

Communication

# A Brief Note on the Nix–Gao Strain Gradient Plasticity Theory

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**Abstract:** The mathematical nature of the flow rule for the strain gradient plasticity theory proposed by Nix and Gao (W.D. Nix and H. Gao, *J Mech Phys Solids* 46(3), 411(1998)) is discussed based on the paradigm developed by Gurtin and Anand (M.E. Gurtin and L. Anand, *J Mech Phys Solids* 57 (3), 405 (2009)). It is shown that, when investigated on the basis of Gurtin–Anand theory, the Nix–Gao flow rule is a combination of constitutive equations for microstresses, balance law, and a constraint. As an accessory, we demonstrate that the strain gradient term introduced in the model is energetic. The results are obtained by combining a virtual-power principle of Fleck and Hutchinson, and the free-energy imbalance under isothermal conditions.

**Keywords:** strain gradient plasticity; principle of virtual power; defect energy; flow rule; material length scale

## 1. Introduction

Many experiments at small scales, including nano/microindentation [1], torsion of thin metallic wires [2–5], and bending of thin foils [6,7], have clearly demonstrated a strong size-dependent strengthening associated with non-uniform plastic deformation. The size-dependent behaviour cannot be captured by the classical plasticity theories, due to their lack of intrinsic material length scales. Besides, the problem of simple plastic shear in thin layers is important for the rapidly developing field of research on severe plastic deformations [8,9]. It has been demonstrated that the flow loses stability, and vortex-like motion occur due to large stress gradients in the plastic shear in thin layers [10–12]. Such a phenomenon also cannot be described by the conventional theories of plasticity [13]. Therefore, many theoretical works have been carried out to enclose strain gradient effects into a continuum theory of plasticity. Apparently, the earliest attempt at a phenomenological theory of strain gradient plasticity can be attributed to Aifantis [14,15], although the pioneering works on continuum dislocation theories which implicitly include length scales established for elastic-plastic crystals, date back to Kröner [16], Teodosiu [17], Lardner [18], and others in the 1960s and 1970s. Aifantis [8,9] proposed a flow rule by simply adding the nonlocal term to the conventional flow resistance. Thereafter, inspired by the concept of geometrically necessary dislocations (GNDs) [16,18–20], a number of strain gradient plasticity theories have been developed. Reviews on the current state of the art have been given by Fleck et al. [21], Lubarda [22], Bardella [23], and Liu and Dunstan [24]. It should be emphasized that the treatment throughout the paper is limited to small strains and isotropic solids. More physically realistic models, that account for nonlinearity and anisotropy of elasticity and slip, including the strain

gradient crystal plasticity theories [25–27] and the continuum theory of dislocations [28–30], are not considered at this stage.

The phenomenological theory of strain gradient plasticity developed by Fleck and Hutchinson [31] is a simple extension of rate-independent  $J_2$  theory. This model shares similar features with an earlier version proposed by Mühlhaus and Aifantis [32]. However, Gudmundson [33] firstly noted that the Fleck–Hutchinson theory [31] does not always satisfy the thermodynamic requirement on plastic dissipation. Afterward, Gurtin and Anand [34] investigated the physical nature of flow rules for theories of strain gradient plasticity proposed by Aifantis [14,15] and by Fleck and Hutchinson [31]. The authors concluded that the flow rule of the Fleck–Hutchinson theory is incompatible with thermodynamic restrictions related to the requirement of nonnegative plastic dissipation, unless the involved nonlocal term is dropped. Moreover, the authors also found that the flow rule of the gradient theory of Aifantis represents microscopic force balances supplemented by appropriate constitutive equations, and that the nonlocal term in the model is energetic. Alternatively, Gudmundson [33] and Gurtin and Anand [35] developed another class of formulations of strain gradient plasticity free of the thermodynamic deficiency. Recently, in order to eliminate the thermodynamic deficiency mentioned above, Hutchinson [36] also proposed a modified version of the theory of Fleck and Hutchinson [31], in which the higher order microstresses are partitioned into energetic (or recoverable) and dissipative (or unrecoverable) components.

