Strain localization and dynamic recrystallization in polycrystalline metals: thermodynamic theory and simulation framework

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Abstract

We describe a theoretical and computational framework for adiabatic shear banding (ASB) and dynamic recrystallization (DRX) in polycrystalline materials. The Langer-Bouchbinder-Lookman (LBL) thermodynamic theory of polycrystalline plasticity, which we recently reformulated to describe DRX via the inclusion of the grain boundary density or the grain size as an internal state variable, provides a convenient and self-consistent way to represent the viscoplastic and thermal behavior of the material, with minimal ad-hoc assumptions regarding the initiation of yielding or onset of shear banding. We implement the LBL-DRX theory in conjunction with a finite-element computational framework. Favorable comparison to experimental measurements on a top-hat AISI 316L stainless steel sample compressed with a split-Hopkinson pressure bar suggests the accuracy and usefulness of the LBL-DRX framework, and demonstrates the crucial role of DRX in strain localization.

Keywords: Constitutive behavior, Dynamic recrystallization, Shear banding, Steel, Finite-element simulation, Taylor-Quinney coefficient

1. Introduction

Under severe loading conditions, adiabatic shear bands (ASBs) often develop in ductile metallic materials. The concentration of plastic deformation...
into narrow bands of the material, often preceding ductile fracture (e.g., Sabnis et al., 2012; Rousselier and Quilici, 2015; Arriaga and Waisman, 2017), has obvious implications for many industrial and defense applications such as metal-forming processes, shock absorption, and structural engineering. The need for an accurate representation of adiabatic shear bands, a thorough understanding of the physics of shear localization, and a predictive description of the formation and growth of shear bands has triggered a large amount of theoretical, numerical, and experimental research; excellent overviews are provided by the treatises of Wright (2002) and Dodd and Bai (2012).

Numerical representation of ASBs presents a major challenge because of the short length and time scales involved. Mesh sensitivity issues naturally arise from direct finite-element implementations which impart a length scale equal to the element size in the shear band. Recent developments have made substantial progress in addressing these issues, through embedding the shear-band width into the problem by non-local techniques (Anand et al., 2012; Ahad et al., 2014; Abed and Voyiadjis, 2005; Voyiadjis et al., 2004; Abed and Voyiadjis, 2007; Voyiadjis and Abed, 2005, 2007; Voyiadjis and Faghihi, 2013). A recent effort by two of us and collaborators (Mourad et al., 2017; Jin et al., 2018) sought to eliminate mesh dependency through the sub-grid method, which permits the nucleation of shear bands narrower than the mesh size, effectively circumventing mesh dependency.

The physical mechanisms underlying adiabatic shear localization pose a profound challenge very distinct from that on the numerical front; advances in numerical methods alone do not provide an understanding of ASB mechanisms, or a predictive description of the shear-banding process. There is growing evidence in the literature that dynamic recrystallization (DRX) – the process by which fine, nano-sized grains with few or no dislocations form in the ASB – provides an additional softening mechanism and supplements the role of thermal softening in shear band initiation. DRX has been observed in conjunction with adiabatic shear localization in a broad range of metals and alloys, including titanium and titanium alloys (e.g., Rittel et al., 2008; Osovski et al., 2012, 2013; Li et al., 2017), magnesium (Rittel et al., 2006), copper (Rittel et al., 2002), and steel (e.g., Meyers et al., 2000, 2001, 2003).

Numerous authors have developed hypotheses for the underlying cause of dynamic recrystallization. Brown and Bammann (2012) attributes DRX to the diffusive motion of grain boundaries for relatively slow loading rates where diffusional time scales are relevant. For conditions of loading consid-
ered here, subgrain rotation and the lineup of dislocations forming new grain boundaries have been invoked as a contributing mechanism for the occurrence of DRX (Hines and Vecchio 1997; Hines et al. 1998; Meyers et al. 2000, 2003; Li et al. 2017). Others (Popova et al. 2015, e.g.,) have argued that DRX is probabilistic in nature and is driven by a local mismatch of the dislocation density. In light of these hypotheses, varied efforts have been made to develop theoretical descriptions of the DRX process. These include phenomenological models (e.g., Galindo-Nava and del Castillo 2014; Galindo-Nava and Rae 2015; Mourad et al. 2017), internal state variable theories (e.g., Brown and Bammann 2012; Puchi-Cabrera et al. 2018; Sun et al. 2018), cellular automaton models (e.g., Popova et al. 2015), phase-field descriptions (e.g., Takaki et al. 2008, 2009), or a hybrid of several of these such as a combination of phase-field modeling and crystal plasticity (e.g., Zhao et al. 2016, 2018).

Important physical ingredients seem to be inadequately included in many of the existing models in the literature. Firstly, many of these theories do not account for energy balance, a crucial physical ingredient in a deforming material because of the input work of deformation and the thermal effects arising from the input work. Some of these theories (e.g., the MTS model used in (Mourad et al. 2017)) partition the stress into components accounting for different physical mechanisms such as the different types of barriers to dislocation motion. Because energy is conserved while there is no analogous conservation law for the stress, the input energy is the only quantity that can be additively partitioned into components stored or dissipated via different mechanisms without invoking additional implicit assumptions. Secondly, conventional theories employ flow rules that are largely phenomenological; examples include power-law fits of the type $\sigma \propto \dot{\epsilon}^\delta$ between the stress $\sigma$ and the strain rate $\dot{\epsilon}$, or between the strain rate and some internal slip resistance. These are based on extensive observations and a search for quantitative trends, and are good mathematical approximations; yet they shed no light on the underlying physical principles for such behavior, and may not apply with greater generality to other materials or loading rate regimes. Finally, while many of these models rightfully adopt a statistical view of dislocations, the assumed evolution of the dislocation density may be problematic on physical grounds. For example, the Kocks-Mecking equation (Kocks 1966; Mecking and Kocks 1981) for the temporal evolution of the dislocation density $\rho$, employed in many of the references (e.g., Takaki et al. 2008, 2009),
The equation is of the form
\[
\frac{d\rho}{de} = k_1 \sqrt{\rho} - k_2 \rho,
\]
where \(k_1\) and \(k_2\) are parameters, and \(\epsilon\) is the total strain. The first term on the right-hand side of Eq. (1) is a storage rate, while the second term is the depletion rate of stored dislocations. This equation does not conform with time reversal and reflection symmetries, as seen immediately if one reverses the strain rate which, strictly speaking, is a tensor. While one may circumvent this problem by replacing \(\epsilon\) with \(|\epsilon|\), this introduces a mathematical singularity at \(\epsilon = 0\) which cannot be correct for physically well-posed and predictive evolution equations. These problems with the conventional literature suggest a vital need for physical input in multiscale descriptions of large deformations in metallic materials.

