A unified model for metal failure capturing shear banding and fracture

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Abstract

Dynamic fracture of metals may be brittle or ductile depending on factors such as material properties, loading rate and specimen geometry. At high strain rates, a thermo plastic instability known as shear banding may occur, which typically precedes fracture.

Experiments on notched plate impact show a ductile - brittle failure transition, where lower impact velocities lead to brittle behavior, while higher impact velocities lead to shear banding. For more complex problems such as armor penetration, both brittle fracture and shear banding have been observed in the same specimen, however, current failure models can either account for fracture or shear banding. For predictive numerical simulations of dynamic failure, it is thus crucial to account for both failure modes, since exclusion of either mode neglects important physics observed in experiments.

In this work a thermodynamically consistent model which accounts for both shear banding and dynamic fracture and can thus capture both failure modes at intermediate strain rates, is presented. The model consists of an elastic-viscoplastic material with strain hardening, strain rate hardening, and thermal softening. Fracture is modeled with the phase field method, for which a novel modification is presented here to account for the creation of fracture surfaces by inelastic work. Numerical examples are presented to illustrate the basic behavior of the model, and to compare it to three special cases: a damage free case, an isothermal case, and an isothermal case where the contribution of inelastic work to fracture is excluded.

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1 Introduction

Metals subjected to high strain rates may become unstable due to shear banding or fracture. 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 fracture, since the thermal softening leads to profound and rapid loss of load carrying capability, the shear band is considered a failure mode in its own right (Bai, 1982; Fressengeas and Molinari, 1987; Ling and Belytschko, 2009).

There are several examples of scenarios where high strain rate failure involves both shear bands and cracks. Shear banding as a precursor to void growth and fracture has been documented in several experimental works such as (Backman and Finnegan, 1973; Dormeal, 1987; Irwin, 1972; Odeshi et al., 2005; Shockey). In addition, a ductile - brittle failure transition has been observed in the impact of notched plates by (Kalthoff, 2000; Kalthoff and Winkler, 1987; Zhou et al., 1996). It was found that failure by shear banding occurred above a critical impact velocity, while brittle fracture resulted from lower impact velocities. A final example is the impact of metal plate with a projectile, where shear bands have been identified propagating parallel to the impact direction, and cracks propagate perpendicular to the impact direction (Nickodemus et al., 2002), and shown schematically in Figure 1. For predictive numerical simulations of dynamic failure, it is thus crucial to account for both failure modes, since exclusion of either mode neglects important physics observed in experiments.

Existing models for ductile fracture include two broad categories, the first of which being empirical or semi empirical criteria based on the experimentally observed effects of variables such as the stress state and the extent of inelastic strain or inelastic work (Bai and Wierzbicki, 2008; Brünig et al., 2008; Khan and Liu, 2012a; Wierzbicki et al., 2005). The stress state variables used in these models are typically related to stress invariants. Examples are the hydrostatic stress, stress triaxiality, Lode angle parameter, and magnitude of the stress vector. This type of criteria has also been modified to incorporate rate and temperature effects (Johnson and Cook, 1985; Khan and Liu, 2012b). In the second category are coupled damage models, which incorporate constitutive relations governing the progressive degradation of material strength through the growth of micro voids or micro cracks. Early examples are the well-known Gurson-Tvergaard-Needleman model for void nucleation, growth, and coalescence (Gurson, 1977; Tvergaard, 1990) and the continuum damage model of Lemaitre (Lemaitre, 1985). More recent models include (Lassance et al., 2007; Lecarme et al., 2011; Shojaei et al., 2013; Xue, 2007). These models account for various sources of micro degradation, which is coupled to the macro response through one or more damage parameters which degrade the overall load carrying capacity of the material leading to failure. Generally speaking, the first category of models are simple to implement in a computational code and to calibrate to experimental data. On the other hand, models of the second type are considered to have a more solid micromechanical basis. Models of both types are discussed further and assessed in the works of (Li et al., 2011; Malcher et al., 2012).

In this paper a combined thermal softening shear banding and phase field fracture model is presented, which falls into the coupled damage model category. The shear band model consists

of an elastic - 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, 1987; Batra and Jin, 1994; Batra and Kim, 1991; Batra and Ravinsankar, 2000; Batra and Zhang, 2004; McAuliffe and Waisman, 2012, 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., 2008; Francfort and Marigo, 1998; Miehe et al., 2010a,b). The crack is approximated as a continuous entity, whose width is defined by a small process zone parameter, see Figure 1. 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., 2000; Francfort and Marigo, 1998) 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., 2011).

Growth of cracks in the phase field models cited above is driven by the elastic free energy. The elastic energy can then be split into portions which contribute to fracture and portions which do not. For example (Borden et al., 2012; Miehe et al., 2010a,b) decompose the strain energy using the principal strains, where only the tensile principal strains contribute to fracture. Inelasticity has been introduced to the phase field model by (Borden, 2012) who combined the phase field model for dynamic fracture with the finite deformation plasticity models in (Simo and Hughes, 1998). In addition, modeling of thermo mechanical damage in tungsten subject to conditions found in a fusion reactor was conducted by (Crosby and Ghoniem, 2012), who combined the phase field model with small deformation plasticity. For an inelastic material, the growth of the elastic free energy will be limited by yielding; in fact the elastic free energy can decrease once thermal softening begins. For metals, where the inelastic response is independent of volumetric deformations, it is conceivable that the elastic free energy due to tensile volumetric deformation will be large enough to initiate a crack. However, the contribution of the extensive inelastic working that occurs during the shear banding process will not be modeled. To remedy this, the model presented here includes an enhancement of the phase field model to account for the contribution of energy of internal inelastic variables to the fracture energy. This leads to the addition of source terms in the phase field evolution equation which are due to inelastic deformation.

An interesting aspect of this enhancement to the phase field model is the partition of the inelastic work into heat and cold work, which is energy stored by defects in the metal's lattice (Bever et al., 1973). In the present model, heat production drives thermal softening and shear bands, while cold work terms along with the elastic energy drives cracks. The partition of the inelastic work is thus significant in determining the eventual mode of failure. Citing the experimental work of (Farren and Taylor, 1925; Taylor and Quinney, 1937), shear band models nearly universally assume that the fraction of inelastic work converted to heat is a constant in the neighborhood of 0.9. This constant is frequently referred to as the Taylor Quinney fraction. However, more recent experiments by (Hodowany et al., 2000; Macdougall, 2000; Mason et al., 1994) have convincingly demonstrated that the fraction of inelastic work converted to heat depends on strain, strain rate and temperature. Furthermore, theoretical objections to constant partition of inelastic work have

been pointed out in (Wright, 2002).

Several studies have been conducted which aim to theoretically or experimentally determine the partition of inelastic work. Early examples are (Aravas et al., 1990), where an expression for the partition is derived from residual stress theory, (Zehnder and Rosakis, 1991). More recently, (Schreyer and Maudlin, 2005) used a dislocation density strain hardening model within a thermodynamic framework similar to the one presented here to model the stored energy. Another approach is that of (Clayton, 2005), calculated the stored energy of cold work from dislocation theory and incorporated this into a crystal plasticity, high rate failure model. A dislocation theory approach was also taken in (Benzerga et al., 2005), who concluded that the stored energy of cold work depends not only on the dislocation density but on the dislocation structure as well. A method for experimental determination of the partition is given in (Rosakis et al., 2000), where the stored energy of cold work as a function of plastic strain for a few metal alloys is calculated from the experiments of (Hodowany et al., 2000). Lastly, (Longere and Dragon, 2007, 2009) calculate the partition from the phenomenological plasticity model employed therein.

Using a rigid plastic model, Wright and Walter (Wright and Walter, 1987) studied the strain to failure of a thermal softening, rate dependent material over several decades of strain rate. This is illustrated here in Figure 3. The failure strain plotted against the strain rate results in a U shape, since thermal diffusion inhibits localization at low strain rates, and inertia inhibits it at high strain rates. This leaves a range of strain rates where thermal softening shear bands occur most readily, which will be referred to in this work as the critical shear band zone (zone 3 in Figure 3). Other zones on the U curve are the diffusion stabilized zone (zone 1 in Figure 3), where no localization occurs, and the two transition zones on either side of the critical shear band zone (zones 2 and 4 in Figure 3). Further studies on the effect of strain rate on shear banding have been conducted by (Fressengeas, 1989; Grady and Kipp, 1987).

