = 25$ m/s

Fig. 4. Surface plots of phase field parameter and equivalent plastic strain, showing fracture at approximately 77° and mild shear band localization at the notch tip due to impact velocity of $v_0 = 20$ m/s. With an increase of the impact velocity to $v_0 = 25$ m/s, an intense shear band localization appears without fracture.

Fig. 5. Maximum value of temperature vs maximum value of phase field parameter in the notch tip

Fig. 6. The subdomain Θ , over which work quantities are integrated.

Fig. 7. Dissipative (solid lines) and non dissipative (dashed lines) parts of the mechanical work. The dissipative portion consists of the inelastic work and the fracture energy i.e. $\mathcal{M}^p + \mathcal{S}$, and the reversible portion consists of the elastic work $\mathcal{M}^e$. The thermal part of the work is negligible.

Fig. 8. Breakdown of the irreversible part of the mechanical work, consisting of the inelastic work (solid lines) and the fracture energy (dashed lines).

Fig. 9. Phase field parameter distribution (top) and equivalent plastic strain distribution (bottom) along the crack length at several times during the deformation. While there is some plasticity that develops at the notch tip before unstable crack growth, after the crack initiates plasticity is negligible. The applied velocity is $20m/s$.

(a) Time = 18.02 μs

(b) Time = 25.93 μs

Fig. 10. Principal elastic stretches along the crack length, indicating that the deformation in the crack is dominated by a single principal stretch, i.e. mode I. The applied velocity is 20m/s.

(a) Extension

(b) Simple Shear

Fig. 11. Fracture contributing free energy for the hyperelastic model and the linearized theory

Acknowledgment

The financial support of the U.S Department of Energy office of Science, through the Early Career Research Program, No. DE-SC-0008196, and the Army Research Office, under grant No. W911NF1310238, is gratefully acknowledged.

References

- Anand, L. On h. hencky's approximate strain-energy function for moderate deformations. *Journal of Applied Mechanics*, 46(1):78–82, Mar. 1979. ISSN 0021-8936. doi: 10.1115/1.3424532.
- Areias, P. M. A. and Belytschko, T. Two-scale shear band evolution by local partition of unity. *International Journal for Numerical Methods in Engineering*, 66(5):878–910, Apr. 2006. ISSN 0029-5981, 1097-0207. doi: 10.1002/nme.1589.
- Areias, P. M. A. and Belytschko, T. Two-scale method for shear bands: thermal effects and variable bandwidth. *International Journal for Numerical Methods in Engineering*, 72(6):658–696, Nov. 2007. ISSN 00295981, 10970207. doi: 10.1002/nme.2028.
- Arriaga, M., McAuliffe, C., and Waisman, H. Onset of shear band localization by a local generalized eigenvalue analysis. *Computer Methods in Applied Mechanics and Engineering*, 289: 179–208, June 2015. ISSN 0045-7825. doi: 10.1016/j.cma.2015.02.010.
- Auricchio, F. and Taylor, R. A return-map algorithm for general associative isotropic elastoplastic materials in large deformation regimes. *International Journal of Plasticity*, 15(12): 1359–1378, Jan. 1999. ISSN 07496419. doi: 10.1016/S0749-6419(99)00044-3.
- Babuška, P. I. Error-bounds for finite element method. *Numerische Mathematik*, 16(4):322–333, Jan. 1971. ISSN 0029-599X, 0945-3245. doi: 10.1007/BF02165003.
- Bai, Y. L. Thermo-plastic instability in simple shear. *Journal of the Mechanics and Physics of Solids*, 30(4):195–207, Aug. 1982. ISSN 0022-5096. doi: 10.1016/0022-5096(82)90029-1.
- Balay, S., Gropp, W. D., McInnes, L. C., and Smith, B. F. Efficient management of parallelism in object oriented numerical software libraries. In Arge, E., Bruaset, A. M., and Langtangen, H. P., editors, *Modern Software Tools in Scientific Computing*, pages 163–202. Birkhäuser Press, 1997.
- Balay, S., Abhyankar, S., Adams, M. F., Brown, J., Brune, P., Buschelman, K., Eijkhout, V., Gropp, W. D., Kaushik, D., Knepley, M. G., McInnes, L. C., Rupp, K., Smith, B. F., and Zhang, H. PETSc users manual. Technical Report ANL-95/11 - Revision 3.5, Argonne National Laboratory, 2014a.
- Balay, S., Abhyankar, S., Adams, M. F., Brown, J., Brune, P., Buschelman, K., Eijkhout, V., Gropp, W. D., Kaushik, D., Knepley, M. G., McInnes, L. C., Rupp, K., Smith, B. F., and Zhang, H. PETSc web page. 2014b.
- Batra, R. and Lear, M. Adiabatic shear banding in plane strain tensile deformations of 11 thermoelastoviscoplastic materials with finite thermal wave speed. *International Journal of Plasticity*, 21(8):1521–1545, Aug. 2005. ISSN 07496419. doi: 10.1016/j.ijplas.2004.07.004.