Related to the question of energy balance in a deforming polycrystalline solid is the accounting for the Taylor-Quinney coefficient, or the fraction of input work expended in heating up the material. Heat is primarily generated and confined within the ASB, causing local material softening that further reduces the resistance to dislocation glide, creating a positive feedback mechanism that results in more severe deformation. In spite of available experimental measurements (e.g., Farren and Taylor, 1925; Taylor and Quinney, 1934; Hartley et al., 1987; Marchand and Duffy, 1988; Duffy and Chi, 1992; Rittel et al., 2017), the accurate prediction of the thermal response of a plastically deforming material is of practical importance and remains an open question (e.g., Zehnder, 1991; Rosakis et al., 2000; Benzerga et al., 2005; Longère and Dragon, 2008b,a; Stainier and Ortiz, 2010; Zaera et al., 2013; Anand et al., 2015; Luscher et al., 2018). Plasticity theories that directly address the issue of energy balance are most promising in this respect.

We recently proposed a minimal, thermodynamic description of DRX in polycrystalline solids during adiabatic shear localization (Lieou and Bronkhorst, 2018), based on the Langer-Bouchbinder-Lookman (LBL) theory of dislocation plasticity (Langer, 2015). The LBL theory directly addresses the issues with conventional dislocation theories, through the notion of a thermodynamically-defined effective temperature that describes the configurational state of the material in question, and the use of well-posed evolution equations for internal state variables. The fact that the LBL theory provides an accurate fit to strain hardening in copper over eight decades of strain rate with minimal assumptions (Langer, 2015), among other re-
cent applications (e.g., Langer, 2016, 2017a,b; Le et al., 2018), attests to its usefulness and predictive capabilities. In Lieou and Bronkhorst (2018), we augmented the LBL theory with a state variable for the grain boundary density, or the grain boundary area per unit volume. A very generic assumption for the interaction between grain boundaries and dislocations – that the interaction is proportional to their respective densities – immediately produces recrystallized grains in the ASB, and provides a good fit to experimental measurements in ultrafine-grained titanium, in a proof-of-principle calculation. DRX is seen to be an entropic effect; under severe loading conditions, the material forgoes dislocations in favor of an increased grain boundary density, the configuration which minimizes the free energy. Following the simple shear calculation in that manuscript, a natural extension is the implementation of the LBL-DRX theory in a simulation framework appropriate for more complex geometries and loading conditions in solid mechanics experiments and practical problems.

The present paper is devoted to a finite-element implementation and verification of the LBL-DRX theory in simulations; the rest of this paper is organized as follows. In Section 2 we present an overview of the LBL-DRX theory of dislocation plasticity and dynamic recrystallization, and discuss the physical basis of the thermodynamic approach. We also propose a simple way to compute the Taylor-Quinney coefficient of a deforming polycrystalline material. We describe in detail the computational framework in Section 3, and the experiment on the 316L stainless steel in Section 4. Section 5 summarizes the computational results and demonstrates good agreement with experiments. We conclude with a brief summary in Section 6.

A list of symbols used throughout the paper is included in Table 1 for the reader’s convenience.

2. Thermodynamic theory of dislocation plasticity and dynamic recrystallization: an overview

In this section, we provide an overview of the LBL theory of dislocations and the recent extension we developed to describe dynamic recrystallization. The LBL theory (Langer et al., 2010; Langer, 2015) provides a simple, minimal description of polycrystalline plasticity, consistent with the laws of thermodynamics. The recent extension of the theory to describe DRX, and a proof-of-principle calculation, are documented in our recent paper (Lieou and Bronkhorst, 2018).
Table 1: List of mathematical symbols

| Symbol(s)          | Meaning or definition                                                   |
|--------------------|------------------------------------------------------------------------|
| $\sigma_{ij}, s_{ij}$ | Total and deviatoric stress tensors                                    |
| $\dot{\varepsilon}_{ij}, \dot{\varepsilon}_{ij}$ | Total and deviatoric strain rate                                       |
| $\dot{\varepsilon}^e_{ij}, \dot{\varepsilon}^p_{ij}$ | Total and deviatoric elastic strain rate                               |
| $\dot{\varepsilon}^{el}_{ij}, \dot{\varepsilon}^{el}_{ij}$ | Total and deviatoric elastic strain rate                               |
| $\dot{\varepsilon}^{pl}_{ij}, \dot{\varepsilon}^{pl}_{ij}$ | Total and deviatoric plastic strain rate                               |
| $\tilde{s}, \tilde{\dot{\varepsilon}}_{pl}$ | Stress and plastic strain rate invariants                             |
| $\rho_M$ | Mass density                                                          |
| $\mu$ | Shear modulus                                                         |
| $\lambda$ | First Lamé parameter                                                 |
| $\nu$ | Poisson’s ratio                                                       |
| $\mu_0, D_0, T_0$ | Parameters in shear modulus                                           |
| $\beta$ | Taylor-Quinney factor                                                |
| $c_v, c_p$ | Specific heat capacity, per unit volume and per unit mass            |
| $c_0, c_1$ | Parameters in heat capacity $c_p$                                     |
| $d$ | Grain size                                                            |
| $a$ | Atomic length scale                                                  |
| $v$ | Average dislocation speed                                             |
| $\tau$ | Atomic vibration time scale                                          |
| $e_P$ | Dislocation depinning energy barrier                                  |
| $T, \theta$ | Thermal temperature, in Kelvins and energy units (\(\theta = k_B T\)) |
| $s_T$ | Taylor stress barrier                                                |
| $\alpha_T, \mu_T$ | Taylor parameter, and effective shear modulus (\(\mu_T = \alpha_T \mu\)) |
| $q$ | Dimensionless plastic strain rate (= 2\(\tau \dot{\varepsilon}^{pl}\)) |
| $\rho, \tilde{\rho}$ | Dislocation density and its dimensionless version (\(\tilde{\rho} = a^2 \rho\)) |
| $\bar{e}_D, \bar{\xi}_G$ | Typical grain boundary energy and its rescaled version (\(\bar{e}_G = e_G/e_D\)) |
| $e_N, \bar{\xi}_N$ | Typical dislocation-grain boundary interaction energy and its rescaled version (\(\bar{e}_N = e_N/e_D\)) |
| $\bar{\rho}$ | Dimensionless density and its dimensionless version (\(\bar{\rho} = a^2 \rho\)) |
| $\bar{\xi}$ | Grain boundary density and its dimensionless version (\(\bar{\xi} = a \xi\)) |
| $\chi, \tilde{\chi}$ | Effective temperature in energy units and its dimensionless version (\(\tilde{\chi} = \chi/e_D\)) |
| $\chi_0, \tilde{\chi}_0$ | Steady-state effective temperature and its dimensionless version (\(\tilde{\chi}_0 = \chi_0/e_D\)) |
| $\tilde{\rho}_{ss}, \tilde{\xi}_{ss}, d_{ss}$ | Steady-state dimensionless dislocation density, dimensionless grain boundary density, and grain size |
| $U_C, S_C$ | Configurational energy and entropy                                    |
| $U_K, S_K$ | Kinetic-vibrational energy and entropy                                |
| $U_{tot}$ | Total energy                                                          |
| $U_D, U_C, U_{int}$ | Energy density of dislocations, grain boundaries, and their interaction |
| $S_D, S_G$ | Entropy density of dislocations and grain boundaries                  |
| $K$ | Thermal transport coefficient between configurational and kinetic-vibrational degrees of freedom |
| $\kappa_1, \kappa_0, \kappa_r$ | Dislocation storage parameters                                        |
| $\kappa_2$ | Disorder storage parameter                                            |
| $\kappa_d$ | Grain boundary storage parameter                                      |
| $q_r$ | Strain hardening parameter                                           |
2.1. Kinematics and elasto-viscoplasticity

