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Size-effects due to Burgers tensor in classical deformation of isotropic thermoplastic materials

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Abstract. This work considers size-effects phenomena associated with Burgers tensor and heat transfer in isotropic plastic materials under thermal loading. The virtual power principle, the first and second laws of thermodynamics are used to obtain the balance of forces, the balance of energy, and the free-energy imbalance in local forms. Also, the constitutive relations for microscopic stresses associated with the Burgers tensor are obtained. The balance of microscopic forces is supplemented with the constitutive relations for the stresses to form the plastic flow rule. The presence of material length scale in the flow rule shows that it is possible to study size effects through the Burgers tensor.

Introduction

Investigations have shown that within the micron range of about 500 nanometers to 50 micrometers, most metals generally exhibit size-dependent behaviors. These size-effects are not known within the context of the classical plasticity because of its inability to accommodate intrinsic material length scales. The theories of strain gradient plasticity have been developed to address this shortcoming.

There are a number of phenomenological gradient theories in the literature, with the earliest attempt by Aifantis [1] whose theory incorporates and energetic length scale via the Laplacian of the accumulated plastic strain within a modified von Mises yield criterion for the stress. Other well established theories oinclude the works of Gurtin [2], Gudmundson [3] and Gurtin and Anand [4].

Recently, Borokinni *et.al.,*[5] investigated size-effects in isotropic materials associated with the divergence of plastic distortion. The work shows that the divergence of the transpose of plastic distortion is a measure of the skew part of the Burgers tensor. However, it is observed that such size-effect does not include the symmetric part of the Burgers tensor which also plays a role in investigating size-effects.

Furthermore, many theories of gradient plasticity are purely mechanical, and so not much attention is given to thermoplastic materials exhibiting size-dependent behaviors.

This paper present a coupled thermo-mechanical theory of distortion gradient plasticity that accounts for the Burgers tensor.

Basic Kinematics Relations

Suppose a point $\boldsymbol{X}$ of a body B in a region of space E has a displacement $\boldsymbol{u}$ at time t. The small deformation theory of continuum plasticity allows the displacement gradient $\nabla\boldsymbol{u}$ to be additively decomposed

$$\nabla\boldsymbol{u} = \boldsymbol{H}^{e} + \boldsymbol{H}^{p} \quad (1)$$

into elastic distortion $\boldsymbol{H^e}$ and plastic distortion $\boldsymbol{H^p}$. The second order tensor $\boldsymbol{H^e}$ measures the stretch and rotation of the underlying material structure, in this case, a lattice. The second order tensor $\boldsymbol{H^p}$ measures defects in that material structure arising from the motion of dislocations through the lattice. The Burgers tensor $\boldsymbol{G}$ is defined as the second order tensor

$$\boldsymbol{G} = \nabla \times \boldsymbol{H^p}, \tag{2}$$

which is also a measure of defect in the material associated with geometrically necessary dislocation densities (GNDs). For most metals, the volumetric change is not accompanied by plastic deformation, and so the trace of $\boldsymbol{H^p}$ is zero. That is,

$$tr\boldsymbol{H^p} = 0. \tag{4}$$

Macroscopic and Microscopic Forces

Here, we introduce power expended through the Burgers tensor rate $\dot{\boldsymbol{G}}$ by a second order microscopic stress denoted as $\boldsymbol{S}$. Thus, we shall assume the following:

- The Cauchy stress $\boldsymbol{T}$ is work-conjugate to the elastic distortion $\boldsymbol{H^e}$;
- The symmetric and deviatoric plastic microscopic stress $\boldsymbol{T^p}$ is work-conjugate to the plastic distortion $\boldsymbol{H^p}$; and
- The second order microscopic stress $\boldsymbol{S}$ is work-conjugate to the Burgers tensor $\boldsymbol{G}$.

In addition to work done by the body force $\boldsymbol{b}$ and macrotraction force $\boldsymbol{t}$, we assume that there exist a microtraction stress tensor $\boldsymbol{K}$ which is work-conjugate to the plastic distortion rate.
The macroscopic force balance is the classical momentum equation in local form given by

$$\text{div}\boldsymbol{T} + \boldsymbol{b} = \boldsymbol{0} \ \text{ in } P, \text{ and } \ \boldsymbol{Tn} = \boldsymbol{t} \ \text{ in } \ \partial P, \tag{5}$$

where P is an arbitrary small portion of the body B and ∂P is the boundary of P.
To obtain the microscopic force balance, we note that the rate-like kinematic relation is given by

$$\nabla\dot{\boldsymbol{u}} = \dot{\boldsymbol{H}}^e + \dot{\boldsymbol{H}}^p. \tag{6}$$