- 1
- 2
- 3
- 4 Batra, R. C. The initiation and growth of, and the interaction among, adiabatic shear bands
- 5 in simple and dipolar materials. *International Journal of Plasticity*, 3(1):75–89, 1987. ISSN
- 6 0749-6419. doi: 10.1016/0749-6419(87)90019-2.
- 7
- 8 Batra, R. C. and Chen, L. Instability analysis and shear band spacing in
- 9 gradient-dependent thermoviscoplastic materials with finite speeds of thermal waves.
- 10 *Archives of Mechanics*, 53(2):167 – 192, Jan. 2001. ISSN 0373-2029. URL
- 11 <http://am.ippt.pan.pl/am/article/view/v53p167>.
- 12
- 13 Batra, R. C. and Gummalla, R. R. Effect of material and geometric parameters on deformations
- 14 near the notch-tip of a dynamically loaded prenotched plate. *International Journal of Fracture*,
- 15 101(1-2):99–140, Jan. 2000. ISSN 0376-9429, 1573-2673. doi: 10.1023/A:1007504431357.
- 16
- 17 Batra, R. C. and Kim, C. H. Adiabatic shear banding in elastic-viscoplastic nonpolar and
- 18 dipolar materials. *International Journal of Plasticity*, 6(2):127–141, 1990. ISSN 0749-6419.
- 19 doi: 10.1016/0749-6419(90)90018-A.
- 20
- 21 Batra, R. C. and Kim, C. H. Effect of thermal conductivity on the initiation, growth and
- 22 bandwidth of adiabatic shear bands. *International Journal of Engineering Science*, 29(8):
- 23 949–960, 1991. ISSN 0020-7225. doi: 10.1016/0020-7225(91)90168-3.
- 24
- 25 Berger-Vergiat, L., McAuliffe, C., and Waisman, H. Parallel preconditioners for monolithic
- 26 solution of shear bands. Submitted, 2015.
- 27
- 28 Bodner, S. R. and Partom, Y. Constitutive equations for elastic-viscoplastic strain-hardening
- 29 materials. *Journal of Applied Mechanics*, 42(2):385–389, June 1975. ISSN 0021-8936. doi:
- 30 10.1115/1.3423586.
- 31
- 32 Borden, M. J. Isogeometric analysis of phase-field models for dynamic brittle and ductile fracture.
- 33 2012.
- 34
- 35 Borden, M. J., Verhoosel, C. V., Scott, M. A., Hughes, T. J., and Landis, C. M. A phase-
- 36 field description of dynamic brittle fracture. *Computer Methods in Applied Mechanics and*
- 37 *Engineering*, 217:77–95, 2012. doi: 10.1016/j.cma.2012.01.008.
- 38
- 39 Bourdin, B., Francfort, G. A., and Marigo, J.-J. The variational approach to fracture. *Journal*
- 40 *of Elasticity*, 91(1-3):5–148, Apr. 2008a. ISSN 0374-3535, 1573-2681. doi: 10.1007/s10659-007-
- 41 9107-3. URL <http://link.springer.com/article/10.1007/s10659-007-9107-3>.
- 42
- 43 Bourdin, B., Francfort, G. A., and Marigo, J.-J. The variational approach to fracture. *Journal*
- 44 *of Elasticity*, 91(1-3):5–148, Apr. 2008b. ISSN 0374-3535, 1573-2681. doi: 10.1007/s10659-007-
- 45 9107-3.
- 46
- 47 Bourdin, B., Larsen, C. J., and Richardson, C. L. A time-discrete model for dynamic fracture
- 48 based on crack regularization. *International Journal of Fracture*, 168(2):133–143, Nov. 2010.
- 49 ISSN 0376-9429, 1573-2673. doi: 10.1007/s10704-010-9562-x.
- 50
- 51 Brezzi, F. On the existence, uniqueness and approximation of saddle-point problems arising from
- 52 lagrangian multipliers. *ESAIM: Mathematical Modelling and Numerical Analysis - Modélisa-*
- 53 *tion Mathématique et Analyse Numérique*, 8(R2):129–151, 1974. ISSN 0764-583X.
- 54
- 55 Buehler, M. J. and Gao, H. Dynamical fracture instabilities due to local hyperelasticity at crack
- 56 tips. *Nature*, 439(7074):307–310, Jan. 2006. ISSN 0028-0836. doi: 10.1038/nature04408.
- 57
- 58 Buehler, M. J., Abraham, F. F., and Gao, H. Hyperelasticity governs dynamic fracture at a
- 59 critical length scale. *Nature*, 426(6963):141–146, 2003.
- 60
- 61 Caminero, M. Á., Montáns, F. J., and Bathe, K.-J. Modeling large strain anisotropic elasto-
- 62 plasticity with logarithmic strain and stress measures. *Computers & Structures*, 89(11–12):
- 63 826–843, June 2011. ISSN 0045-7949. doi: 10.1016/j.compstruc.2011.02.011.
- 64
- 65