Let $\sigma_{ij}$ and $\dot{\epsilon}_{ij}$ denote the Cauchy stress and total strain rate tensors, and let $s_{ij}$ and $\dot{e}_{ij}$ denote their deviatoric counterparts. These are related to each other by

$$s_{ij} = \sigma_{ij} - \frac{1}{3} \sigma_{kk} \delta_{ij}, \quad \dot{e}_{ij} = \dot{\epsilon}_{ij} - \frac{1}{3} \dot{\epsilon}_{kk} \delta_{ij}. \quad (2)$$

(The repeated indices indicate the Einstein summation convention.) In polycrystalline metals, where the elastic strain is expected to be small, we decompose the total strain rate tensor additively into elastic and plastic parts, $\dot{e}_{ij}^{el}$ and $\dot{e}_{ij}^{pl}$:

$$\dot{\epsilon}_{ij} = \dot{\epsilon}_{ij}^{el} + \dot{\epsilon}_{ij}^{pl}. \quad (3)$$

Plastic incompressibility, or the notion that plastic deformation preserves volume, implies that the plastic strain-rate tensor is trace-free, or

$$\dot{e}_{ij}^{pl} = \dot{e}_{ij}^{pl}. \quad (4)$$

Assuming isotropic elasticity, the total stress rate is then given by

$$\dot{\sigma}_{ij} = 2\mu(\dot{\epsilon}_{ij} - \dot{\epsilon}_{ij}^{pl}) + \lambda \dot{\epsilon}_{kk} \delta_{ij}. \quad (5)$$

Here, $\mu$ is the shear modulus, and $\lambda$ is the first Lamé parameter, related to $\mu$ and the Poisson ratio $\nu$ by $\lambda = 2\mu \nu / (1 - 2\nu)$.

In this study, we assume that the shear modulus is temperature-dependent:

$$\mu = \mu_0 - \frac{D_0}{\exp(T/T_0) - 1}, \quad (6)$$

where $\mu_0$ and $D_0$ are parameters with the dimensions of stress, and $T_0$ is a reference temperature. We also assume that the Poisson ratio $\nu$ is a constant, and that $\lambda$ varies with the temperature accordingly.

2.2. Dislocation motion

Define the deviatoric stress invariant

$$\bar{s} = \sqrt{\frac{1}{2} s_{ij} s_{ij}}. \quad (7)$$

Dislocation motion is governed by the Orowan relation, which says that the plastic strain rate is proportional to the dislocation density or dislocation line
length per unit volume $\rho$, their average velocity $v$, and some atomic length scale $a$:

$$\dot{\epsilon}^{\text{pl}}_{ij} = \frac{\rho}{2} \frac{s_{ij}}{\bar{s}} a v,$$

(8)

The Orowan relation, as written in Eq. (8), assumes isotropic plasticity and co-directionality of plastic strain rate with the deviatoric stress. This is a fairly reasonable simplification in a polycrystalline material, where the crystal orientation varies between adjacent grains. In conventional literature, $a$ is usually the Burgers vector; we however take the view that $a$ is an atomic length scale, and absorb any uncertainties into the time scale associated with the velocity $v$.

A dislocation moves when it hops from one pinning site to another. The distance $l$ between pinning sites is related to the dislocation density $\rho$ by $l = 1/\sqrt{\rho}$. We take the view that depinning is a thermally activated process with energy barrier $e_P$ and stress barrier $s_T$, so that the pinning time $\tau_P$ is given by

$$\frac{1}{\tau_P} = \frac{1}{\tau} \exp\left( -\frac{e_P}{\theta} e^{-\frac{s}{s_T}} \right).$$

(9)

Here, $\tau \sim 10^{-12}$ s, being the only relevant atomic time scale, is on the order of the inverse Debye frequency; we absorb any uncertainties in the length scale $b$ into here. $\theta = k_B T$ is the thermal temperature $T$ in energy units, with $k_B$ being the Boltzmann constant. The stress barrier $s_T$ equals the shear stress needed to unpin a dislocation and move it by a fraction of the length scale $a$ when the average separation between dislocations is $l = 1/\sqrt{\rho}$. The shear strain associated with this operation is a fraction of the quantity $a/l = a\sqrt{\rho}$, so that it is given by the Taylor expression $s_T = \mu_T a \sqrt{\rho}$, where $\mu_T = \alpha T \mu$ with $\alpha_T$ being on the order of 0.1. Combining Eqs. (8) and (9), the expression for the plastic strain rate is

$$\dot{\epsilon}^{\text{pl}}_{ij} = \sqrt{\frac{\rho}{2\tau}} \frac{s_{ij}}{\bar{s}} \exp\left( -\frac{e_P}{\theta} e^{-\frac{s}{s_T}} \right),$$

(10)

which conveniently defines the dimensionless dislocation density $\bar{\rho} = a^2 \rho$. It is useful to define the dimensionless plastic strain rate

$$q \equiv 2\tau \dot{\epsilon}^{\text{pl}} = \sqrt{\bar{\rho}} \exp\left[ -\frac{e_P}{\theta} e^{-\frac{s}{(\mu_T \sqrt{\bar{\rho}})}} \right].$$

(11)

from the strain rate invariant $\dot{\epsilon}^{\text{pl}} \equiv \sqrt{(1/2)\dot{\epsilon}^{\text{pl}}_{ij}\dot{\epsilon}^{\text{pl}}_{ij}}$. 