In the numerical experiments shown in this study, a constant partition of the inelastic work is assumed, and the failure strain and energy dissipation of a one dimensional model is studied over a wide range of strain rates and values of the Taylor Quinney fraction. **Two dimensional studies of a plate in tension were also conducted to test the capability of the various models to produce different failure directions with changing strain rate.** Significant differences in the failure behavior of the shear band, and combined model are present in all zones except the critical shear band zone. Of particular interest are the transition zones, where differences between the two formulations becomes most important for high rate failure modeling.

2 Proposed Model Derivation

In this section the proposed modeling framework is developed. The combined phase field and shear band model consists of macro and micro force balance equations, the energy balance equation, and the entropy inequality. In addition, elastic and inelastic constitutive relations are needed. A brief review of the requisite kinematics is given before developing the governing equations.

2.1 Kinematics

A multiplicative decomposition of the deformation gradient F_{iA} is assumed (see also Figure 2) so that

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

Where elastic deformations are included in F_{ia}^e , thermal deformations in F_{aq}^t and irreversible, inelastic deformations are in F_{qA}^p . The velocity gradient, which is defined as

$$l_{ij} = \dot{F}_{iA} F_{Aj}^{-1} \quad (2)$$

can thus be expanded as

$$l_{ij} = \dot{F}_{ia}^e F_{aj}^{e,-1} + F_{ia}^e \dot{F}_{aq}^t F_{qb}^{t,-1} F_{bj}^{e,-1} + F_{ia}^e F_{aq}^t \dot{F}_{qA}^p F_{Ar}^{p,-1} F_{rb}^{t,-1} F_{bj}^{e,-1} \quad (3)$$

This can be viewed as an additive split of the velocity gradient, where the first term on the right hand side of (3) is the elastic part of l_{ij} , the second term is the thermal part and the third is the inelastic part, i.e.

$$l_{ij}^e = \dot{F}_{ia}^e F_{aj}^{e,-1} \quad (4)$$

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

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

Isotropic thermal expansion is considered, allowing for simplification of the thermal and inelastic velocity gradients in equations (5) and (6). The thermal deformation gradient and its time derivative are

$$F_{iq}^t = \lambda(T) \delta_{iq} \quad (7)$$

$$\dot{F}_{iq}^t = \frac{\partial \lambda}{\partial T} \dot{T} \delta_{iq} \quad (8)$$

Where $\lambda(T)$ 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 $\alpha = \frac{1}{\lambda} \frac{\partial \lambda}{\partial T}$. The thermal and plastic velocity gradients are now

$$l_{ij}^t = \alpha \dot{T} \delta_{ij} \quad (9)$$

$$l_{ij}^p = F_{iq}^e \dot{F}_{qA}^p F_{Ar}^{p,-1} F_{rj}^{e,-1} \quad (10)$$

The symmetric part of the velocity gradient is called the rate of deformation and is defined so that

$$d_{ij} = \frac{1}{2} (l_{ij} + l_{ji}) \quad (11)$$

Using (3), the elastic rate of deformation is

$$d_{ij}^e = \frac{1}{2} (l_{ij}^e + l_{ji}^e) = \frac{1}{2} (\dot{F}_{ia}^e F_{aj}^{e,-1} + \dot{F}_{ja}^e F_{ai}^{e,-1}) \quad (12)$$

In addition, the elastic Right Cauchy Green tensor is

$$C_{qr}^e = F_{kq}^e F_{kr}^e \quad (13)$$

giving the elastic Green strain as

$$E_{qr}^e = \frac{1}{2} (C_{qr}^e - \delta_{qr}) \quad (14)$$

Differentiating (14) with respect to time gives the rate of Green strain

$$\dot{E}_{qr}^e = \frac{1}{2} (\dot{F}_{kq}^e F_{kr}^e + F_{kq}^e \dot{F}_{kr}^e) \quad (15)$$

Note that the first and second terms of this equation can be written respectively as

$$\dot{F}_{kq}^e F_{kr}^e = F_{iq}^e \dot{F}_{ja}^e F_{ai}^{e,-1} F_{jr}^e = F_{iq}^e l_{ji}^e F_{jr}^e \quad (16)$$

$$F_{kq}^e \dot{F}_{kr}^e = F_{iq}^e \dot{F}_{ia}^e F_{aj}^{e,-1} F_{jr}^e = F_{iq}^e l_{ij}^e F_{jr}^e \quad (17)$$

and thus the elastic deformation rate and the rate of elastic Green strain have the relation

$$\dot{E}_{qr}^e = \frac{1}{2} F_{iq}^e (l_{ji}^e + l_{ij}^e) F_{jr}^e = F_{iq}^e d_{ij}^e F_{jr}^e \quad (18)$$

The inelastic velocity gradient is defined later, as the inelastic constitutive relations are developed.

2.2 Balance laws and entropy inequality

There are three balance laws governing the physical system. They are the macro force balance, the micro force balance, and the energy balance. In addition, the entropy inequality must be satisfied. The macro force balance is

$$\rho_0 \ddot{u}_i = P_{iI,I} + B_i \quad (19)$$

where ρ_0 is the reference density, u_i is the displacement, B_i is the body force per reference volume, and P_{iA} is the first Piola Kirchhoff stress. Cracks, which are characterized by the phase field parameter c , are assumed to evolve under the influence of micro forces (Stumpf and Hackl, 2003), which are governed by the following equation

$$\rho_0 \theta \ddot{c} = H_{I,I} - K + G \quad (20)$$

Here, θ is the micro inertia, which accounts for the local inertia of accelerating material at the crack tip. The external micro force, G , which may be used to model bond breakage due to reactive

materials or internally pressurized cracks. The internal micro force is denoted as K , which is the main driving force of the crack. It will be shown later that K depends on the elastic free energy and, a novel feature of the present model, the stored energy of internal inelastic variables. Lastly, H_I is the micro traction.

The energy balance law is given by

$$\rho_0 \dot{e} = S_{IJ} \dot{E}_{IJ} + K \dot{c} + H_I \dot{c}_{,I} + \rho_0 R - Q_{I,I} \quad (21)$$

where S_{IJ} is the second Piola Kirchhoff stress, $\dot{E}_{IJ}$ is the rate of Green strain, R is the heat supply and Q_I is the heat flux through the reference area.

Lastly the entropy inequality is (Marsden and Hughes, 1993)

$$\rho_0 \dot{\eta} \geq - \left(\frac{Q_I}{T} \right)_{,I} + \rho_0 \frac{R}{T} \quad (22)$$

where η is the specific entropy, and T is the temperature.

The free energy per unit mass is

$$\psi = e - T\eta \quad (23)$$

or in rate form

$$\dot{\psi} = \dot{e} - \dot{T}\eta - T\dot{\eta} \quad (24)$$

Substituting (24) into (22) and using (21) leads to the inequality

$$S_{IJ} \dot{E}_{IJ} + H_I \dot{c}_{,I} + K \dot{c} - \rho_0 (\dot{\psi} + \dot{T}\eta) \geq \frac{Q_I T_{,I}}{T} \quad (25)$$

The term on the right hand side is the dissipation due to heat transfer, while the terms on the left hand side account for the internal energy dissipation per unit reference volume, $\mathcal{D} \geq 0$ so that

$$\mathcal{D} = \tau_{ij} d_{ij} + H_I \dot{c}_{,I} + K \dot{c} - \rho_0 (\dot{\psi} + \dot{T}\eta) \quad (26)$$

where we have used the identity $S_{IJ} \dot{E}_{IJ} = \tau_{ij} d_{ij}$, with τ_{ij} being the Kirchhoff stress. The rate of deformation d_{ij} and conjugate stress measure τ_{ij} are convenient because it permits the use of the additive decomposition in (3). Using (26), along with (24), the energy equation (21) can be written in an alternative form, which will prove to be convenient later

$$\rho_0 T \dot{\eta} = \mathcal{D} - Q_{I,I} + \rho_0 R \quad (27)$$

Using the additive decomposition of d_{ij} in (3), the stress power term in (25) is expanded so that entropy inequality becomes

$$\tau_{ij} d_{ij}^e + \tau_{ij} d_{ij}^t + \tau_{ij} d_{ij}^p + H_I \dot{c}_{,I} + K \dot{c} - \rho_0 (\dot{\psi} + \dot{T}\eta) \geq \frac{Q_I T_{,I}}{T} \quad (28)$$