- 1
- 2
- 3
- 4 Comi, C. and Perego, U. A unified approach for variationally consistent finite elements in
- 5 elastoplasticity. *Computer Methods in Applied Mechanics and Engineering*, 121(1-4):323–344,
- 6 Mar. 1995. ISSN 00457825. doi: 10.1016/0045-7825(94)00703-P.
- 7
- 8 Crosby, T. and Ghoniem, N. Phase-field modeling of thermomechanical damage in tungsten
- 9 under severe plasma transients. *Computational Mechanics*, 50(2):159–168, Aug. 2012. ISSN
- 10 0178-7675, 1432-0924. doi: 10.1007/s00466-012-0733-7.
- 11
- 12 Dafalias, Y. F. Plastic spin: necessity or redundancy? *International Journal of Plasticity*, 14(9):
- 13 909–931, Dec. 1998. ISSN 0749-6419. doi: 10.1016/S0749-6419(98)00036-9.
- 14
- 15 Davis, T. A. Algorithm 832: UMFPACK v4.3—an unsymmetric-pattern multifrontal
- 16 method. *ACM Trans. Math. Softw.*, 30(2):196–199, June 2004. ISSN 0098-3500. doi:
- 17 10.1145/992200.992206.
- 18
- 19 Duda, F. P., Ciarbonetti, A., Sánchez, P. J., and Huespe, A. E. A phase-field/gradient damage
- 20 model for brittle fracture in elastic–plastic solids. *International Journal of Plasticity*, 65:269–
- 21 296, Feb. 2015. ISSN 0749-6419. doi: 10.1016/j.ijplas.2014.09.005.
- 22
- 23 Francfort, G. A. and Marigo, J. J. Revisiting brittle fracture as an energy min-
- 24 imization problem. *Journal of the Mechanics and Physics of Solids*, 46(8):1319–
- 25 1342, Aug. 1998a. ISSN 0022-5096. doi: 10.1016/S0022-5096(98)00034-9. URL
- 26 <http://www.sciencedirect.com/science/article/pii/S0022509698000349>.
- 27
- 28 Francfort, G. A. and Marigo, J. J. Revisiting brittle fracture as an energy minimization problem.
- 29 *Journal of the Mechanics and Physics of Solids*, 46(8):1319–1342, Aug. 1998b. ISSN 0022-5096.
- 30 doi: 10.1016/S0022-5096(98)00034-9.
- 31
- 32 Fressengeas, C. and Molinari, A. Instability and localization of plastic flow in shear at high strain
- 33 rates. *Journal of the Mechanics and Physics of Solids*, 35(2):185–211, 1987. ISSN 0022-5096.
- 34 doi: 10.1016/0022-5096(87)90035-4.
- 35
- 36 Griffith, A. A. The phenomena of rupture and flow in solids. *Philosophical Transactions of the*
- 37 *Royal Society A: Mathematical, Physical and Engineering Sciences*, 221(582-593):163–198,
- 38 Jan. 1921. ISSN 1364-503X, 1471-2962. doi: 10.1098/rsta.1921.0006.
- 39
- 40 Henderson, A. *ParaView Guide, A Parallel Visualization Application*, Kitware Inc. 4 edition,
- 41 2012. ISBN 978-1-1930934-24-5.
- 42
- 43 Hunter, J. Matplotlib: A 2d graphics environment. *Computing in Science Engineering*, 9(3):
- 44 90–95, May 2007. ISSN 1521-9615. doi: 10.1109/MCSE.2007.55.
- 45
- 46 Johnson, G. R. and Cook, W. H. Fracture characteristics of three metals subjected to various
- 47 strains, strain rates, temperatures and pressures. *Engineering Fracture Mechanics*, 21(1):31–
- 48 48, 1985. ISSN 0013-7944. doi: 10.1016/0013-7944(85)90052-9.
- 49
- 50 Kalthoff, J. F. Modes of dynamic shear failure in solids. *International Journal of Fracture*, 101
- 51 (1-2):1–31, 2000.
- 52
- 53 Kalthoff, J. F. and Winkler, S. Failure mode transition at high rates of shear loading. In
- 54 Chiem, C., Kunze, H. D., and Meyer, L. W., editors, *Impact Loading and Dynamic Behavior*
- 55 *of Materials*, vol. 1, pages 185–195. DGM Informationsgesellschaft Verlag, 1987.
- 56
- 57 Khan, A. S. and Huang, S. Experimental and theoretical study of mechanical behavior of 1100
- 58 aluminum in the strain rate range 10⁻⁵-10⁴s⁻¹. *International Journal of Plasticity*, 8(4):397–
- 59 424, 1992. ISSN 0749-6419. doi: 10.1016/0749-6419(92)90057-J.
- 60
- 61 Khan, A. S. and Liang, R. Behaviors of three BCC metal over a wide range of strain rates
- 62 and temperatures: experiments and modeling. *International Journal of Plasticity*, 15(10):
- 63 1089–1109, 1999. ISSN 0749-6419. doi: 10.1016/S0749-6419(99)00030-3.
- 64
- 65