If the motion is microscopic then $\dot{\boldsymbol{u}} = \boldsymbol{0}$, so that $\dot{\boldsymbol{H}}^e = -\dot{\boldsymbol{H}}^p$. The power balance is given by

$$\int_P \left(\boldsymbol{T}:\dot{\boldsymbol{H}}^e + \boldsymbol{T^p}:\dot{\boldsymbol{H}}^p + \boldsymbol{S}:\dot{\boldsymbol{G}}\right)dV = \int_P \boldsymbol{b}\cdot\dot{\boldsymbol{u}}\,dv + \int_{\partial P}\left(\boldsymbol{t}\cdot\dot{\boldsymbol{u}} + \boldsymbol{K}:\dot{\boldsymbol{H}}^p\right)dA. \tag{7}$$

For microscopic motion, we have

$$\int_P \left((\boldsymbol{T^p} - \boldsymbol{T_o}):\dot{\boldsymbol{H}}^p + \boldsymbol{S}:\dot{\boldsymbol{G}}\right)dV = \int_{\partial P} \boldsymbol{K}:\dot{\boldsymbol{H}}^p\,dA, \tag{8}$$

where the quantity $\boldsymbol{T_o}$ is the deviatoric part of the Cauchy stress tensor $\boldsymbol{T}$.
We note that

$$\boldsymbol{S}:\dot{\boldsymbol{G}} = S_{ij}\mathcal{E}_{irs}H^p_{js,r}.$$

Define the component M_{jsr} of the hyperstress $\mathbb{M}$ as

$$M_{jsr} = S_{ij}\mathcal{E}_{irs}. \tag{9}$$

The power balance in Eq. 8 can be written as

$$\int_P \left((\boldsymbol{T^p} - \boldsymbol{T_o}): \dot{\boldsymbol{H}}^p + \mathbb{M} \vdots \nabla\dot{\boldsymbol{H}}^{\boldsymbol{p}}\right) dV = \int_{\partial P} \boldsymbol{K}: \dot{\boldsymbol{H}}^p \, dA. \tag{10}$$

By Gauss divergence theorem, the microscopic force balance in local form is given as

$$\boldsymbol{T_o} = \boldsymbol{T^p} - \mathrm{div}\mathbb{M}, \tag{11}$$

with microtraction condition given as

$$\mathbb{M}\boldsymbol{n} = \boldsymbol{K}. \tag{12}$$

Balance of Energy

The balance of energy is essentially the first law of thermodynamics which is mathematically written as

$$\int_P \dot{\mathcal{E}}\, dV = \int_P \boldsymbol{T}: \dot{\boldsymbol{H}}^{\boldsymbol{e}}\, dV + \int_P \boldsymbol{T^p}: \dot{\boldsymbol{H}}^{\boldsymbol{p}}\, dV + \int_P \mathbb{M} \vdots \nabla\dot{\boldsymbol{H}}^{\boldsymbol{p}}\, dV - \int_{\partial P} \boldsymbol{q}\cdot\boldsymbol{n}\, dV + \int_P Q\, dV, \tag{13}$$

where $\mathcal{E}$ is the internal energy measured per unit volume, $\boldsymbol{q}$ is the heat flux measured per unit area, and Q is the heat supply measures per unit volume.
By using the Gauss divergence theorem and noting that P is arbitrary, then the balance of energy in local form is given by

$$\dot{\mathcal{E}} = \boldsymbol{T}: \dot{\boldsymbol{H}}^{\boldsymbol{e}} + \boldsymbol{T^p}: \dot{\boldsymbol{H}}^{\boldsymbol{p}} + \mathbb{M} \vdots \nabla\dot{\boldsymbol{H}}^{\boldsymbol{p}} - \mathrm{div}\boldsymbol{q} + Q. \tag{14}$$

Entropy Imbalance

Let η be the entropy at an arbitrary point of P. The second law of thermodynamics in local form is the given by the Clausius-Duhem inequality

$$\dot{\eta} \geq -\mathrm{div}\left(\frac{\boldsymbol{q}}{\vartheta}\right) + \frac{Q}{\vartheta}, \tag{15}$$

where $\vartheta > 0$ is the absolute temperature.
The free-energy φ is defined via the relation

$$\mathcal{E} = \varphi + \vartheta\eta,$$

so that we have

$$\dot{\mathcal{E}} = \dot{\varphi} + \vartheta\dot{\eta} + \dot{\vartheta}\eta. \tag{16}$$