the elastic part of the stress power, using (18) can alternatively be written as

$$\tau_{ij} d_{ij}^e = \tau_{ij} F_{qi}^{e,-1} F_{rj}^{e,-1} \dot{E}_{qr}^e \quad (29)$$

also, by using (9) and noting that the thermal velocity gradient is symmetric so that $l_{ij}^t = d_{ij}^t$, the thermal part of the stress power can be replaced with

$$\tau_{ij} d_{ij}^t = \tau_{ij} \delta_{ij} \alpha \dot{T} \quad (30)$$

Where α is the coefficient of thermal expansion. Defining the elastic second Piola Kirchhoff stress, which is the second Piola Kirchhoff stress with respect to the elastic configuration, as

$$S_{qr}^e = \tau_{ij} F_{qi}^{e,-1} F_{rj}^{e,-1} \quad (31)$$

Eq. (29) can be written as

$$\tau_{ij} d_{ij}^e = S_{qr}^e \dot{E}_{qr}^e = \frac{1}{2} S_{qr}^e \dot{C}_{qr}^e \quad (32)$$

substituting (32) and (30) into the entropy inequality (28) gives

$$\frac{1}{2} S_{qr}^e \dot{C}_{qr}^e + \tau_{ij} \delta_{ij} \alpha \dot{T} + \tau_{ij} d_{ij}^p + H_I \dot{c}_{,I} + K \dot{c} - \rho_0 (\dot{\psi} + \dot{T} \eta) \geq \frac{Q_I T_{,I}}{T} \quad (33)$$

Now, the free energy is assumed to be a function of elastic right Cauchy Green tensor C_{qr}^e , T , c , $c_{,j}$, and n internal variables ξ_i for $i = 1, n$ so that

$$\psi = \psi(C_{qr}^e, T, c, c_{,j}, \xi_1, \dots, \xi_n) \quad (34)$$

The internal variables quantify microstructural details of the material which affect the mechanical response (Rice, 1971). Common examples of internal variables are dislocation density, isotropic hardening parameter, and back stress (Nemat-Nasser, 2004). The time derivative of the free energy is now

$$\dot{\psi} = (\partial_{C^e} \psi)_{qr} \dot{C}_{qr}^e + \partial_T \psi \dot{T} + \partial_c \psi \dot{c} + \partial_{c_{,I}} \psi \dot{c}_{,I} + \sum_{i=1}^n \Xi_i \dot{\xi}_i \quad (35)$$

Where the $\Xi_i = \partial_{\xi_i} \psi$ are the thermodynamic forces conjugate to the ξ_i . substituting this into (33) gives

$$\begin{aligned} \mathcal{D} &= \left(S_{qr}^e - 2\rho_0 (\partial_{C^e} \psi)_{qr} \right) \dot{C}_{qr}^e + (\tau_{kk} \alpha - \rho_0 \partial_T \psi - \rho_0 \eta) \dot{T} \\ &\quad + (K - \rho_0 \partial_c \psi) \dot{c} + \left(H_I - \rho_0 \partial_{c_{,I}} \psi \right) \dot{c}_{,I} + \tau_{ij} d_{ij}^p - \rho_0 \sum_{i=1}^n \Xi_i \dot{\xi}_i \\ &\geq \frac{Q_I T_{,I}}{T} \end{aligned} \quad (36)$$

The above inequality must hold for an arbitrary thermodynamic process, which is to say that $\dot{C}_{qr}^e$, $\dot{T}$, $\dot{c}$, $\dot{c}_{,I}$ can assume arbitrary values. It is assumed that the internal microforce K depends on $K^*(C_{IJ}, \dot{C}_{IJ}, c, \dot{c}, c_{,I}, T)$, a function accounting for dissipation. These considerations impose the following conditions:

$$S_{qr}^e = 2\rho_0 (\partial_{C^e} \psi)_{qr} \quad (37)$$

$$H_I = \rho_0 \partial_{c_{,I}} \psi \quad (38)$$

$$\eta = \tau_{kk} \frac{\alpha}{\rho_0} - \partial_T \psi = \Pi - \partial_T \psi \quad (39)$$

and

$$K = K^* \left(C_{IJ}, \dot{C}_{IJ}, c, \dot{c}, c_{,I}, T \right) + \rho_0 \partial_c \psi \quad (40)$$

The internal dissipation is now

$$\mathcal{D} = \mathcal{D}^p + \mathcal{D}^f \geq \frac{Q_I T_{,I}}{T} \quad (41)$$

$$\mathcal{D}^p = \tau_{ij} d_{ij}^p - \rho_0 \sum_{i=1}^n \Xi_i \dot{\xi}_i \geq 0 \quad (42)$$

$$\mathcal{D}^f = K^* \dot{c} \geq 0 \quad (43)$$

Where $\mathcal{D}^p$ and $\mathcal{D}^f$ are the contributions to the internal dissipation from inelasticity and fracture respectively. The inelastic dissipation is thus interpreted as the inelastic stress power less the rate of energy stored by changing internal variables. In light of (39), the rate of entropy production can be expanded using the chain rule

$$\dot{\eta} = \partial_T \Pi \dot{T} - \left[(\partial_{TC^e} \psi)_{qr} \dot{C}_{qr}^e + \partial_{TT} \psi \dot{T} + \partial_{Tc} \psi \dot{c} + \partial_{Tc_{,I}} \psi \dot{c}_{,I} + \sum_{i=1}^n \partial_T \Xi_i \dot{\xi}_i \right] \quad (44)$$

substitution of (41) and (44) into the energy equation (27) leads to

$$\begin{aligned} \rho_0 T (\partial_T \Pi - \partial_{TT} \psi) \dot{T} &= \rho_0 T (\partial_{TC^e} \psi)_{qr} \dot{C}_{qr}^e + \tau_{ij} d_{ij}^p - \rho_0 \sum_{i=1}^n (\Xi_i - T \partial_T \Xi_i) \dot{\xi}_i \\ &\quad + \rho_0 T \partial_T H_I \dot{c}_I + \rho_0 T \partial_T K \dot{c} + K^* \dot{c} \\ &\quad - Q_{I,I} + \rho_0 R \end{aligned} \quad (45)$$

We let the specific heat be a constant, defined as

$$\hat{c} = \frac{\partial e}{\partial T} = \frac{\partial e}{\partial \eta} \frac{\partial \eta}{\partial T} = T \left(\frac{\partial \Pi}{\partial T} - \frac{\partial^2 \psi}{\partial T^2} \right) = \text{constant} \quad (46)$$

The energy equation can thus be written as

$$\begin{aligned} \rho_0 \hat{c} \dot{T} &= \rho_0 T (\partial_{TC^e} \psi)_{qr} \dot{C}_{qr}^e + \tau_{ij} d_{ij}^p - \rho_0 \sum_{i=1}^n (\Xi_i - T \partial_T \Xi_i) \dot{\xi}_i \\ &\quad + \rho_0 T \partial_T H_I \dot{c}_I + \rho_0 T \partial_T K \dot{c} + K^* \dot{c} \\ &\quad - Q_{I,I} + \rho_0 R \end{aligned} \quad (47)$$

This equation accounts for heat storage, thermo elastic heating, inelastic work, energy storage by internal variables, reversible and dissipative heat generation due to fracture, thermal diffusion, and heat supply.