- 1
- 2
- 3
- 4 Li, S., Liu, W. K., Rosakis, A. J., Belytschko, T., and Hao, W. Mesh-free galerkin simulations
- 5 of dynamic shear band propagation and failure mode transition. *International Journal of*
- 6 *Solids and Structures*, 39(5):1213–1240, Mar. 2002. ISSN 0020-7683. doi: 10.1016/S0020-
- 7 7683(01)00188-3.
- 8
- 9 Ling, X. and Belytschko, T. Thermal softening induced plastic instability in rate-dependent
- 10 materials. *Journal of the Mechanics and Physics of Solids*, 57(4):788–802, Apr. 2009. ISSN
- 11 00225096. doi: 10.1016/j.jmps.2008.04.010.
- 12
- 13 Lubarda, V. A. Constitutive theories based on the multiplicative decomposition of deformation
- 14 gradient: Thermoelasticity, elastoplasticity, and biomechanics. *Applied Mechanics Reviews*,
- 15 57(2):95, 2004. ISSN 00036900. doi: 10.1115/1.1591000.
- 16
- 17 McAuliffe, C. and Waisman, H. Mesh insensitive formulation for initiation and growth of shear
- 18 bands using mixed finite elements. *Computational Mechanics*, 51(5):807–823, May 2013. ISSN
- 19 0178-7675, 1432-0924. doi: 10.1007/s00466-012-0765-z.
- 20
- 21 McAuliffe, C. and Waisman, H. A pian–sumihara type element for modeling shear bands at
- 22 finite deformation. *Computational Mechanics*, 53(5):925–940, May 2014. ISSN 0178-7675,
- 23 1432-0924. doi: 10.1007/s00466-013-0940-x.
- 24
- 25 McAuliffe, C. and Waisman, H. On the importance of nonlinear elastic effects in shear band
- 26 modelling. *International Journal of Plasticity*, 71:10–31, 2015a.
- 27
- 28 McAuliffe, C. and Waisman, H. A unified model for metal failure capturing shear banding and
- 29 fracture. *International Journal of Plasticity*, 65:131–151, Feb. 2015b. ISSN 0749-6419. doi:
- 30 10.1016/j.ijplas.2014.08.016.
- 31
- 32 Miehe, C. On the representation of prandtl-reuss tensors within the framework of multiplicative
- 33 elastoplasticity. *International Journal of Plasticity*, 10(6):609–621, 1994. ISSN 0749-6419. doi:
- 34 10.1016/0749-6419(94)90025-6.
- 35
- 36 Miehe, C. and Schänzel, L.-M. Phase field modeling of fracture in rubbery polymers. part i:
- 37 Finite elasticity coupled with brittle failure. *Journal of the Mechanics and Physics of Solids*,
- 38 65:93–113, Apr. 2014. ISSN 0022-5096. doi: 10.1016/j.jmps.2013.06.007.
- 39
- 40 Miehe, C., Hofacker, M., and Welschinger, F. A phase field model for rate-
- 41 independent crack propagation: Robust algorithmic implementation based
- 42 on operator splits. *Computer Methods in Applied Mechanics and Engi-*
- 43 *neering*, 199(45):2765–2778, 2010a. doi: 10.1016/j.cma.2010.04.011. URL
- 44 <http://www.sciencedirect.com/science/article/pii/S0045782510001283>.
- 45
- 46 Miehe, C., Hofacker, M., and Welschinger, F. A phase field model for rate-independent
- 47 crack propagation: Robust algorithmic implementation based on operator splits. *Com-*
- 48 *puter Methods in Applied Mechanics and Engineering*, 199(45):2765–2778, 2010b. doi:
- 49 10.1016/j.cma.2010.04.011.
- 50
- 51 Miehe, C., Welschinger, F., and Hofacker, M. Thermodynamically consistent phase-field models
- 52 of fracture: Variational principles and multi-field FE implementations. *International Journal*
- 53 *for Numerical Methods in Engineering*, 83(10):1273–1311, 2010c. doi: 10.1002/nme.2861. URL
- 54 <http://onlinelibrary.wiley.com/doi/10.1002/nme.2861/abstract>.
- 55
- 56 Miehe, C., Welschinger, F., and Hofacker, M. Thermodynamically consistent phase-field models
- 57 of fracture: Variational principles and multi-field FE implementations. *International Journal*
- 58 *for Numerical Methods in Engineering*, 83(10):1273–1311, 2010d. doi: 10.1002/nme.2861.
- 59
- 60 Needleman, A. and Tvergaard, V. Analysis of a brittle-ductile transition under dynamic shear
- 61 loading. *International Journal of Solids and Structures*, 32(17–18):2571–2590, Sept. 1995. ISSN
- 62
- 63
- 64
- 65