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2.3. Nonequilibrium thermodynamics and steady-state defect densities

One of the most important aspects of the LBL theory of dislocation plasticity is the compliance with the laws of thermodynamics, based upon which the steady-state defect densities and the evolution of state variables are derived. This is the place where the present theory diverges from traditional descriptions of polycrystalline plasticity and dynamic recrystallization. The deforming polycrystalline material is by definition in a nonequilibrium state because of the nonzero external work rate arising from deformation itself. The configurational degrees of freedom – those pertaining to the positions of atoms – fall out of equilibrium with the kinetic-vibrational degrees of freedom pertaining to the atoms’ thermal motion, whose time scale given by the Debye frequency is often many orders of magnitude above the strain rate. As such, we partition the total energy density $U_{\text{tot}}$ and entropy density $S_{\text{tot}}$ into configurational (C) and kinetic-vibrational (K) contributions:

$$U_{\text{tot}} = U_C + U_K; \quad S_{\text{tot}} = S_C + S_K.$$  \hspace{1cm} (12)

Dislocations and grain boundaries (GBs) clearly belong to the configurational degrees of freedom. Denote by $\xi$ the GB density, or the GB area per unit volume, and its dimensionless counterpart $\tilde{\xi} = a\xi$. (The characteristic grain size $d$ is related to the GB density by $d = 1/\xi$.) The configurational energy and entropy densities $U_C$ and $S_C$ can then be written as

$$U_C(S_C, \tilde{\rho}, \tilde{\xi}) = U_D(\tilde{\rho}) + U_G(\tilde{\xi}) + U_{\text{int}}(\tilde{\rho}, \tilde{\xi}) + U_1(S_1);$$ \hspace{1cm} (13)

$$S_C(U_C, \tilde{\rho}, \tilde{\xi}) = S_D(\tilde{\rho}) + S_G(\tilde{\xi}) + S_1(U_1).$$ \hspace{1cm} (14)

$U_D$ and $S_D$ are the energy and entropy densities associated with dislocations; their counterparts for GBs are $U_G$ and $S_G$. $U_1$ and $S_1$ are the energy and entropy densities of all other configurational degrees of freedom. We implicitly assume that the contributions of dislocations and GBs to the entropy are independent, while there is a contribution $U_{\text{int}}$ from the interaction between dislocations and GBs to the total energy density. Define the effective temperature

$$\chi \equiv \frac{\partial U_C}{\partial S_C}.$$ \hspace{1cm} (15)

The first law of thermodynamics says that

$$\dot{U}_{\text{tot}} = \sigma_{ij} \dot{\epsilon}_{ij} = \dot{U}_C + \dot{U}_K$$  \hspace{1cm} (16)

$$= \chi \dot{S}_C + \left( \frac{\partial U_C}{\partial \dot{t}} \right)_{S_C, \tilde{\rho}, \tilde{\xi}} + \left( \frac{\partial U_C}{\partial \tilde{\rho}} \right)_{S_C, \tilde{\xi}} \dot{\tilde{\rho}} + \left( \frac{\partial U_C}{\partial \tilde{\xi}} \right)_{S_C, \tilde{\rho}} \dot{\tilde{\xi}} + \theta \dot{S}_K.$$ \hspace{1cm} (17)
Because deformation at constant defect densities $\rho$, $\xi$ and configurational entropy $S_C$ is by definition elastic (Bouchbinder and Langer, 2009), the elastic work $(\partial U_C/\partial t)_{S_C,\hat{\rho},\hat{\xi}} = \sigma_{ij}\varepsilon_{ij}^{el}$ cancels out of both sides of Eq. (16), so that

$$\sigma_{ij}\varepsilon_{ij}^{pl} = \chi \dot{S}_C + \left( \frac{\partial U_C}{\partial \rho} \right)_{S_C,\hat{\xi}} \dot{\rho} + \left( \frac{\partial U_C}{\partial \xi} \right)_{S_C,\hat{\rho}} \dot{\xi} + \theta \dot{S}_K. \quad (18)$$

Move on to the second law of thermodynamics, according to which

$$\dot{S}_{tot} = \dot{S}_C + \dot{S}_K \geq 0. \quad (19)$$

Eliminating $\dot{S}_C$ using the energy balance equation, one finds

$$\sigma_{ij}\varepsilon_{ij}^{pl} - \left( \frac{\partial U_C}{\partial \rho} \right)_{S_C} \dot{\rho} - \left( \frac{\partial U_C}{\partial \xi} \right)_{S_C} \dot{\xi} + (\chi - \theta) \dot{S}_K \geq 0. \quad (20)$$

The Coleman-Noll argument (Coleman and Noll, 1963) stipulates non-negativity of each independently variable term in this inequality. This is automatically satisfied for the plastic work rate $\sigma_{ij}\varepsilon_{ij}^{pl} = s_{ij}\varepsilon_{ij}^{pl}$ according to Eq. (8). The constraint $(\chi - \theta) \dot{S}_K \geq 0$ will be discussed in Section 2.5 in connection with the Taylor-Quinney coefficient which determines the fraction of plastic work dissipated as heat. For now, we are left with

$$- \left( \frac{\partial U_C}{\partial \rho} \right)_{S_C} \dot{\rho} \geq 0; \quad - \left( \frac{\partial U_C}{\partial \xi} \right)_{S_C} \dot{\xi} \geq 0. \quad (21)$$

These inequalities say that the time rates of change of the defect densities $\dot{\rho}$ and $\dot{\xi}$ change sign when $U_C$ at constant $S_C$ is a minimum. Once we write explicitly that

$$\left( \frac{\partial U_C}{\partial \rho} \right)_{S_C} = \frac{\partial U_D}{\partial \rho} + \frac{\partial U_{int}}{\partial \rho} - \chi \frac{\partial S_D}{\partial \rho} \equiv \frac{\partial F_C}{\partial \rho}; \quad (22)$$

$$\left( \frac{\partial U_C}{\partial \xi} \right)_{S_C} = \frac{\partial U_G}{\partial \xi} + \frac{\partial U_{int}}{\partial \xi} - \chi \frac{\partial S_G}{\partial \xi} \equiv \frac{\partial F_C}{\partial \xi}, \quad (23)$$

where

$$F_C(\hat{\rho}, \hat{\xi}) = U_D(\hat{\rho}) + U_G(\hat{\xi}) + U_{int}(\hat{\rho}, \hat{\xi}) - \chi(S_D(\hat{\rho}) + S_G(\hat{\xi})) \quad (24)$$
is the configurational free energy density, the requirement in (21) is immediately seen to amount to the dynamic minimization of the configurational free energy.