2.3 Specification of the Free Energy

The constitutive relations now depend on the specified form of the elastic and fracture contributions to the free energy. We use a general form, where the free energy is additively decomposed into thermal, elastic, fracture, and internal variable parts: ψ^t , ψ^e , ψ^f , and ψ^ξ respectively, giving

$$\psi = \psi^t + \psi^e + \psi^f + \psi^\xi \quad (48)$$

The elastic and internal variable portions are further broken into portions which contribute to fracture and portions which do not. Splitting the free energy is typically done to permit modeling of fracture in tension only. In accordance with the constant specific heat assumption eq. (46), the thermal part of the free energy is given by (Clayton, 2005)

$$\rho_0 \psi^t = -\rho_0 \hat{c} T \log T/T_0 \quad (49)$$

The elastic part of the free energy is

$$\rho_0 \psi^e = W + [m(c) - 1] W^+ \quad (50)$$

Where W is a function of the elastic deformation and the elastic material properties and W^+ is the damaged free energy. The degradation function $m(c)$ models the loss of strength in the material due to fracture, and is often chosen to be a quadratic. Note that this is notationally different from most phase field models where the elastic free energy is defined as

$$\rho_0 \psi^e = W^- + m(c) W^+ \quad (51)$$

Where W^- is the undamaged free energy. The reason for this difference is that the resulting definition of the elastic second Piola Kirchhoff stress, after using equation (37) in equation (50), will look familiar to the shear band only model, but with an additional term appended accounting for degradation of the stress due to fracture. Examples of W used in the literature for small strain analysis are a volumetric - deviatoric split of the strain energy used in (Amor et al., 2009), which is

$$W = \frac{1}{2} C_{ijkl}^{elas} \epsilon_{ij} \epsilon_{kl} \quad (52)$$

$$W^+ = (\lambda + 2\mu/3) \langle \epsilon_{ii}^2 \rangle + \mu \epsilon_{ij}^{dev} \epsilon_{ij}^{dev} \quad (53)$$

Where ϵ_{ij} is the small strain tensor, the deviatoric strain tensor is $\epsilon_{ij}^{dev} = \epsilon_{ij} - \frac{1}{3} \epsilon_{kk} \delta_{ij}$, λ and μ are Lamé's constants, and $\langle \rangle$ are Macaulay brackets, defined as

$$\langle x \rangle = \begin{cases} 0, & \text{if } x \leq 0 \\ x, & \text{if } x > 0 \end{cases} \quad (54)$$

In this split tensile volumetric and deviatoric strains contribute to damage. The finite deformation analogue of this split was used in a phase field model with plasticity in (Borden, 2012).

A second popular split, used in (Borden et al., 2012; Miehe et al., 2010a,b) is based on principal strains so that

$$W^+ = \frac{\lambda}{2} \langle \epsilon_1^{pr} + \epsilon_2^{pr} + \epsilon_3^{pr} \rangle^2 + \mu \left(\langle \epsilon_1^{pr} \rangle^2 + \langle \epsilon_2^{pr} \rangle^2 + \langle \epsilon_3^{pr} \rangle^2 \right) \quad (55)$$

where the principal strains ϵ_a^{pr} and principal directions p_a are given by the spectral decomposition of the small strain tensor

$$\epsilon = \epsilon_{ij} e_i \otimes e_j = \sum_{a=1}^3 \epsilon_a^{pr} p_a \otimes p_a \quad (56)$$

The fracture energy is given by the phase field theory (Bourdin et al., 2008; Francfort and Marigo, 1998; Miehe et al., 2010a,b) as

$$\rho_0 \psi^f = \mathcal{G}_c \left[\frac{c^2}{4l_0} + l_0 c_{,I} c_{,I} \right] \quad (57)$$

As noted earlier, the phase field approximation to the fracture energy converges to that of the discontinuous crack in the limit as the process zone parameter l_0 goes to zero (Bourdin et al., 2000; Francfort and Marigo, 1998). Lastly, the free energy due to internal variables is

$$\rho_0 \psi^\xi = \sum_{i=1}^n \left(\Xi_i \xi_i + [m(c) - 1] \Xi_i \xi_i^+ \right) \quad (58)$$

Where the ξ_i^+ are the internal variables whose evolution contributes to fracture. Thus, this modeling framework allows the choice of which internal variables contribute to the generation of fracture surfaces and which do not. In addition, similar to the notion of splitting the elastic free energy, the contribution of a single internal variable may be split into a fracture producing part and a part which is does produce fracture. This is where the present formulation departs significantly from existing phase field models which incorporate plasticity (Borden, 2012; Crosby and Ghoniem, 2012), and as shown below, these contributions to the free energy will lead to additional source terms in the phase field evolution equation. The physical motivation for inclusion of these terms in the modeling framework is due to the well known relationship between fracture and barriers to dislocation motion such as dislocation density and grain size. This leads to a model for fracture which is explicitly rate and temperature dependent, due to the rate and temperature dependence of the internal variables. Adopting as an example a volumetric - deviatoric split of the elastic strain energy (Simo and Hughes, 1998), the elastic second Piola Kirchhoff stress, and thus the Kirchhoff stress, can be determined. The elastic energy is thus composed of a volumetric contribution $U(J^e)$, dependent on the elastic volume change J^e , and a deviatoric contribution $\bar{W}(\bar{C}_{qr}^e)$, dependent on the deviatoric part of elastic right Cauchy Green tensor $\bar{C}_{qr}^e = J^{e,-2/3} F_{kq}^e F_{kr}^e$. W , U , and $\bar{W}$ are defined as

$$W = U(J^e) + \bar{W}(\bar{C}_{qr}^e) \quad (59)$$

$$U(J^e) = \frac{1}{2} k \left[\frac{1}{2} (J^{e,2} - 1) - \ln J^e \right] \quad (60)$$

$$\bar{W}(\bar{C}_{qr}^e) = \frac{1}{2} \mu \left(\text{trace} [\bar{C}_{qr}^e] - 3 \right) \quad (61)$$

W is split so that W^+ , the fracture producing portion, depends on the volumetric expansion so

that

$$W^+ = \begin{cases} 0, & \text{if } J^e \leq 0 \\ U(J^e), & \text{if } J^e > 0 \end{cases} \quad (62)$$

Using (37) with the above definitions and the relation $\tau_{ij} = S_{qr}^e F_{iq}^e F_{jr}^e$ the Kirchhoff stress becomes

$$\tau_{ij} = \tau_{ij}^{sb} + \tau_{ij}^f \quad (63)$$

Where τ_{ij}^{sb} is the contribution of the familiar elastic - plastic material law, and is defined as

$$\tau_{ij}^{sb} = \frac{k}{2} (J^{e,2} - 1) \delta_{ij} + \mu \text{dev} [\bar{b}^e] \quad (64)$$

Where $\text{dev} [\bar{b}_{ij}^e]$ is the deviatoric part of the tensor $\bar{b}_{ij}^e = J^{e,-2/3} F_{iq}^e F_{jq}^e$, with the elastic left Cauchy Green tensor being $b_{ij}^e = F_{iq}^e F_{jq}^e$. The decrement in stress due to cracking τ_{ij}^f is then

$$\tau_{ij}^f = \begin{cases} 0, & \text{if } J^e \leq 0 \\ [m(c) - 1] \frac{k}{2} (J^{e,2} - 1) \delta_{ij}, & \text{if } J^e > 0 \end{cases} \quad (65)$$

There are other options for splitting the energy, for example the deviatoric part of the elastic free energy can be included, which would result in an extra term in τ_{ij}^f

With the elastic constitutive relation specified, the terms of the micro force balance must now be developed. The micro force traction in the present formulation is identical to that of other phase field models. This is

$$H_I = \rho_0 \frac{\partial \psi}{\partial c_{,I}} = 2\mathcal{G}_c l_0 c_{,I} \quad (66)$$

However, the internal micro force contains extra source terms as follows

$$K = \rho_0 \frac{\partial \psi}{\partial c} + K^* = \frac{\partial m}{\partial c} \left(W^+ + \sum_{i=1}^n \Xi_i \xi_i^+ \right) + \mathcal{G}_c \frac{c}{2l_0} + K^* \quad (67)$$

Now, substituting (66) and (67) into (20) the micro force strong form becomes

$$\rho_0 \theta \ddot{c} = 4l_0 c_{,II} - c - \frac{2l_0}{\mathcal{G}_c} \frac{\partial m}{\partial c} \left(W^+ + \sum_{i=1}^n \Xi_i \xi_i^+ \right) - \frac{2l_0}{\mathcal{G}_c} K^* \quad (68)$$

Note that the addition of the terms $\sum_{i=1}^n \Xi_i \xi_i^+$ results in the possibility of cracking due to evolving internal inelastic variables, in contrast to the classical phase field method, where only the elastic free energy W^+ contributes to fracture.