In most of the modern SGP frameworks, both the energetic and dissipative gradient contributions have been introduced [33,35,37–39]. Especially, positive plastic dissipation has been ensured by the gradient theory of Gudmundson [33], thanks to the peculiar structure of the constitutive laws for the dissipative stresses, smartly relating the rates of the plastic strain and its gradient to finite stress measures. The role of energetic and dissipative gradient effects has been studied numerically by several authors [40–44]. However, as indicated by Fleck and Willis [45], the degree to which strain gradient effect is mainly energetic or dissipative remains unclear. The exact mechanisms by which GNDs lead to material strengthening are still controversial. On the one hand, GNDs may be considered to translate into an increase in free energy of the solid [38]. On the other hand, several experiments suggest that the core energy of dislocations stored during plastic deformation is much smaller than the plastic work dissipated in dislocation motion, such that the movement of GNDs in the lattice may contribute more to plastic dissipation [38].

Another attractive formulation of strain gradient plasticity is the mechanism-based gradient plasticity (MSG) proposed by Gao and co-workers [1,46], based on a multiscale framework linking the microscale concept of statistically stored dislocation (SSDs) and GNDs to the mesoscale notion of plastic strains and strain gradients. Inspired by the indentation experiments at small scales, Nix and Gao [1] firstly proposed a flow rule for strain gradient plasticity based on the Taylor-based hardening,

$$\tau = \sqrt{Y^2(e^p) + \beta |\nabla e^p|}, \quad (1)$$

where  $Y(e^p)$  is the conventional flow resistance,  $e^p$  is the accumulated plastic strain, and  $|\nabla e^p| = \sqrt{\nabla e^p \cdot \nabla e^p}$  is the effective strain gradient introduced by Aifantis and co-workers [14,32]. Note that the original expression of the Nix and Gao flow rule is  $\sigma_{flow} = Y_0 \sqrt{f^2(e^p) + l \eta_p} = \sqrt{[Y_0 f(e^p)]^2 + Y_0^2 l \eta_p}$ . In Equation (1), we assume  $Y(e^p) = Y_0 f(e^p)$ ,  $\eta_p = |\nabla e^p|$ , and  $\beta = Y_0^2 l$ , with  $Y_0$  being the initial flow resistance and  $l$  a material length scale introduced for dimension consistency. Moreover, the measure of strain gradient used here is different from that adopted by Nix and Gao [1], in which the contribution of elastic strain gradient is involved. The flow rule, Equation (1), is derived from the Taylor relation of the shear strength and the dislocation density. It has been widely used by many authors for developing various theories of strain gradient plasticity, e.g., MSG [46,47], the conventional theory of mechanism-based strain gradient plasticity (MSG) [48], the Taylor-based nonlocal theory of plasticity (TNT) [49,50], and the physically based gradient plasticity

theory (PGP) [51], etc. However, we are unaware of any detailed discussion of the thermodynamics related to Equation (1). Following Gurtin and Anand [34], one may ask:

1. Is Equation (1) a constitutive relation, a balance law, or a combination of both?
2. Whether the nonlocal term  $\beta|\nabla e^p|$  is energetic or dissipative, or even whether or not the theory is consistent with thermodynamics?

By combining the thermodynamical principle under isothermal conditions and the virtual-power principle of Fleck and Hutchinson [31], we perform a discussion on the mathematical nature of the famous flow rule for strain gradient plasticity proposed by Nix and Gao [1]. In order to elucidate whether the plastic-strain gradient term involved is energetic or dissipative, the general flow rule established by Gurtin and Anand [34] is adopted, and a form of quadratic defect energy is also assumed. It is our choice to investigate the Nix–Gao theory in light of the Gurtin–Anand theory. This will also afford us an opportunity to determine the differences between the two theories.