A very generic assumption is that the energy density of dislocations $U_D$ and GBs $U_G$ increase linearly with the dislocation and GB densities, and that the interaction energy $U_{\text{int}}$ is bilinear in the defect densities; i.e.,

$$U_D = \frac{e_D \tilde{\rho}}{a^3}, \quad U_G = \frac{e_G \tilde{\xi}}{a^3}, \quad U_{\text{int}} = \frac{e_N \tilde{\rho} \tilde{\xi}}{a^3}.$$  \hspace{1cm} (25)

This defines the characteristic formation energies $e_D$ and $e_G$ for a dislocation line of length $a$ and a GB of area $a^2$, respectively, and the energy scale $e_N$. The length scale $a$ is therefore the minimum average separation between dislocation lines and between GBs, or the minimum length for which dislocation and GB densities are meaningful quantities, and should be roughly 10-20 atomic spacings. The entropies $S_D$ and $S_G$ can be computed by a simple counting argument detailed in, for example, Lieou and Bronkhorst (2018), with the result

$$S_D(\tilde{\rho}) = \frac{1}{a^3}(\tilde{\rho} \ln \tilde{\rho} + \tilde{\rho}), \quad S_G(\tilde{\xi}) = \frac{1}{a^3}(\tilde{\xi} \ln \tilde{\xi} + \tilde{\xi}).$$  \hspace{1cm} (26)

As such, the steady-state defect densities are given by

$$\tilde{\rho}^{ss} = \exp \left( -\frac{e_D + e_N \tilde{\xi}}{\chi} \right);$$  \hspace{1cm} (27)

$$\tilde{\xi}^{ss} = \exp \left( -\frac{e_G + e_N \tilde{\rho}}{\chi} \right).$$  \hspace{1cm} (28)

It is seen that whenever $e_D > e_G$ and $e_N > 0$, dynamically recrystallized grains with depleted dislocations correspond to the steady state. Of course, there needs to be a pathway, i.e., large enough strain rate, for the polycrystalline material to reach this DRX state to begin with.

It is convenient to rescale the effective temperature $\chi$ and the defect energies $e_G$ and $e_N$ by the dislocation formation energy $e_D$:

$$\tilde{\chi} \equiv \frac{\chi}{e_D}, \quad \tilde{e}_G \equiv \frac{e_G}{e_D}, \quad \tilde{e}_N \equiv \frac{e_N}{e_D}. \hspace{1cm} (29)$$
Then
\[
\tilde{\rho}^{ss} = \exp \left( -\frac{1 + \tilde{e}_N \tilde{\xi}}{\chi} \right); \tag{30}
\]
\[
\tilde{\xi}^{ss} = \exp \left( -\frac{\tilde{e}_G + \tilde{e}_N \tilde{\rho}}{\chi} \right). \tag{31}
\]

2.4. Evolution of defect densities and the effective temperature

Energy is stored in dislocations and grain boundaries that are formed over the course of deformation. In order to express a direct connection between the rate at which mechanical work is done on the material and the rates at which defects are created or annihilated, the rates of change of the defect densities, \( \dot{\tilde{\rho}} \) and \( \dot{\tilde{\xi}} \), are manifestly proportional to the plastic work rate \( \sigma_{ij} \dot{\epsilon}_{ij}^{pl} = s_{ij} \dot{\epsilon}_{ij}^{pl} \), which is the only relevant scalar invariant with the dimensions of energy per unit volume per time. The equation for the dislocation density evolution towards the steady-state value \( \tilde{\rho}^{ss} \) reads
\[
\dot{\tilde{\rho}} = \kappa_1 \frac{\sigma_{ij} \dot{\epsilon}_{ij}^{pl}}{\nu^2 \mu T} \left( 1 - \frac{\tilde{\rho}}{\tilde{\rho}^{ss}} \right). \tag{32}
\]

Here, the quantity
\[
\bar{\nu} \equiv \frac{\bar{s}}{\mu T \sqrt{\tilde{\rho}}} = \ln \left( \frac{e_P}{\theta} \right) - \ln \left[ \ln \left( \frac{\sqrt{\tilde{\rho}}}{q} \right) \right], \tag{33}
\]
where \( q \) is the dimensionless strain rate defined in Eq. (11), controls the strain-hardening rate. The \( \bar{\nu}^{-2} \) dependence on the right-hand side of Eq. (32) can be derived by computing the hardening rate at the onset of plasticity, when \( \bar{s} \approx s_T = \mu T \sqrt{\tilde{\rho}} \), \( \dot{\epsilon}_{ij} \approx \dot{\epsilon}_{ij}^{pl} \), and \( \tilde{\rho} \ll \tilde{\rho}^{ss} \) [Langer et al., 2010; Langer, 2015]. \( \kappa_1 \) is a storage factor which increases with the strain rate, and increases with decreasing grain size because grain corners serve as a source of dislocations; as in [Lieou and Bronkhorst, 2018], we assume the form
\[
\kappa_1(d, q) = \kappa_0 + \frac{\kappa_r}{\sqrt{d}} \left( 1 + \frac{q}{q_r} \right), \tag{34}
\]
where \( q_r \) determines the onset of rate hardening, and \( \kappa_0, \kappa_r \) are hardening parameters.
The evolution equation for the GB density is
\[
\dot{\tilde{\xi}} = \kappa_d \frac{\sigma_{ij} \epsilon_{ij}^{pl}}{\mu_T} \left(1 - \frac{\tilde{\xi}}{\tilde{\xi}_{ss}}\right),
\]
(35)
where \(\kappa_d\) is a dimensionless GB storage parameter. Note that in contrast to our earlier work \cite{Lieou2018}, here we inserted an overall factor of \(\tilde{\xi}\) on the right hand side. This factor appears to be necessary to ensure timely recrystallization going from micron-sized grains to grains with diameter \(d \sim 100\) nm. If one prefers to track the evolution of the grain size \(d = a/\xi\) as opposed to \(\tilde{\xi}\), the evolution equation is
\[
\dot{d} = \kappa_d \frac{\sigma_{ij} \epsilon_{ij}^{pl}}{\mu_T} (d^{ss} - d),
\]
(36)
where \(d^{ss} = a/\tilde{\xi}_{ss}\) is the steady-state grain size.