The final equations needed for the strong form are the inelastic constitutive equations. The equivalent plastic strain evolves according to the following equation

$$\dot{\gamma}^p = \sqrt{\frac{2}{3} d_{ij}^p d_{ij}^p} \quad (69)$$

To specify l_{ij}^p and hence d_{ij}^p , first the inelastic velocity gradient with respect to the intermediate plastic configuration is defined as $\hat{l}_{qr}^p = \dot{F}_{qA}^p F_{Ar}^{p,-1}$. The symmetric part of this velocity gradient is defined as (Miehe, 1994; Simo and Miehe, 1992)

$$\hat{d}_{qr}^p = \frac{1}{2} (\hat{l}_{qr}^p + \hat{l}_{rq}^p) = g(\bar{\sigma}, T, \xi_i) \hat{n}_{qs} C_{sr}^e \quad (70)$$

Where $g(\bar{\sigma}, T, \xi_i)$ 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. Note however that rigid body rotations on the intermediate configuration have no effect upon the hyperelastic constitutive laws employed here. Thus the antisymmetric part of $\hat{l}_{qr}^p$ 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 (70) into (10) gives

$$l_{ij}^p = g(\bar{\sigma}, T, \xi_i) F_{iq}^e \hat{n}_{qs} C_{sr}^e F_{rj}^{e,-1} \quad (71)$$

$$= g(\bar{\sigma}, T, \xi_i) n_{ij} \quad (72)$$

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

$$n_{ij} = \frac{3s_{ij}}{2\bar{\tau}} \quad (73)$$

where $s_{ij} = \tau_{ij} - \frac{1}{3}\tau_{kk}\delta_{ij}$ is the deviatoric Kirchhoff stress and $\bar{\tau} = \sqrt{\frac{3}{2}s_{ij}s_{ij}}$ is the effective Kirchhoff stress. Since n_{ij} is symmetric, then $l_{ij}^p = d_{ij}^p$. Using (73) and (72) in (69) gives

$$\dot{\gamma}^p = g(\bar{\sigma}, T, \xi_i) \quad (74)$$

and thus the constitutive function $g(\bar{\sigma}, T, \xi_i)$ gives the equivalent plastic strain rate as a function of stress, temperature and internal variables. Lastly, the constitutive relations for the ξ_i are (Rice, 1971)

$$\dot{\xi}_i = \mathcal{X}_i(\bar{\tau}, T, \xi_i) \quad (75)$$

An example of which, that has been used for shear band modeling by (Batra and Kim, 1991) is (using the present notation)

$$\dot{\xi} = \bar{\tau}\dot{\gamma}^p / (1 + \xi/\xi_0)^n \quad (76)$$

In this case, there is one internal variable ξ which represents the extent of work hardening in the material.

Putting all of these equations together, the strong form consists of the balance laws

$$\rho_0 \ddot{u}_i = P_{i,I} + B_i \quad (77)$$

$$\begin{aligned} \rho_0 \dot{\hat{c}} = & \rho_0 T (\partial_{TE^e} \psi)_{qr} \dot{E}_{qr}^e + \bar{\tau} g(\bar{\sigma}, T, \xi_i) - \rho_0 \sum_{i=1}^n (\Xi_i - T \partial_T \Xi_i) \dot{\xi}_i \\ & + K^* \dot{c} - Q_{I,I} + \rho_0 R \end{aligned} \quad (78)$$

$$\rho_0 \theta \ddot{c} = 4l_0 c_{,II} - c - \frac{2l_0}{\mathcal{G}_c} \frac{\partial m}{\partial c} \left(W^+ + \sum_{i=1}^n \Xi_i \xi_i^+ \right) - \frac{2l_0}{\mathcal{G}_c} K^* \quad (79)$$

and the constitutive relations

$$\tau_{ij} = \tau_{ij}^{sb} + \tau_{ij}^f \quad (80)$$

$$\tau_{ij}^{sb} = \frac{k}{2} (J^{e,2} - 1) \delta_{ij} + \mu \text{dev} [\bar{b}^e] \quad (81)$$

$$\tau_{ij}^f = \begin{cases} 0, & \text{if } J^e \leq 0 \\ [m(c) - 1] \frac{k}{2} (J^{e,2} - 1) \delta_{ij}, & \text{if } J^e > 0 \end{cases} \quad (82)$$

$$\dot{\gamma}^p = g(\bar{\sigma}, T, \xi_i) \quad (83)$$

$$\dot{\xi}_i = \mathcal{X}_i(\bar{\sigma}, T, \xi_i) \quad (84)$$

3 Numerical Solutions With Constant Partition of Inelastic Work

To illustrate the basic behavior of the present model, several numerical experiments in one and two dimensions are given below. Small strains are considered so that all stress measures are equivalent, and represented by σ_{ij} . There is no micro inertia or fracture dissipation, i.e. $\theta = 0$ and $K^* = 0$. A quadratic degradation function is employed: $m(c) = (1 - c)^2$, which is the most commonly used degradation function, though others are available, subject to certain restrictions (Borden, 2012). The equivalent plastic strain is taken as the only internal variable, and represents the extent of work hardening of the material. As pointed out in the introduction, in general the Taylor Quinney fraction is not a material constant but depends on strain, strain rate, and temperature, as shown experimentally by (Hodowany et al., 2000; Mason et al., 1994). According to the previous section, the fraction of inelastic work converted to heat is

$$\chi = 1 - \frac{\rho_0 \sum_{i=1}^n (\Xi_i - T \partial_T \Xi_i) \dot{\xi}_i}{\bar{\sigma} g(\bar{\sigma}, T, \bar{\gamma}^p)} \quad (85)$$

When the equivalent plastic strain is the only internal variable, $n = 1$ and

$$\dot{\xi} = g(\bar{\sigma}, T, \bar{\gamma}^p) \quad (86)$$

The conjugate force to $\bar{\gamma}^p$ is a stress like variable related to isotropic strain hardening (Lubliner, 1990), and is defined as

$$\Xi = \partial_{\bar{\gamma}^p} \psi \quad (87)$$

Then equation (85) becomes

$$\chi = 1 - \frac{\Xi - T\partial_T\Xi}{\bar{\sigma}} \quad (88)$$

This approach for computing χ has been taken by (Longere and Dragon, 2007, 2009), but the predicted values of χ for steels tends to be significantly lower than the experimental predictions of (Mason et al., 1994). In what follows, it is assumed that a constant fraction of the inelastic work is converted to heat, and that the remaining plastic work is expended by creating new fracture surfaces.

The strong form (77) - (84) becomes

$$\rho\ddot{u}_i = \sigma_{ij,j} \quad (89)$$

$$\rho\dot{\bar{c}}\dot{T} = \kappa T_{,jj} + \chi\bar{\sigma}g(\bar{\sigma}, T, \bar{\gamma}^p) \quad (90)$$

$$c = 4l_0c_{,jj} + \frac{4l_0}{\mathcal{G}_c}c(W^+ + P^+) \quad (91)$$

$$\sigma_{ij} = \sigma_{ij}^{sb} + \sigma_{ij}^f \quad (92)$$

$$\dot{\bar{\gamma}}^p = g(\bar{\sigma}, T, \bar{\gamma}^p) \quad (93)$$

For all test problems shown below, insulated thermal boundary conditions are chosen and a velocity is applied to problem domain. The domains are initially at rest, with a temperature of $315K$. The stress due to shear banding σ_{ij}^{sb} is

$$\sigma_{ij}^{sb} = \lambda\epsilon_{kk}^e\delta_{ij} + 2\mu\epsilon_{ij}^e \quad (94)$$

where an additive decomposition of the strain has been used so that

$$\epsilon_{ij}^e = sym(u_{i,j}) - \epsilon_{ij}^p \quad (95)$$

and the plastic strain is

$$\epsilon^p = \int_0^t \frac{3s_{ij}}{2\bar{\sigma}}g(\bar{\sigma}, T, \bar{\gamma}^p) dt' \quad (96)$$

where t' is a dummy integration parameter and t is time. Thermal expansion has been ignored. To define σ_{ij}^f , first W^+ is defined with a volumetric - deviatoric split as follows

$$W^+ = \frac{1}{2}\lambda\langle\epsilon_{kk}^e\rangle^2 + \mu\epsilon_{ij}^e\epsilon_{ij}^e \quad (97)$$

Thus the deviatoric part of the strain energy contributes to fracture and the volumetric part contributes to fracture only if it corresponds to dilatation. Now, σ_{ij}^f is given by

$$\sigma_{ij}^f = \left[(1-c)^2 - 1\right] \frac{\partial W^+}{\partial \epsilon_{ij}^e} = \left[(1-c)^2 - 1\right] \left[\lambda\langle\epsilon_{kk}^e\rangle\delta_{ij} + 2\mu\epsilon_{ij}^e\right] \quad (98)$$

Lastly the inelastic free energy is defined, and is related to the accumulated plastic work

$$P^+ = \int_0^t (1-\chi)\bar{\sigma}g(\bar{\sigma}, T, \bar{\gamma}^p) dt' \quad (99)$$