## 2. Kinematic Relations

Let  $\mathbf{u}(x, t)$  be the displacement vector at point  $x$  and time  $t$  of a particle in a body  $B$  undergoing infinitesimal deformation. By convention, the displacement gradient  $\nabla \mathbf{u}$  admits an additive decomposition

$$\nabla \mathbf{u} = \mathbf{H}^e + \mathbf{H}^p, \text{tr} \mathbf{H}^p = 0, \quad (2)$$

where  $\mathbf{H}^e$  is the elastic distortion,  $\mathbf{H}^p$  is the plastic distortion, and  $\text{tr} \mathbf{H}^p$  is the trace of plastic distortion. The elastic distortion accounts for both lattice stretching and rotation, while the plastic distortion accounts for the local deformation of material as a result of the formation and motion of dislocations through the material structure.  $\mathbf{H}^e$  and  $\mathbf{H}^p$  can be further decomposed, additively and uniquely, into symmetric and skew parts in the sense,  $\mathbf{H}^e = \mathbf{E}^e + \mathbf{W}^e$ ;  $\mathbf{H}^p = \mathbf{E}^p + \mathbf{W}^p$ , where  $\mathbf{E}^e = \text{sym} \mathbf{H}^e$ ,  $\mathbf{E}^p = \text{sym} \mathbf{H}^p$  and  $\mathbf{W}^e = \text{skw} \mathbf{H}^e$ ,  $\mathbf{W}^p = \text{skw} \mathbf{H}^p$ . Here,  $\text{sym} \mathbf{A}$  and  $\text{skw} \mathbf{A}$  are the symmetric and skew parts of tensor  $\mathbf{A}$ , respectively. We limit the discussion to a plastically irrotational material, i.e.,  $\mathbf{W}^p = 0$ . Hence, Equation (2) can be written as

$$\nabla \mathbf{u} = \mathbf{H}^e + \mathbf{E}^p, \text{tr} \mathbf{E}^p = 0 \quad (3)$$

In Gurtin and Anand [34], the flow direction  $\mathbf{N}^p$  is defined by

$$\mathbf{N}^p = \frac{\dot{\mathbf{E}}^p}{|\dot{\mathbf{E}}^p|}, \text{with } \dot{\mathbf{E}}^p \neq 0 \quad (4)$$

We denote the accumulated plastic strain by  $e^p$ , which is a function of space and time. The accumulated plastic strain is defined through its evolution equation

$$\dot{e}^p(\mathbf{x}, t) = |\dot{\mathbf{E}}^p(\mathbf{x}, t)| \text{ with } e^p(\mathbf{x}, 0) = 0 \quad (5)$$

By Equations (4) and (5), the plastic strain rate  $\dot{\mathbf{E}}^p$  has the form

$$\dot{\mathbf{E}}^p = \dot{e}^p \mathbf{N}^p \quad (6)$$

Taking the time derivative of Equation (3) and using Equation (6), we obtain the basic kinematic rate equation

$$\nabla \dot{\mathbf{u}} = \dot{\mathbf{H}}^e + \dot{e}^p \mathbf{N}^p, \text{tr} \mathbf{N}^p = 0 \quad (7)$$

Equation (7) is useful in the derivation of the force balances established by Gurtin and Anand [34].

### 3. Virtual-Power Principle and Force Balances

The virtual-power principle of Fleck and Hutchinson [31] and the force balances have been presented in Ref. [34]. We give a brief summary here. Microscopic stresses include plastic microscopic stress  $T^p$  power-conjugate to plastic strain rate  $\dot{E}^p$  and third-order microscopic hyperstress  $\mathbb{K}^p$  power-conjugate to the plastic strain gradient rate  $\nabla\dot{E}^p$ . Note that  $T^p$  is dissipative and deviatoric, and  $\mathbb{K}^p$  is symmetric and deviatoric in its first two indices.

The codirectionality hypothesis states that the deviatoric part of the macroscopic stress  $T_o$  and the plastic strain rate flow in the same direction in the sense

$$\frac{T_o}{|T_o|} = \frac{\dot{E}^p}{|\dot{E}^p|} \equiv N^p \quad (8)$$

The resolved shear denoted by  $\tau$  is defined by

$$\tau = T : N^p = T_o : N^p \text{ with } T_o = \tau N^p \quad (9)$$

here,  $T$  is known as the Cauchy stress, power-conjugate to the elastic distortion rate  $\dot{H}^e$ . The local power expended within an arbitrary portion of the body by the microscopic stresses  $T^p$  and  $\mathbb{K}^p$  can be written as

$$T^p : \dot{E}^p + \mathbb{K}^p : \nabla\dot{E}^p = \tau^p \dot{e}^p + \zeta^p \cdot \nabla\dot{e}^p \quad (10)$$

here,  $\tau^p$  and  $\zeta^p$  are scalar and vector microstresses, respectively. These are defined by

$$\tau^p = T_{ij} N_{ij}^p + K_{ijk}^p N_{ijk}^p \text{ and } \zeta_k^p = K_{ijk}^p N_{ij}^p \quad (11)$$

where  $K_{ijk}^p$  and  $N_{ij}^p$  are components of  $\mathbb{K}^p$  and  $N^p$  respectively. The microscopic stresses  $\tau^p$  and  $\zeta^p$  can be additively decomposed into dissipative and energetic parts.