- 0020-7683. doi: 10.1016/0020-7683(94)00283-3.
- Needleman, A. and Tvergaard, V. Numerical modeling of the ductile-brittle transition. *International Journal of Fracture*, 101(1-2):73–97, Jan. 2000. ISSN 0376-9429, 1573-2673. doi: 10.1023/A:1007520917244.
- Simo, J. C. and Miehe, C. Associative coupled thermoplasticity at finite strains: formulation, numerical analysis and implementation. *Computer Methods in Applied Mechanics and Engineering*, 98(1):41–104, 1992.
- Taylor, R. L. FEAP—A Finite Element Analysis Program. Univ. of Calif., Berkeley, 2011.
- Weber, G. and Anand, L. Finite deformation constitutive equations and a time integration procedure for isotropic, hyperelastic-viscoplastic solids. *Computer Methods in Applied Mechanics and Engineering*, 79(2):173–202, Mar. 1990. ISSN 0045-7825. doi: 10.1016/0045-7825(90)90131-5.
- Wright, T. W. The physics and mathematics of adiabatic shear bands. Cambridge monographs on mechanics. Cambridge University Press, Cambridge, UK ; New York, 2002. ISBN 0521631955.
- Wright, T. W. and Walter, J. W. On stress collapse in adiabatic shear bands. *Journal of the Mechanics and Physics of Solids*, 35(6):701–720, 1987. ISSN 0022-5096. doi: 10.1016/0022-5096(87)90051-2.
- Zerilli, F. J. and Armstrong, R. W. Dislocation-mechanics-based constitutive relations for material dynamics calculations. *Journal of Applied Physics*, 61(5):1816–1825, Mar. 1987. ISSN 0021-8979, 1089-7550. doi: 10.1063/1.338024.
- Zhou, M., Ravichandran, G., and Rosakis, A. J. Dynamically propagating shear bands in impact-loaded prenotched plates—II. numerical simulations. *Journal of the Mechanics and Physics of Solids*, 44(6):1007–1032, 1996a.
- Zhou, M., Ravichandran, G., and Rosakis, A. J. Dynamically propagating shear bands in impact-loaded prenotched plates—i. experimental investigations of temperature signatures and propagation speed. *Journal of the Mechanics and Physics of Solids*, (6):981–1006, 1996b. ISSN 0022-5096. doi: 10.1016/0022-5096(96)00003-8.