Five versions of the above model are considered, the first being the model as it is written, which will be called the combined phase field and shear band model (PFSB) and accounts for both shear banding and fracture. In the second version the phase field parameter is fixed at 0, which reduces the PFSB model to previously studied thermal softening shear band models. The abbreviation used for this is SB. The third version considers isothermal conditions (PFIT), implying that $\chi = 0$, which excludes the possibility of thermal softening, leaving fracture due to accumulation of inelastic work as the only source of failure. The fourth version is the same as the PFSB model, but with the inelastic contribution to fracture P^+ neglected, and is abbreviated PFSBNP. Results from this model are only shown in 2D, since the model produces results that are indistinguishable from the SB model in 1D. The fifth and final version is the same as the PFIT model, but also neglects the inelastic contribution to fracture P^+ , and so is abbreviated PFITNP. This model is most similar to existing combined phase field models with plasticity (Borden, 2012; Crosby and Ghoniem, 2012) since both of these models do not account for thermal softening or P^+ . The differences are that (Crosby and Ghoniem, 2012) account for thermal expansion while PFITNP does not and (Borden, 2012) employ large strain kinematics while PFITNP is for small strains. A summary of the models is shown in table 1

The material parameters are chosen to be representative of HY 100 steel, where the Johnson Cook flow law has been used so that

$$g(\bar{\sigma}, T, \bar{\gamma}^p) = g_0 \exp \left\{ \frac{1}{c} \left[\frac{\bar{\sigma}}{\left[A + B (\bar{\gamma}^p)^N \right] \left[1 - \left(\frac{T - T_0}{T_m - T_0} \right)^m \right]} - 1 \right] \right\} \quad (100)$$

The phase field length scale parameter, which defines the width of the diffuse crack process zone, was chosen to be 5.0E-5 m. In the elastic setting, this parameter affects the peak stress obtained by the material before softening. In the one dimensional, quasi static case, homogeneous solutions of the elastic phase field model predict the critical stress as (Borden et al., 2012)

$$\sigma_c = \frac{9}{16} \sqrt{\frac{E \mathcal{G}_c}{6l_0}} \quad (101)$$

It is apparent that the critical stress tends to infinity as l_0 tends to zero. Physically, this corresponds to the well known crack tip singularity present in linear elastic fracture mechanics with discrete crack topology. In real materials however, experiments show finite fracture process regions. Process zone modeling dates back to the well known Barenblatt-Dugdale model which introduces the concept of a bounded stress within the cohesive zone at the crack tip (Barenblatt, 1962; Dugdale, 1960).

In this study, l_0 simply serves as a regularization parameter. It's value does not determine the stress at which fracture occurs, because the stress in the specimen is limited by the yield stress. However, smaller values of l_0 lead to higher fracture strains. Determination of a physically motivated choice of l_0 is an ongoing area of research for the present authors.

3.1 1D Results: a rod under tension

The 1D problem studied is a 0.001 m rod with a central imperfection in the yield strength and critical energy release rate $\mathcal{G}_c$ and a velocity applied at each end. A wide range of nominal strain rates are tested, from 10^{-1} to 10^5 , with the intent of examining the effect of rate on the mode and strain at failure. The effect of the Taylor Quinney fraction χ on the response is also studied over a range of values.

3.1.1 Failure and post localization behavior

Given sufficient input strain, the combined phase field and shear band model will eventually lead to fracture. However, since stress collapse due to thermal softening is an instability in its own right, failure is divided into three categories based qualitatively on the extent of thermal softening before fracture. The failure categories and in Table 3.

Fracture without thermally induced stress collapse tends to occur at the low range of the strain rates modeled here, which lie in the diffusion stabilized zone of the shear band model. At these strain rates thermal diffusion has enough time to spread the heat generated by inelastic deformation throughout the domain, resulting in nearly homogeneous conditions within the rod. However, despite the fact that the heat production is not sufficient to produce failure, the continued inelastic straining leads to fracture. In this range of strain rates, the shear band only model is essentially stable, and large strains are needed to produce significant softening. This is evident from Figure 4a, where the stress strain curves from the four formulations, PFSB, SB, PFIT, and PFITNP are plotted side by side with the phase field parameter vs strain and the temperature vs strain. The total temperature rise from the beginning of the simulation to the point of fracture is about 150 degrees, which does not lead to significant thermal softening. The PFSB and SB models perform nearly identically up until the point of fracture, with a slightly slower rate of temperature rise for the PFSB model. This is because the increase of the phase field parameter degrades the stress, which in turn results in less inelastic straining and thus less heat production. Note that inelastic straining and heat production cannot continue in the fully fractured phase since by definition the equivalent plastic strain rate is zero for an unstressed material, i.e. $g(\bar{\sigma} = 0, T, \bar{\gamma}^p) = 0$. The PFITNP model is similar to the other models only at small strains, and continues to harden without failure. This is due to the fact that the only source term for fracture in the PFITNP model is the elastic free energy, the growth of which is limited by yielding. The implications of this are discussed further in the next section. The PFIT model fails at the earliest strain, since all of the inelastic work contributes to fracture, as opposed to the PFSB model, where a tenth of the inelastic work is generates fracture and the remainder is converted to heat.

Failure due to thermally induced stress collapse with early transition to fracture tend to occur in the transition zone between the diffusion stabilized zone and the critical shear band zone, and is probably where the differences between the PFSB and SB formulations are most important for failure modeling. In these intermediate rates, thermal softening induced stress collapse occurs at

roughly the nominal strain for both the SB and the PFSB formulations, but the post localization behavior of the two models is very different.

For the SB model, after an initial rapid stress collapse the rate of softening decreases significantly and a great deal of additional input strain is needed to continue to soften the material, see Figure 4b. In contrast for the PFSB model, the stress collapse causes the stress to drop to zero without a decrease in the softening rate. This is because the phase field parameter has grown to a significant value, roughly 0.6, during the plateau region of the stress strain curve, and the subsequent intense inelastic straining resulting from thermal softening stress collapse causes the material to quickly transition to fracture. The differences in the post localization behavior of the two models is of particular importance in higher dimensions, where the propagation characteristics of the shear band depend on the unloading rate. Again, the PFIT model, which is most appropriate for small strain rates, fails at very low strains. The PFITNP model is not shown since no failure is predicted by this model.

Thermally induced stress collapse with late transition to fracture occurs in the critical shear band zone, and there are only minor differences between the two models in this range until late in the stress collapse process. Due to slower heat production, the PFSB model shows slightly higher strain to failure than the SB model, see Figure 4c. The post localization behavior of the two models is also similar, since thermal softening is prevalent at these rates and thus fracture will not occur until late in the stress collapse process. Further details on the effect of the strain rate and Taylor Quinney fraction on the failure characteristics are given in section 3.1.3.

3.1.2 Inelastic contribution to fracture

A comparison of the elastic and inelastic contributions to fracture vs nominal strain for the PFSB model are shown in Figure 5, with the same strain rates as were shown in the previous section. These are the inelastic free energy, the elastic free energy, and the sum of the two, defined as

$$\text{inelastic energy} \quad \psi^i = (1 - c)^2 P^+ \quad (102)$$

$$\text{elastic energy} \quad \psi^e = (1 - c)^2 W^+ \quad (103)$$

$$\text{total energy} \quad \psi^{tot} = \psi^i + \psi^e = (1 - c)^2 [P^+ + W^+] \quad (104)$$

Up until the point of fracture, the contribution of the inelastic free energy is much higher than the elastic contribution, due to the fact that the elastic strain is small compared to the inelastic strain. After fracture, inelastic straining ceases and the inelastic free energy drops to zero due to the degradation function $(1 - c)^2$, while the elastic strain increases rapidly. The increase in the elastic strain is because the strain increments in the fully fractured phase are modeled as pure elastic, even though they physically represent a separated material.

In the one dimensional setting, it is clear that the growth of the elastic free energy will be quadratic in the elastic range, but the onset of yielding will limit further growth of this term. In fact, with thermally induced softening, the elastic free energy can decrease as the material unloads. Thus, unless fracture occurs before yielding, crack formation will not be possible in the

one dimensional setting unless the contribution of inelastic deformation to fracture is accounted for as in the present formulation. This is evident from Figure 6, where the free energies are shown vs strain for the PFSB, PFIT, and PFITNP models.