The internal power expenditure  $W_{int}(P)$  within a portion  $P$  of a body  $B$  is given by

$$\begin{aligned} W_{int}(P) &= \int_P (T : \dot{E}^e + T^p : \dot{E}^p + \mathbb{K}^p : \nabla\dot{E}^p) dV \\ &= \int_P (T : \dot{E}^e + \tau^p \dot{e}^p + \zeta^p \cdot \nabla\dot{e}^p) dV \end{aligned} \quad (12)$$

To obtain the power expended on  $P$  of  $B$  by external forces, we denote  $t(\mathbf{n})$  as the macrotraction on the boundary  $\partial P$  and  $\mathbf{b}$  the body force, both conjugate to the velocity  $\dot{\mathbf{u}}$ . Due to the presence of gradient term  $\nabla\dot{e}^p$ , considering the divergence theorem, we denote  $k(\mathbf{n})$  as the microtraction on  $\partial P$  conjugate to  $\dot{e}^p$ . The vector  $\mathbf{n}$  denotes the outward unit normal to the boundary  $\partial P$ .

The power expended  $W_{ext}(P)$  on  $P$  by the external agencies is given by

$$W_{ext}(P) = \int_{\partial P} \mathbf{t} \cdot \dot{\mathbf{u}} da + \int_P \mathbf{b} \cdot \dot{\mathbf{u}} dV + \int_{\partial P} k \dot{e}^p da \quad (13)$$

Gurtin and Anand [34] introduced a generalized virtual velocity in the form of a list  $\vartheta = \{\tilde{\mathbf{u}}, \tilde{E}^e, \tilde{e}^p\}$  consistent with the equation

$$\text{sym}\nabla\tilde{\mathbf{u}} = \tilde{E}^e + \tilde{e}^p N^p \quad (14)$$

The principle of virtual power states that

$$\int_P (T : \tilde{E}^e + \tau^p \tilde{e}^p + \zeta^p \cdot \nabla\tilde{e}^p) dV = \int_{\partial P} \mathbf{t} \cdot \tilde{\mathbf{u}} da + \int_P \mathbf{b} \cdot \tilde{\mathbf{u}} dV + \int_{\partial P} k \tilde{e}^p da \quad (15)$$

Consequences of the virtual power balance Equation (15) are

1. Macroscopic force balance with concomitant macrotraction condition

$$\text{Div} \mathbf{T} + \mathbf{b} = 0 \text{ in } P, \mathbf{T} \mathbf{n} = \mathbf{t} \text{ on } \partial P \quad (16)$$

2. Microscopic force balance and its concomitant microtraction condition

$$\boldsymbol{\tau} = \tau^p - \text{Div} \boldsymbol{\zeta}^p \text{ in } P, \boldsymbol{\zeta}^p \cdot \mathbf{n} = k(\mathbf{n}) \text{ on } \partial P \quad (17)$$

#### 4. Free Energy, Constitutive Relations, and Gurtin–Anand Flow Rule [34]

Let  $\psi$  be the free energy measured per unit volume in an arbitrary region  $P$  of a body. The combination of the first and the second laws of thermodynamics under isothermal condition implies that the temporal increase of the free energy over the subregion  $P$  cannot exceed the external power expended on  $P$ . Following Gurtin and Anand [34], the local free energy imbalance is given as

$$\dot{\psi} - \mathbf{T} : \dot{\mathbf{E}}^e - \tau^p \dot{e}^p - \boldsymbol{\zeta}^p \cdot \nabla \dot{e}^p \leq 0 \quad (18)$$