The effective temperature \(\tilde{\chi}\) increases as deformation induces configurational disorder, and saturates at some \(\tilde{\chi}_0\):
\[
\dot{\tilde{\chi}} = \frac{\kappa_2}{\mu_T} \sigma_{ij} \epsilon_{ij}^{pl} \left(1 - \frac{\tilde{\chi}}{\tilde{\chi}_0}\right),
\]
(37)
with \(\kappa_2\) being a dimensionless parameter. At saturation, \(\tilde{\rho}^{ss} \approx e^{-1/\tilde{\chi}_0}\), and the average separation between dislocation lines should be about \(10a\), in the spirit of the Lindemann melting criterion \cite{Lindemann1910}; this gives \(\tilde{\chi}_0 \approx 0.25\).

Finally, the true, thermal temperature increases at a rate proportional to the plastic work rate:
\[
\dot{\theta} = k_B \dot{T} = \frac{\beta k_B}{c_v} \sigma_{ij} \epsilon_{ij}^{pl},
\]
(38)
In the adiabatic approximation, we neglect the flow of heat within the material, and between the material and the surroundings. This is valid as long as heat is generated more quickly than the speed of heat conduction, and is a good approximation at sufficiently high strain rates. The Taylor-Quinney coefficient \(\beta\) is the fraction of plastic work converted into heat. \(c_v\) is the heat capacity per unit volume of the material; it is related to the heat capacity per unit mass \(c_p\) and the mass density \(\bar{\rho}_M\) by \(c_v = c_p \bar{\rho}_M\); in this study we assume temperature dependence of the form
\[
c_p(T) = c_0 + c_1 T,
\]
(39)
where \(c_0\) and \(c_1\) are constants.
2.5. Taylor-Quinney coefficient

Incidentally, the thermodynamic description outlined in Section 2.3 provides a simple estimate of the Taylor-Quinney coefficient $\beta$, a long-standing challenge in the materials science and solid mechanics communities (e.g., Zehnder, 1991; Rosakis et al., 2000; Benzerwa et al., 2005; Longère and Dragon, 2008b,a; Stainier and Ortiz, 2010; Zaera et al., 2013; Anand et al., 2015; Lüscher et al., 2018) despite a vast amount of experimental efforts (e.g., Farren and Taylor, 1925; Taylor and Quinney, 1934; Hartley et al., 1987; Marchand and Duffy, 1988; Duffy and Chi, 1992; Rittel et al., 2017). The thermodynamic constraint $(\chi - \theta)S_K \geq 0$, a direct consequence of the second-law inequality (20), stipulates that
\begin{equation}
  c_v \dot{\theta} = \theta \dot{S}_K = -K \left(1 - \frac{\chi}{\theta}\right),
\end{equation}
where $K$ is a non-negative thermal transport coefficient (Bouchbinder and Langer, 2009). To calculate $K$, consider the nonequilibrium steady state, at which the effective temperature $\chi$, as well as the dislocation and GB densities $\tilde{\rho}$ and $\tilde{\xi}$, have reached their respective steady-state values, i.e., $\chi_0 \equiv e_D \tilde{\chi}_0$, and $\dot{\chi} = 0$, $\dot{\tilde{\rho}} = \dot{\tilde{\xi}} = 0$. Substitution of these and Eq. (40) into the first-law statement, Eq. (18), gives
\begin{equation}
  K = \sigma_{ij} c_{ij}^{pl} \frac{\theta}{\chi_0 - \theta},
\end{equation}
Suppose that this also holds true beyond the nonequilibrium steady state, by virtue of consistency. Then
\begin{equation}
  c_v \dot{\theta} = \sigma_{ij} c_{ij}^{pl} \frac{\chi - \theta}{\chi_0 - \theta},
\end{equation}
from which we directly read off the Taylor-Quinney coefficient
\begin{equation}
  \beta = \frac{\chi - \theta}{\chi_0 - \theta}.
\end{equation}
Because thermal fluctuations of energy $\theta = k_B T$ are insufficient to create dislocations and grain boundaries, $\theta \ll e_G \simeq e_D \lesssim \chi \lesssim \chi_0$. As such,
\begin{equation}
  \beta \approx \frac{\chi}{\chi_0} = \frac{\tilde{\chi}}{\chi_0}.
\end{equation}
The present argument says that the Taylor-Quinney coefficient, or the fraction of plastic work expended in heating up the material, is entirely controlled by the state of its configurational disorder, increasing towards unity as the deforming material approaches the nonequilibrium steady state, at which all of the input work is dissipated as heat.

3. Computational method

To solve evolution equations, which include Eq. (5) for the stress, and Eqs. (32), (36), (35), and (38) for the dislocation density \( \tilde{\rho} \), grain size \( d \), effective temperature \( \tilde{\chi} \), and thermal temperature \( T \), we implement the following implicit algorithm within the explicit branch of the finite element code ABAQUS [Smith 2014]. The symmetry and geometry of the hat-shaped sample permits the use of axisymmetric formulation where we represent the material by a vertical cross section, partitioned into quadrilateral elements with four nodes each, two degrees of freedom (radial and axial displacement) per node, and four independent components for the stress and strain rate tensors associated with each element (the \( rr \), \( \theta \theta \), \( zz \), and \( rz \) components).

The implicit algorithm is as follows. Denote by \( \Lambda_\alpha \) the collection of state variables \( \tilde{\rho} \), \( d \), \( \tilde{\chi} \), and \( T \) at each element. At each time step \( t \), we first perform an explicit update to make a best guess for the state variables at the next time step at \( t + \Delta t \):

\[
\Lambda_\alpha^*(t + \Delta t) = \Lambda_\alpha(t) + \Delta t \cdot \dot{\Lambda}_\alpha(\sigma_{ij}(t), \Lambda_\beta(t)).
\] (45)

If \( t = 0 \), we perform an explicit update to compute the stress value \( \sigma_{ij} \) at the next time step. Otherwise, we perform the following Newton-type iterative algorithm to compute the stress. If \( \Delta \epsilon_{ij} \) is the strain increment accrued through time \( \Delta t \), define

\[
R_{ij}(\sigma_{kl}(t + \Delta t)) \equiv \sigma_{ij}(t + \Delta t) - \sigma_{ij}(t) - 2\mu \left[ \Delta \epsilon_{ij} - \Delta t \dot{\epsilon}_{ij}^{pl}(t + \Delta t) \right] - \lambda \delta_{ij} \Delta \epsilon_{kk}.
\] (46)