Here it is shown that when the inelastic free energy is not accounted as a source term in the phase field equation, the elastic free energy does not increase beyond the peak stress, thus prohibiting the occurrence of a crack, as shown by the light blue curve in Figure 6. In contrast, when the inelastic free energy is accounted for, the phase field source term will continue to increase, even during thermal softening. Additionally, continued growth of the phase field parameter degrades the stress as previously mentioned, which leads to smaller increments of inelastic strain, which means a larger portion of the total strain increment will be elastic. This is why the elastic free energy is larger and why it continues to grow after yielding when the inelastic contribution to fracture is accounted for, as shown in Figure 5.

In multi dimensional simulations of elastic plastic materials, it is possible for cracks to occur without consideration of P^+ if the loading is sufficiently triaxial. This is shown in the next section where fracture is observed without P^+ , but only after shear band formation. However, exclusion of P^+ or a similar term as presented in the previous section would model fracture as independent of the state of the material's microstructure. This is in contrast to the fact that microstructural characteristics which impede dislocation motion such as dislocation density and grain size are related to fracture.

3.1.3 *Effect of strain rate and Taylor Quinney fraction on failure strain*

The combined phase field and shear band model has been tested for Taylor Quinney fractions of 0.5, 0.7, and 0.9, with strain rates varying from 10^{-1} to 10^5 . Here, we define failure as a drop in the integral averaged stress to 0.9 of the peak value in its history

$$\int_{\Omega} \sigma(x, t) d\Omega = 0.9 \max \left[\int_{\Omega} \sigma(x, t) d\Omega \right] \quad (105)$$

and as a second condition, there must be severe strain localization at the center of the rod. The range of strain rates was chosen to illustrate the zones in Figure 3, which are the diffusion stabilized zone, the critical shear band zone, and the two transition zones above and below the critical shear band zone, as illustrated in Figure 1. In the transition zone above the critical shear band zone inertia effects are significant and the conditions in the domain are highly non uniform due to elastic wave propagation. For the current test problem, strain rates beyond $1.0\text{E}+5$ 1/s lead to significant thermal softening at the ends of the rod, which can occur while the center of the rod has not yet been loaded. Since the aim of studying the one dimensional test problem is to compare the four formulations in the simplest possible setting, we leave these higher rates to future studies.

The failure strain vs strain rate is shown in Figure 7. For the shear band only model, the diffusion stabilized, first transition, and critical shear band zones can be clearly identified. The second transition zone can not be clearly shown due to the effect described in the previous paragraph. For

a Taylor Quinney parameter of 0.9, which is the value used typically in the literature, differences in the failure strain in the diffusion stabilized zone are due to fracture occurring without much thermal softening. In the first transition zone, some differences in failure strain are present, but the response of the PFSB and SB formulations mainly differs beyond the failure point recorded for this plot. Lastly, the PFSB and SB formulations are most similar in the critical shear band zone, where there are only slight differences in the failure strains of the two models. It is worth noting that since the inelastic source term in the phase field equation is strain, strain rate, and temperature dependent, the fracture response is also dependent on these quantities as well.

For the isothermal PFIT model, increased strain rate is found to always decrease the strain to failure with χ held fixed. In the context of the model, this is due to the rate dependence of the Johnson Cook model, where higher strain rates lead to higher yield stresses, which causes the plastic work term in equation (99) to accumulate faster. The presence of thermal softening in the PFSB model leads to larger failure strains compared to the PFIT model, and in addition there is a minimum strain to failure in the critical shear band zone for the PFSB model.

While a fully variable fraction is not modeled, a parametric study of constant Taylor Quinney fraction has been conducted, and this parameter was found to have a significant effect on the results. A lower Taylor Quinney fraction not only leads to a higher fraction of the inelastic work available as a source term in the phase field equation, but less heat will be generated, resulting in a lower susceptibility to thermal softening induced stress collapse. In the results shown in Figure 7, lowering the fraction significantly biases the results toward fracture.

Experimental work on carbon steels by (Dixon and Parry, 1991) show a transition from essentially isothermal conditions to essentially adiabatic conditions over the course of three decades of strain rate. This was used by (Vural et al., 2003), to develop an expression for χ as a function of strain rate as a smooth step function. We use a similar expression here, namely

$$\chi = 0.45 + 0.45 \tanh \left(0.6 \log \left(\frac{\dot{\epsilon}_0}{50} \right) \right) \quad (106)$$

Which is the same as the function used by (Vural et al., 2003), but the limiting values of χ used here are 0.0 and 0.9, instead of 0 and 1. The transition region from $\chi = 0.0$ to $\chi = 0.9$ is thus $1.0 \text{ 1/s} - 1.0\text{E}+3 \text{ 1/s}$. The results of this are shown in Figure 7d, which demonstrates that the PFSB and PFIT models are identical at low strain rates, where the effects of temperature are very small. For the same reason, there is no failure predicted by the SB model. As the strain rate is increased, the strain to failure predicted by PFSB and PFIT begins to increase, due to the fact that the fraction of inelastic work that generates fracture decreases. This trend is in qualitative agreement with experiments on HY 100 steel by (Rajendran et al., 1995), where the failure strains at intermediate strain rates were found to be larger than failure strain of quasi static tests. In this region, the failure strain of the PFSB model is higher than the PFIT model, indicating that temperature rise is improving the ductility of the material. The PFSB and SB model meet in the critical shear band zone, where thermal softening is most prevalent. Thus the PFSB model coincides with the PFIT model at low strain rates where the thermal softening is negligible, and with the SB model in the critical shear band zone, where thermal softening induced stress collapse occurs most readily. In the transition region, which is of the most interest,

failure strains for the PFSB model are higher than the PFIT model, but significantly lower than the SB model.

To quantitatively validate the model, further study to calibrate the model parameters such as χ , l_0 , and the flow law parameters are needed for various materials over a wide range of strain rates. Note, that flow law parameters are fit to experimental data with consideration only for thermal softening rather than the combined effect of thermal softening and damage. In this work, it is our intention to present the theoretical development of the model and to present basic numerical results demonstrating the model capabilities.

3.2 2D Results: plate under tension

The 2D problem studied is a 2E-4 m by 2E-4 m plate with an applied velocity to the upper and lower edges. Due to symmetry, only the upper right quadrant has been modeled. Since the problem domain is smaller than the 1D case, l_0 has been reduced to $1.0E - 5$. Similar to the 1D case, a material imperfection is applied at the center of the plate, which corresponds to the lower left corner of the modeled domain.

Figure 8 shows σ_{22} , the normal stress in the direction of the applied displacement, at the lower left corner of the plate vs nominal strain for two different strain rates.

The full PFSB model predicts fracture at both the lower and higher strain rates. In contrast, if the inelastic contribution to fracture is excluded, fracture is only predicted by the PFSBNP model at the higher rate, after severe localization due to shear banding has occurred. At the lower strain rate where fracture without significant thermal softening is expected, no fracture is observed up to very high nominal strains. Thus while the PFSBNP model is capable of predicting a shear band transitioning to a crack, the full PFSB model with inelastic contribution to fracture is also capable of predicting fracture without significant thermal softening and is thus a more appropriate model for predicting a failure transition.

The presence of multidirectional loading leads to the main difference between the 1D and 2D implementations. In 1D, it was noted that plasticity limits the growth of the elastic free energy W^+ preventing the occurrence of fracture for models which do not account for P^+ . Growth of W^+ is also limited by plasticity in multiple dimensions, but since J2 plasticity is considered, the volumetric component of the strain can cause W^+ to grow without causing yielding. This is why the PFSBNP model is capable of predicting fracture after yielding in 2D. After severe loss of stiffness in the material due to shear banding, significant volumetric deformations are encountered due to the boundary conditions, resulting in fracture. Thus, shear banding expedites the fracture process through growth in both the elastic and inelastic contribution terms to fracture. No significant effect of fracture was found in the PFITNP model, however it is likely fracture would occur if the simulations were carried out to very large strains.

The crack direction predicted by the PFSB model was found to change with strain rate, as shown in Figure 9. At the lower strain rate, a crack is observed at 90 degrees, which corresponds to a

mode I fracture behavior, while at the higher strain rate, the shear band dominates and a crack is forms on top of the shear band at 45 degrees.

4 Conclusion

A formulation for simultaneously modeling shear bands and fracture was developed using conservation laws and thermodynamic principles. The formulation combines a thermally softening shear band model with the phase field method for fracture. The phase field method presented here differs from existing ones in that it includes a term accounting for the creation of fracture surfaces stored energy of cold work, which is energy stored by imperfections in the crystal lattice of a metal upon inelastic straining. Thus, the inelastic work is partitioned into heat, which contributes to thermal softening, and stored energy of cold work, which contributes to fracture.