It is known that the energetic microstresses are obtained from terms relating to the partial derivatives of the free energy with respect to the conjugated kinematic variables, while the dissipative microscopic stresses usually satisfy dissipation inequality, and are related to the kinematic rate variables. Gurtin and Anand [34] assumed the free-energy is decomposed into elastic free energy  $\psi^e(E^e)$  and plastic free-energy  $\psi^p(e^p, \mathbf{g})$ , where  $\mathbf{g} = \nabla e^p$ . By convention, the elastic stress  $\mathbf{T}$  is defined by

$$\mathbf{T} = \frac{\partial \psi^e(E^e)}{\partial E^e} \quad (19)$$

and the energetic parts of  $\tau^p$  and  $\boldsymbol{\zeta}^p$  denoted, respectively, as  $\tau_{en}^p$  and  $\boldsymbol{\zeta}_{en}^p$ . They are defined by

$$\tau_{en}^p = \frac{\partial \psi^p}{\partial e^p} \text{ and } \boldsymbol{\zeta}_{en}^p = \frac{\partial \psi^p}{\partial \mathbf{g}} \quad (20)$$

Denote the dissipative part of the microscopic stresses  $\tau^p$  and  $\boldsymbol{\zeta}^p$  by  $\tau_{dis}^p$  and  $\boldsymbol{\zeta}_{dis}^p$ , respectively. Define

$$\tau_{dis}^p = \tau^p - \tau_{en}^p \text{ and } \boldsymbol{\zeta}_{dis}^p = \boldsymbol{\zeta}^p - \boldsymbol{\zeta}_{en}^p \quad (21)$$

Substituting Equations (19)–(21) into Equation (18), we have the local dissipation inequality

$$\tau_{dis}^p \dot{e}^p + \boldsymbol{\zeta}_{dis}^p \cdot \nabla \dot{e}^p \geq 0 \quad (22)$$

The general flow rule of Gurtin and Anand [34], for the strain gradient plasticity involving the accumulated plastic strain, is obtained by substituting the constitutive relations for the microscopic stresses, Equations (20) and (21), into the microscopic force balance, Equation (17). The flow rule is given as

$$\boldsymbol{\tau} = \tau_{dis}^p + \frac{\partial \psi^p}{\partial e^p} - \text{Div} \left( \boldsymbol{\zeta}_{dis}^p + \frac{\partial \psi^p}{\partial \mathbf{g}} \right) \quad (23)$$

Hence the flow rule consists of the microscopic force balance augmented with thermodynamically consistent constitutive relation for the microscopic stresses.

In order to derive the Aifantis model, Gurtin and Anand [34] assumed a quadratic defect energy of the form

$$\psi^p(\mathbf{g}) = \frac{1}{2} \beta^* |\mathbf{g}|^2 \quad (24)$$

where  $\beta^* > 0$  is a constant. This form of defect energy implies that  $\tau_{en}^p = 0$ . By Equation (20), the microscopic stress vector  $\boldsymbol{\zeta}_{en}^p$  is deduced as

$$\xi_{en}^p = \beta^* g \quad (25)$$

In addition, Gurtin and Anand [4] also assumed that

$$\tau_{dis}^p = Y(e^p) \text{ and } \xi_{dis}^p = 0 \quad (26)$$

where  $Y(e^p)$  is the coarse grain flow resistance. Substituting Equations (25) and (26) into Equation (23), we obtain the Aifantis flow rule

$$\tau = Y(e^p) - \beta^* \Delta e^p \quad (27)$$

The nonlocal term  $\beta^* \Delta e^p$  is energetic, since it is related to the defect free energy. It is obvious that the Aifantis model is thermodynamically consistent.

### 5. Mathematical Nature of the Nix–Gao Flow Rule

In what follows, we discuss the mathematical nature of Nix–Gao flow rule based on the Gurtin–Anand general flow rule, Equation (23), and the quadratic defect energy, Equation (24). As we mentioned earlier, the Nix–Gao flow rule has the form

$$\tau = \sqrt{Y^2(e^p) + \beta |\nabla e^p|} \quad (28)$$

We have raised the following questions:

1. Is the Nix–Gao flow rule, Equation (28), a constitutive relation, a balance law, or a combination of both?
2. Whether the nonlocal term  $\beta |\nabla e^p|$  is energetic or dissipative, or even whether or not the theory is consistent with the laws of thermodynamics?