The balance of energy in term of free-energy and entropy is given by

$$\dot{\varphi} + \vartheta\dot{\eta} + \dot{\vartheta}\eta = \boldsymbol{T}:\dot{\boldsymbol{H}}^{\boldsymbol{e}} + \boldsymbol{T}^{\boldsymbol{p}}:\dot{\boldsymbol{H}}^{\boldsymbol{p}} + \mathbb{M} \vdots \nabla\dot{\boldsymbol{H}}^{\boldsymbol{p}} - \mathrm{div}\boldsymbol{q} + Q$$

$$\Longrightarrow \qquad \boldsymbol{T}:\dot{\boldsymbol{H}}^{\boldsymbol{e}} + \boldsymbol{T}^{\boldsymbol{p}}:\dot{\boldsymbol{H}}^{\boldsymbol{p}} + \mathbb{M} \vdots \nabla\dot{\boldsymbol{H}}^{\boldsymbol{p}} - \mathrm{div}\boldsymbol{q} + Q \geq \dot{\varphi} + \eta\dot{\vartheta} + \frac{\boldsymbol{q}}{\vartheta}\cdot\nabla\vartheta - \mathrm{div}\boldsymbol{q} + Q. \qquad (17)$$

The free-energy imbalance essential for the development of thermodynamically consistent constitutive equations is given by

$$\dot{\varphi} + \eta\dot{\vartheta} - \boldsymbol{T}:\dot{\boldsymbol{H}}^{\boldsymbol{e}} - \boldsymbol{T}^{\boldsymbol{p}}:\dot{\boldsymbol{H}}^{\boldsymbol{p}} - \mathbb{M} \vdots \nabla\dot{\boldsymbol{H}}^{\boldsymbol{p}} + \frac{\boldsymbol{q}}{\vartheta}\cdot\nabla\vartheta \leq 0. \qquad (18)$$

Constitutive Relations

We shall assume that the free-energy φ is additively decomposed into

$$\varphi = \varphi^e + \varphi^p \qquad (19)$$

into elastic and plastic free-energies, and it is assumed that

$\varphi^e = \varphi^e(\boldsymbol{E}^{\boldsymbol{e}}, \vartheta)$ and $\varphi^p = \varphi^p(\boldsymbol{G}, \vartheta)$ so that we have $\varphi = \varphi(\boldsymbol{E}^{\boldsymbol{e}}, \boldsymbol{G}, \vartheta)$. (20)

Furthermore, let the plastic stress $\boldsymbol{T}^{\boldsymbol{p}}$ be purely dissipative and rate-independent, while $\mathbb{M}$ is purely energetic. By chain rule, we have

$$\dot{\varphi} = \frac{\partial\varphi}{\partial\vartheta}\dot{\vartheta} + \frac{\partial\varphi^e}{\partial\boldsymbol{E}^{\boldsymbol{e}}}:\dot{\boldsymbol{E}}^e + \frac{\partial\varphi^p}{\partial\boldsymbol{G}}:\dot{\boldsymbol{G}}. \qquad (21)$$

Observe that

$$\frac{\partial\varphi^p}{\partial\boldsymbol{G}}:\boldsymbol{G}^{\cdot} = \frac{\partial\varphi^p}{\partial G_{ij}}\,\varepsilon_{irs}\,\dot{H}^p_{js,r} \text{ and } \mathbb{M} \vdots \nabla\dot{\boldsymbol{H}}^p = \boldsymbol{S}:\dot{\boldsymbol{G}}.$$

The free energy imbalance becomes

$$\left(\frac{\partial\varphi}{\partial\vartheta} + \eta\right)\dot{\vartheta} + \left(\frac{\partial\varphi^e}{\partial\boldsymbol{E}^{\boldsymbol{e}}} - \boldsymbol{T}\right):\dot{\boldsymbol{E}}^e + \left(\frac{\partial\varphi^p}{\partial\boldsymbol{G}} - \boldsymbol{S}\right):\dot{\boldsymbol{G}} - \boldsymbol{T}^{\boldsymbol{p}}:\dot{\boldsymbol{H}}^{\boldsymbol{p}} + \frac{\boldsymbol{q}}{\vartheta}\cdot\nabla\vartheta \leq 0. \qquad (22)$$

By the Coleman-Noll procedure (Gurtin *et al.,* 2010), the constitutive relations for the entropy, Cauchy stress, plastic stress and polar microstresses are

$$\eta = -\frac{\partial\varphi}{\partial\vartheta}, \ \boldsymbol{T} = \frac{\partial\varphi^e}{\partial\boldsymbol{E}^{\boldsymbol{e}}}, \ \boldsymbol{S} = \frac{\partial\varphi^p}{\partial\boldsymbol{G}}. \qquad (23)$$

Clearly, we have

$$M_{jsr} = \mathcal{E}_{irs}\frac{\partial\varphi^p}{\partial G_{ij}}. \qquad (24)$$

The mechanical dissipation and heat conduction inequalities are thus given as

$$\boldsymbol{T^p}:\dot{\boldsymbol{H}}^{\boldsymbol{p}} \geq 0 \ \text{ and } \ \boldsymbol{q}\cdot\nabla\vartheta \leq 0. \tag{25}$$