A simple, one dimensional parametric study was conducted with constant partition of cold work to illustrate the basic behavior of the model and compare the model with two special cases. Two dimensional studies on a plate in tension were also conducted. The original model, abbreviated as PFSB to indicate that thermal softening and fracture are present, was compared to the isothermal case (PFIT) which models ductile fracture without temperature rise, and the damage free case (SB), which reduces the model to thermal softening shear banding models found in the literature. The final model tested was isothermal with damage, but without the inelastic contribution to fracture introduced in section 2 of this paper. This model was abbreviated at PFITNP and was found to never lead to failure since the only source of damage is the elastic free energy, the growth of which is limited by yielding. Material parameters were chosen for a typical steel and strain rates of 10^{-1} to 10^5 were tested. Using a Taylor Quinney fraction of 0.9, it was found that in the diffusion stabilized zone, where shear banding does not occur, fracture occurs in the PFSB model without much thermal softening. In the first transition zone, there are also very significant differences between the PFSB and the SB models, principally in the post stress collapse behavior, where the unloading rate of the present model is much faster than the shear band only model.

For all strain rates, the PFSB model predicts higher failure strains than the PFIT model, indicating that temperature rise improves the ductility of the material. Using a strain rate dependent Taylor Quinney fraction which ramps smoothly from a value of 0.0 to 0.9 over the strain rates 1.0 1/s to 1.0E+3 1/s, the PFSB model coincides with the PFIT model at low strain rates, where thermal softening is negligible, and with the SB model in the critical shear band zone, where thermal softening is most prevalent. This formulation is very important for accurate failure modeling in higher dimensions, where the unloading rate effects the propagation characteristics of the shear band. In the critical shear band zone, where thermal softening is prevalent, the models behaved quite similarly. Thus, it is expected that the present model will be valid for failure modeling in a much broader range of strain rates than the shear band only model, as well as significantly improve the accuracy of failure modeling in the transition regions. Furthermore, the framework presented here permits modeling of the relationship between fracture and barriers to dislocation motion such as dislocation density and grain size. This leads to a model for fracture

which is explicitly rate and temperature dependent, due to the rate and temperature dependence of the internal variables.

The general trends observed in the 1D modeling were also observed in the 2D model. In addition, the PFSB model showed a transition in the crack direction with strain rate; higher strains lead to a crack forming on top of the shear band at 45 degrees while lower strain rates lead to mode I crack behavior. For the multidimensional model, cracks were produced with the PFSBNP model which neglects the inelastic contribution to fracture term introduced in this work, but only at the highest strain rate tested. The transition in crack behavior was observed only in the full PFSB model.

Future studies will include determination of the most physically reasonable values for the phase field length scale parameter, l_0 , which at present is interpreted as a regularization parameter.

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Table 1

Summary of models tested.

Model Name	Taylor Quinney Parameter	Phase Field	Fracture Source Terms
PFSB	$\chi \neq 0$	Governed by Eq. (91)	P^+ and W^+
SB	$\chi \neq 0$	Fixed at 0	-
PFIT	$\chi = 0$	Governed by Eq. (91)	P^+ and W^+
PFSBNP	$\chi \neq 0$	Governed by Eq. (91)	W^+ only
PFITNP	$\chi = 0$	Governed by Eq. (91)	W^+ only

Table 2

Material Properties and Parameters. Johnson - Cook parameters were taken from (Batra and Kim, 1991) and are for HY 100 steel.

Property Name	Symbol	Value	Unit
Young's Modulus	E	200E9	Pa
Poisson Ratio	ν	0.3	-
Mass Density	ρ	7860	$\frac{kg}{m^3}$
Specific Heat	$\hat{c}$	473	$\frac{J}{kgK}$
Reference Stress	A	111.4E6	Pa
Hardening Parameter	B	579.1E6	Pa
Rate Sensitivity Parameter	c	0.028	-
Reference Strain Rate	g_0	1	s^{-1}
Strain Hardening Exponent	N	0.054	-
Reference Temperature	T_0	300	K
Reference Temperature	T_m	1800	K
Thermal Softening Parameter	m	0.8	-
Critical Energy Release Rate	$\mathcal{G}_c$	1.25E-4	$\frac{J}{m^2}$
Process Zone Parameter	l_0	5.0E-5	m

Table 3

Failure mechanisms and corresponding strain rate loading ranges.

Failure Mechanism with $\chi = 0.9$	Strain Rates [$1/s$]
Fracture without thermally induced stress collapse	$1.0E-1 - 1.0E+2$
Thermally induced stress collapse with early transition to fracture	$1.0E+2 - 1.0E+4$
Thermally induced stress collapse with late transition to fracture	$1.0E+4 - 1.0E+5$

Fig. 1. On the left, a schematic illustration of a projectile penetrating a metal plate, such as those shown in (Nickodemus et al., 2002). Shear failure occurs parallel to the impact direction while crack radiate out perpendicular to the impact direction. On the right, an illustration of the phase field approximation to a crack is shown. Phase field models treat cracks as continuous entities where the extent of the damage to the material is characterized by the phase field parameter c . The parameter is 1 in the fully fractured phase and 0 in the undamaged phase. The width of the diffusive crack is determined by the parameter l_0

Fig. 2. Multiplicative Split of F per equation (1)

Fig. 3. Schematic illustration of the results reported in (Wright and Walter, 1987), for a rigid plastic model. Zone 1 is the diffusion stabilized zone, where thermal diffusion is able to prevent severe localization due to the slow loading rate. Zone 2 is the first transition zone, where severe localization occurs at increasingly low strains. Zone 3 is the critical shear band zone, where thermal softening failure is most prevalent. Lastly, zone 4 is the second transition zone, where inertia effects become important. Inertia has been shown to delay shear localization (Fressengeas, 1989)

(a) $\chi = 0.9, \epsilon_0 = 1.0$

(b) $\chi = 0.9, \epsilon_0 = 5.0E + 3$

(c) $\chi = 0.9, \epsilon_0 = 5.0E + 4$

Fig. 4. Plots illustrating the three failure categories. Stress vs nominal strain is shown in the left column. In the right column the phase field parameter and temperature vs nominal strain is shown. The left axis is for the temperature, which is plotted in red, and the right axis is for the phase field parameter c , which is plotted in blue.

— Elastic Free Energy — Inelastic Free Energy — Total Free Energy

(a) $\chi = 0.9, \epsilon_0 = 1.0$

(b) $\chi = 0.9, \epsilon_0 = 5.0\text{E}+3$

(c) $\chi = 0.9, \epsilon_0 = 5.0\text{E}+4$

Fig. 5. For the PFSB model the elastic, inelastic, and total free energies, which serve as the driving forces for fracture, are shown vs nominal strain.

(a) $\chi = 0.9, \epsilon_0 = 1.0$

(b) $\chi = 0.9, \epsilon_0 = 5.0\text{E}+3$

(c) $\chi = 0.9, \epsilon_0 = 5.0\text{E}+4$

Fig. 6. The total free energy for the PFSB, PFIT, and PFITNP models is shown vs nominal strain. For the PFITNP model, the only fracture producing contribution to the free energy is the elastic energy, shown in light blue, which does not increase significantly beyond the yield point.

Fig. 7. Failure strain vs strain rate for different values of χ . The black dots are from experimental tension tests on HY 100 steel from (Rajendran et al., 1995), which consisted of a quasi static test and a split Hopkinson test at 1500 1/s. The black diamond is the failure strain from a Hopkinson bar torsion test at 3300 1/3.

(a) Nominal strain rate $= 5E1s^{-1}$

(b) Nominal strain rate $= 5E4s^{-1}$

Fig. 8. Stress strain plots at the lower left corner of the domain for nominal strain rates of $5E1s^{-1}$ and $5E4s^{-1}$. Fracture is predicted for the full PFSB model at both strain rates. The PFSBNP model, which does not account for the inelastic contribution to fracture coincides with the SB model at the lower strain rate and predicts fracture only at the higher rate.

Fig. 9. Surface plots of equivalent plastic strain (left side) and phase field parameter (right side) for (a) nominal strain rate of $5E1s^{-1}$ and (b) $5E4s^{-1}$. At the low strain rate mild localization occurs at a 45 degree angle due to plasticity, while the crack propagates at a 90 degree angle. In contrast at the higher rate, there is severe localization due to shear banding at 45 degrees. The shear band transitions into a 45 degree crack