Note that \( \dot{\epsilon}_{ij}^{pl}(t + \Delta t) \) is a function of \( \sigma_{kl}(t + \Delta t) \) and the state variables at time \( t + \Delta t \). \( \sigma_{ij}(t + \Delta t) \) is then found by setting \( R_{ij}(\sigma_{kl}(t + \Delta t)) = 0 \). The iterative solution going from the \( n \)th to the \( (n+1) \)-st iteration is

\[
\sigma_{ij}^{(n+1)}(t + \Delta t) = \sigma_{ij}^{(n)}(t + \Delta t) - (J_{k,l,ij}^F)^{-1}R_{kl}(\sigma_{kl}^{(n)}(t + \Delta t)),
\] (47)
Table 2: Dimensions of the hat-shaped 316L steel sample used in the present experiment and sketched in Fig. 1

| Dimension variable corresponding to Fig. 1 | Value (mm) |
|-------------------------------------------|------------|
| \( r_1 \)                                | 2.095      |
| \( r_2 \)                                | 2.285      |
| \( r_3 \)                                | 4.320      |
| \( h_1 \)                                | 2.540      |
| \( h_2 \)                                | 3.430      |
| \( h_3 \)                                | 5.080      |

where

\[
J_{ij,kl}^F = \frac{\partial R_{ij} \left( \sigma_{kl}^{(n)}(t + \Delta t) \right)}{\partial \sigma_{kl}^{(n)}(t + \Delta t)} = \delta_{ij,kl} + 2\mu \Delta t \frac{\partial \dot{\epsilon}_{ij}^{pl} \left( \sigma_{kl}^{(n)}(t + \Delta t) \right)}{\partial \sigma_{kl}^{(n)}(t + \Delta t)}
\]  \tag{48}

is the 4-by-4 Jacobian of the function \( R_{ij} \left( \sigma_{kl}^{(n)}(t + \Delta t) \right) \) defined above (no summation over the four possible pairs of \( kl \)-indices here), and \( \delta_{ij,kl} = 1 \) when \( (ij) = (kl) \) and 0 otherwise. Upon reaching sufficient accuracy for \( \sigma_{ij}(t + \Delta t) \), we stop the iteration, and perform one final update for the state variables at time \( t + \Delta t \):

\[
\Lambda_\alpha(t + \Delta t) = \Lambda_\alpha(t) + \Delta t \cdot \dot{\Lambda}_\alpha(\sigma_{ij}(t + \Delta t), \Lambda_\beta(t + \Delta t)),
\]  \tag{49}

using the trial values \( \Lambda_\beta(t + \Delta t) \) obtained from Eq. (45) above, and the stress \( \sigma_{ij}(t + \Delta t) \) from Eq. (47).

4. Experiments

The cylindrical hat-shaped sample geometry, first developed by Meyer and Manwaring (1985) and depicted here in Fig. 1, has been exploited in previous work (e.g., Bronkhorst et al., 2006) to study the shear-dominated response of metallic materials, because of the oblique orientation of the shear band relative to the loading direction. Sample dimensions of the AISI 316L stainless steel specimen used in this study are tabulated in Table 2.

In the experiment that we consider in this manuscript and also described in Mourad et al. (2017), a series of identical samples were loaded dynamically from the top, using a split-Hopkinson pressure bar test system. Steel collars were placed around the sample to avoid overdrive and to arrest the sample
at pre-determined displacements. The tests were conducted at an initial temperature of $T = 298$ K and a breech gas pressure of 42 kPa. The striker bar length was 15.24 cm. The initial grain size of each sample was $d = 30\, \mu m$. Fig. 2 shows the downward velocity profile imposed at the top of each specimen.

5. Model results

We present in this section the simulations results based on the traditional finite element method and the implicit algorithm presented in Section 3. Three finite element meshes have been used in this study, with element sizes $h = 90$, 40, and 20 $\mu m$ in the shear section; two of these are shown in Fig. 3. Note that the mesh itself introduces the length scale $h$ into the problem; without using more sophisticated sub-grid methods that constrain the shear-band width, $h$ limits the shear band width, and some length-related parameters, such as the atomic length scale $a$ over which one can define dislocation and GB densities, are presently $h$-dependent. The material parameters used in the present work are listed in Table 3. For steel, many
Figure 2: Imposed top-surface downward velocity on the hat-shaped steel sample. The data points are recorded in the experiment, while the solid red line is the approximation used in our simulation as the top-surface boundary condition.
parameters are known. For example, its heat capacity, mass density, and the parameters associated with the shear modulus $\mu$ are well documented in the literature (e.g., Bronkhorst et al. 2006; Mourad et al. 2017); LBL theory parameters appropriate for steel, such as the depinning energy $e_P$, the ratio $\alpha_T = \mu_T/\mu$, and the storage coefficients $\kappa_1$ and $\kappa_2$, are documented in Le et al. (2018). We only needed to adjust the parameters $\tilde{e}_N$ and $\tilde{e}_G$ for the ratios of the interaction energy and GB energy scales to the dislocation formation energy, and the GB energy storage parameter $\kappa_d$. We also account for the grain-size and strain-rate dependence of the storage parameter $\kappa_1$ through small adjustments in $q_r$ and $\kappa_r$ to keep $\kappa_1$ in the same ballpark as reported in the literature. In addition, we had to adjust the initial conditions for the dislocation density and effective temperature to provide a good fit to the stress-displacement curve, the only piece of experimental measurement directly available to us; we used $\tilde{\rho}(t = 0) = 1.7 \times 10^{-3}$ for the relatively large strain hardening at the initial stage, and $\tilde{\chi}(t = 0) = 0.16$.

Fig. 4 shows the load-displacement curves computed using the conventional finite element method, and the implicit algorithm described above, for the mesh sizes $h = 20$, 40, and 90 $\mu$m in the shear section. Note that the
stress drop increases slightly with decreasing mesh size, which artificially sets the ASB width. This conforms with the intuition that localization of plastic work within a narrower band increases the thermal heating and therefore the thermal softening and recrystallization activity in the band, thereby accounting for the greater stress drop. The mesh-dependence issue can be addressed by embedding the assumed ASB width into the mesh, by means of sub-grid methods (e.g., [Mourad et al., 2017; Jin et al., 2018]; this is beyond the scope of the present work. The stress drop for \( h = 40 \mu \text{m} \) appears to be in closet agreement with the experiment; we shall focus on \( h = 40 \mu \text{m} \) henceforth in this paper.