Isotropic Thermoplastic Solids

Assume the quadratic form of the free energy

$$\varphi = \mu|\boldsymbol{E^e}|^2 + \frac{1}{2}\lambda|\mathrm{tr}\boldsymbol{E^e}|^2 + \frac{1}{2}\mu L^2|\boldsymbol{G}|^2 + (\boldsymbol{M^e}:\boldsymbol{E^e})(\vartheta-\vartheta_o) + (\boldsymbol{A}:\boldsymbol{G})(\vartheta-\vartheta_o) - \frac{c_o(\vartheta-\vartheta_o)^2}{2\vartheta_o}, \tag{26}$$

where $\boldsymbol{M^e}$ and $\boldsymbol{A}$ are the macroscopic and microscopic stress-temperature moduli respectively. Following Eqs. 24 and 26, the constitutive relations for isotropic materials are given as

$$\eta = -\boldsymbol{M^e}:\boldsymbol{E^e} - \boldsymbol{A}:\boldsymbol{G} + \frac{c_o(\vartheta-\vartheta_o)}{\vartheta_o} \tag{27a}$$
$$\boldsymbol{T} = 2\boldsymbol{E^e} + \lambda(\mathrm{tr}\boldsymbol{E^e})\boldsymbol{I} + \boldsymbol{M^e}(\vartheta-\vartheta_o) \tag{27b}$$
$$\boldsymbol{S} = \mu L^2\boldsymbol{G} + \boldsymbol{A}(\vartheta-\vartheta_o). \tag{27c}$$

We shall assume that the plastic stress $\boldsymbol{T^p}$ obeys the codirectionality constraint and the heat flux obeys the Fourier law, given as (Gurtin *et al.,* 2010; Borokinni *et al.,* 2020):

$$\boldsymbol{T^p} = Y_o\frac{\dot{\boldsymbol{H}}^p}{|\dot{\boldsymbol{H}}^p|} \qquad \text{for } \ \dot{\boldsymbol{H}}^p \neq \boldsymbol{0}, \ \text{ and } \ \boldsymbol{q} = -k\nabla\vartheta, \tag{28}$$

where $\boldsymbol{Y_o}$ and $\boldsymbol{k}$ are the flow resistance and coefficient of thermal conductivity respectively.
To obtain the non local plastic flow rule that account for size effect due to Burgers tensor, the following relations between the partial derivative of the Burgers tensor and partial derivatives of the plastic distortion tensor will be useful

$$\mathcal{E}_{irs}G_{ij,r} = H^p_{js,rr} - H^p_{jr,rs}, \tag{29}$$

where

$$\boldsymbol{G_{ij,r}} = \frac{\boldsymbol{\partial G_{ij}}}{\boldsymbol{\partial X_r}}, \qquad \boldsymbol{H^p_{js,rr}} = \frac{\boldsymbol{\partial^2 H^p_{js}}}{\boldsymbol{\partial X_r \partial X_r}} \ \textbf{and} \ \ \boldsymbol{H^p_{js,rr}} = \frac{\boldsymbol{\partial^2 H^p_{jr}}}{\boldsymbol{\partial X_r \partial X_s}}.$$

Also, observe that

$$\mathrm{div}\,\mathbb{M} = \mu L^2[\Delta\boldsymbol{H^p} - \nabla\mathrm{div}\boldsymbol{H^p}] + \boldsymbol{A}^{\mathrm{T}}(\nabla\vartheta\times).$$

Thus by substituting the relevant constitutive relations for the microscopic stresses as deduced from Eqs. 27c and 28, the non-local plastic flow rule accounting for size effect due to Burgers tensor is

$$\boldsymbol{T_o} + \boldsymbol{\mu L^2}[\Delta\boldsymbol{H^p} - \boldsymbol{\nabla}\textbf{div}\boldsymbol{H^p}] + \boldsymbol{A}^{\mathrm{T}}(\boldsymbol{\nabla\vartheta}\times) = \boldsymbol{Y_o}\frac{\dot{\boldsymbol{H}}^{\boldsymbol{p}}}{|\dot{\boldsymbol{H}}^{\boldsymbol{p}}|} \ \ \textbf{provided} \ \dot{\boldsymbol{H}}^{\boldsymbol{p}} \neq \boldsymbol{0}.$$

Conclusion

This paper has only presented plastic flow rule associated with the Burgers tensor. It has shown that the flow rule is non-local as it involves system of second-order partial differential equations in plastic distortion. Consequently, it is required that the plastic flow law be supplemented by appropriate initial-boundary conditions, and further, the system of equations obtained from balance of macroscopic forces, balance of energy and microscopic force balance be translated to variational problem, where well-posedness of the initial-boundary value problem could be investigated, and a finite element model can be provided. A report of the well-posedness and numerical implementations of this problem will be considered as a future work.

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