In view of Gurtin and Anand [34], we take the same assumptions as in Section 4. Comparing the general flow rule Equation (23) and the flow rule Equation (28), one can deduce that  $\text{Div} \xi_{en}^p$  has the form

$$\text{Div} \xi_{en}^p = Y(e^p) - \sqrt{Y^2(e^p) + \beta |\nabla e^p|} \text{ for } e^p \neq 0 \quad (29)$$

here, we have already assumed that  $\tau_{en}^p = 0$  and  $\xi_{dis}^p = 0$ . Note that the solution  $\text{Div} \xi_{en}^p = Y(e^p) + \sqrt{Y^2(e^p) + \beta |\nabla e^p|}$  is not considered, since from  $\tau = \sqrt{Y^2(e^p) + \beta |\nabla e^p|}$ , we have  $\text{Div} \xi_{en}^p = \tau_{dis}^p - \tau = Y(e^p) - \sqrt{Y^2(e^p) + \beta |\nabla e^p|}$ . We recall the following equations [4]:

- (i) Microforce balance

$$\tau - \tau_{dis}^p = -\text{Div} \xi_{en}^p \quad (30)$$

- (ii) Constitutive relations for the microscopic stresses

$$\tau_{dis}^p = Y(e^p), \quad \xi_{en}^p = \frac{\beta l}{Y_0} \nabla e^p \quad (31)$$

where  $\beta = Y_0^2 l$ , and a comparison with Equation (25) implies that  $\beta^*$  has the specific form

$$\beta^* = Y_0 l^2 \quad (32)$$

- (iii) Flow rule of Aifantis (i.e., Equation (27))

$$\tau = Y(e^p) - \frac{\beta l}{Y_0} \Delta e^p \quad (33)$$

substituting Equation (31) into Equation (28), we arrive at

$$\tau^2 - (\tau_{dis}^p)^2 = \beta |\nabla e^p| \quad (34)$$

and making use of Equations (30) and (31), we have

$$(\tau - \tau_{dis}^p)(\tau + \tau_{dis}^p) = -(\tau + \tau_{dis}^p) \frac{\beta l}{Y_0} \Delta e^p \quad (35)$$

Thus,

$$\tau + \tau_{dis}^p = -\frac{Y_0}{l} \frac{|\nabla e^p|}{\Delta e^p} \quad (36)$$

It seems that Equation (36) is a constraint and not a constitutive law, since the constitutive relations and the balance law for the system of microforces are known, a priori. Clearly, we show that the Nix–Gao flow rule Equation (28) is compatible with thermodynamics, if the constraint Equation (36) is satisfied. Actually, we are unaware of any discussion of the thermodynamic aspects of the Nix–Gao flow rule in the literature, although a common viewpoint seems to be that the gradient term is dissipative. However, our analysis, based on the laws of thermodynamics, as expressed in the free-energy imbalance, indicates that the gradient term involved is energetic, which provides a definitive answer to the question.

## 6. Conclusions

The thermodynamic admissibility of the flow rule due to Nix and Gao [1] has been examined within the paradigm set out by Gurtin and Anand [34]. It has been shown that the Nix–Gao theory—in the light of Gurtin and Anand [34]—is a combination of (i) constitutive relations (see Equation (31)) for the microstresses, (ii) balance law given by Equation (30), and (iii) an additional constraint given by Equation (36). This constraint establishes the difference between the Nix–Gao theory and the Aifantis theory. What is important, the material length scale  $l$  is associated with energetic microstress vector  $\zeta_{en}^p$  (see Equation (31)). It is concluded that the term  $\beta|\nabla e^p|$  is energetic, and is consistent with the law of thermodynamics provided the constraint condition and the assumptions leading to the Aifantis theory are always satisfied. It should be noted that, for deriving the constraint condition, we take a specific form of defect energy that corresponds to the Aifantis model. If we alter the form of the defect energy, the resultant constraint may change. However, the physical feature of the Nix–Gao flow rule remains. In summary, fundamental issues which are raised by Gurtin and Anand [4], for Aifantis-type strain gradient plasticity theories, are extended to the Nix–Gao theory. The issues will be interesting and important in the field of small scale plasticity.

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