To demonstrate the softening effect of dynamic recrystallization, we performed the simulation with “pseudo-steel”, for which DRX is prohibited by setting \( \kappa_d = 0 \), but whose material parameters are otherwise identical to those listed in Table 3 for 316L stainless steel. The resulting load-displacement curve is shown in Fig. 5 alongside the result for 316L stainless steel and the experimental measurements; the stress drop upon the formation of the shear band is almost negligible. This result indicates that DRX provides a crucial softening mechanism and may be needed to explain the observed stress drop.

To verify the position of the shear band, we show in Fig. 6 the logarithmic shear strain and accumulated plastic strain \( \tilde{\varepsilon}^{\text{pl}} \equiv \sqrt{(1/2)\epsilon_{ij}^{\text{pl}}\epsilon_{ij}^{\text{pl}}} \), where

### Table 3: List of parameters and initial conditions

| Parameter | Definition or meaning | Value             |
|-----------|-----------------------|-------------------|
| \( \rho_M \) | Mass density          | 7860 kg m\(^{-3}\) |
| \( \mu_0 \) | Shear modulus parameter | 71.46 GPa       |
| \( D_0 \) | Shear modulus parameter | 2.09 GPa       |
| \( T_0 \) | Shear modulus parameter | 204 K           |
| \( \nu \) | Poisson’s ratio       | 0.3              |
| \( c_0 \) | Heat capacity parameter | 391.63 J kg\(^{-1}\) K\(^{-1}\) |
| \( c_1 \) | Heat capacity parameter | 0.237 J kg\(^{-1}\) K\(^{-2}\) |
| \( a \) | Atomic length scale | 12, 1.8, 1 nm for \( h = 90, 40, 20 \mu \text{m} \) |
| \( \tau \) | Atomic time scale | 1 ps               |
| \( \epsilon_P \) | Depinning energy barrier | 7.121 \times 10^{-18} J |
| \( \alpha_T \) | Ratio \( \mu/\mu_T \) | 0.0178              |
| \( \tilde{\epsilon}_G \) | GB energy in units of dislocation energy \( e_D \) | 0.2               |
| \( \tilde{\epsilon}_N \) | GB-dislocation interaction in units of dislocation energy \( e_D \) | 100              |
| \( \dot{X}_0 \) | Steady-state effective temperature in units of \( e_D \) | 0.25              |
| \( \kappa_r \) | Dislocation storage rate parameter | \( 10^{-3} \) |
| \( \varphi_r \) | Rate hardening parameter | \( 2 \times 10^{-9} \) |
| \( \kappa_0 \) | Dislocation storage rate parameter | 7.5               |
| \( \kappa_2 \) | Effective temperature increase rate | 14.3              |
| \( \kappa_d \) | Recrystallization rate parameter | 5                |
Figure 4: Load-displacement curves computed using the finite element method with $h = 20$, 40, and 90 µm, compared to experimental measurements.

$\varepsilon_{ij}^{pl} \equiv \int_0^t dt' \dot{\varepsilon}_{ij}^{pl}(t')$, at the end of the experiment. Model prediction for the temperature rise in the ASB is given by the left panel Fig. 7 which shows the concentration of the heat generated by the plastic work within the shear band. The predicted temperature rise is very close to that given by the MTS model coupled with the sub-grid finite element formulation (Mourad et al., 2017). The right panel of Fig. 7 shows the distribution of the effective temperature $\tilde{\chi}$; The increase and subsequent saturation of $\tilde{\chi}$ within the shear band, or the growth of configurational disorder therein, causes the evolution of both the dislocation density and the grain size to the $\tilde{\chi}$-controlled values $\tilde{\rho}^{ss}$ and $d^{ss}$ given by Eqs. (30) and (31). Because $\tilde{\chi}$ increases at a rate proportional to the plastic work, it changes little far away from the ASB.

Turn now to our predictions for microstructural evolution. Fig. 8 shows four snapshots of the dislocation density and grain size profiles in the hat-shaped sample, at the four instances marked (a) through (d) in the bottom panel 8e in that figure. We see an initial growth of the dislocation density in the shear band, accompanied by a mild decrease of the characteristic grain size, apparently representative of the initial nucleation of DRX grains at grain junctions as described in (Takaki et al., 2008, 2009). When the
Figure 5: Load-displacement curve computed using the finite element method with $h = 40\mu m$, compared to experimental measurements. Also shown is the load-displacement curve computed for “pseudo-steel” that does not undergo dynamic recrystallization, and with otherwise identical material parameters, to indicate the crucial role of DRX in material softening.
strain rate in the ASB becomes large enough, dislocations are converted into new grain boundaries. The grain size $d$ within the ASB at the end of the experiment goes down to 270 nm, two orders of magnitude below the initial grain size, while the dislocation density $\tilde{\rho}$ decreases concomitantly by more than two orders of magnitude, to a value even below that of the initial dislocation density. While our quantitative predictions need further verification from more advanced imaging techniques, which will further constrain the parameters that control the rates of grain size reduction and dislocation depletion, these results suggest the possibility of using severe loading conditions to produce ultrafine-grained material almost free of dislocations.

6. Concluding remarks

This paper presents the first implementation of the thermodynamic theory of dislocation plasticity and dynamic recrystallization in a finite-element simulation framework. Using known parameters for steel, plus a small handful of tunable parameters with available order-of-magnitude estimates, we have been able to fit the experimental stress-strain behavior of 316L stainless
Figure 7: Model prediction for the distribution of the temperature $T$ (left) and dimensionless effective temperature $\tilde{\chi}$ (right) in the hat-shaped sample, at the end of the experiment. Within the adiabatic assumption, thermal heating occurs almost exclusively within the shear band. The effective temperature saturates to $\tilde{\chi}_0 = 0.25$ in the shear band, but not far away from it.
Figure 8: Evolution of the dimensionless dislocation density $\tilde{\rho}$ (left), and the grain size $d$. Snapshots are taken at the instances marked (a) - (d) in panel (e) at the bottom.
steel that undergoes dynamic recrystallization, using only minimal assumptions. In so doing, we have also provided a simple estimate of the Taylor-Quinney coefficient. This serves as an indication of the validity and usefulness of the LBL-DRX theory. Our effort represents a first step in bridging between physical theories and numerical simulations; there remains substantial work to be done in this area, including more sophisticated finite-element implementations that address the issue of shear-band width and mesh dependency. We conclude with a plea for more detailed imaging and thermomechanical measurements of the recrystallization process, in order to shed light on the nature of ASBs and further validate the theory via a more rigorous constraint of parameters appropriate for steel and other materials.

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