A Effect of the hyperelastic law on the elastic free energy

In this appendix, the differences between the elastic free energy resulting from the logarithmic hyperelastic law and the small strain theory. The logarithmic strains have been defined previously, and the small strain tensor is defined from linearized kinematics, and has the form

$$\epsilon_{ij}^{ss} = \frac{1}{2} (F_{ij} + F_{ji}) - \delta_{ij} \quad (\text{A.1})$$

Consider a tensile deformation given by

$$\mathbf{F} = \begin{bmatrix} 1+k & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad (\text{A.2})$$

Where k is a strain parameter. The principal logarithmic and small strains are

$$\ln(\epsilon_1) = \ln[1+k] \quad \ln(\epsilon_2) = 0 \quad \ln(\epsilon_3) = 0 \quad (\text{A.3})$$

$$\epsilon_1^{ss} = k \quad \epsilon_2^{ss} = 0 \quad \epsilon_3^{ss} = 0 \quad (\text{A.4})$$

the fracture contributing part of the free energy is

$$W^{+,log} = \left(\frac{\lambda}{2} + \mu\right) \ln[1+k]^2, \quad W^{+,ss} = \left(\frac{\lambda}{2} + \mu\right) k^2 \quad (\text{A.5})$$

Consider next a shear deformation given by

$$\mathbf{F} = \begin{bmatrix} 1 & k & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad (\text{A.6})$$

The principal logarithmic and small strains are

$$\ln(\epsilon_1) = \ln \left[\sqrt{1 + \frac{k^2}{2} + \frac{k}{2} \sqrt{4+k^2}} \right] \quad \ln(\epsilon_2) = \ln \left[\sqrt{1 + \frac{k^2}{2} - \frac{k}{2} \sqrt{4+k^2}} \right] \quad \ln(\epsilon_3) = 0 \quad (\text{A.7})$$

$$\epsilon_1^{ss} = \frac{k}{2} \quad \epsilon_2^{ss} = -\frac{k}{2} \quad \epsilon_3^{ss} = 0 \quad (\text{A.8})$$

Once again assuming k is positive, the part of the free energy that contributes to fracture is then

$$W^{+,log} = \mu \ln \left[\sqrt{1 + \frac{k^2}{2} + \frac{k}{2} \sqrt{4+k^2}} \right]^2, \quad W^{+,ss} = \mu \frac{k^2}{4} \quad (\text{A.9})$$

1
2
3
4 W^+ is plotted in figure 11 for these two deformations. The difference between the logarithmic
5 hyperelastic free energy and the free energy from linearized kinematics grows as the strain in-
6 creases, with the particular hyperelastic model used here leads to smaller W^+ for a given value
7 of k . There is not much difference for the shear deformation, but for the tensile deformation
8 significant difference become apparent even at moderate deformations.
9
10
11
12
13
14
15
16
17
18
19
20
21
22
23
24
25
26
27
28
29
30
31
32
33
34
35
36
37
38
39
40
41
42
43
44
45
46
47
48
49
50
51
52
53
54
55
56
57
58
59
60
61
62
63
64
65