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Variational gradient plasticity at finite strains. Part I: Mixed potentials for the evolution and update problems of gradient-extended dissipative solids

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This work outlines a theoretical and computational framework of finite inelasticity with length scales based on a rigorous exploitation of *mixed variational principles*. In contrast to classical local approaches to inelasticity based on locally evolving internal variables, order parameter fields are taken into account governed by additional balance-type partial differential equations including micro-structural boundary conditions. This incorporates non-local dissipative effects based on length scales, which reflect properties of the material micro-structure. Typical examples are phase field theories, gradient damage and strain gradient plasticity. We outline unified minimization and saddle point principles for the evolution problem of first-order gradient-type standard dissipative solids. Particular emphasis is put on mixed multi-field representations, where both the microstructural variable itself as well as its dual driving force are present. These settings are needed for models with threshold functions formulated in the space of the driving forces, in particular for finite gradient plasticity. The central aim is to *define constitutive rate-type and algorithmic incremental potentials*, whose variational derivatives govern the coupled macro- and micro-balances in both the continuous as well as the time-discrete setting. Their existence underlines the inherent symmetry of standard dissipative solids. We demonstrate *geometrically consistent constructions* of these potentials for important classes of finite inelasticity, providing a fresh look on models of *multiplicative and additive gradient plasticity* of single crystals and amorphous materials. The potentials provide maximum compact representations of those complex material models, are the cornerstones of a subsequent mixed finite element design and should be considered as the *primary objects* for the theoretical and computational modeling.

1. Introduction

The modeling of size effects in solids, such as the width of shear bands or the grain size dependence of the plastic flow in polycrystals (Hall–Petch effect), need to be based on non-standard continuum theories of inelasticity which incorporate length-scales. With the ongoing trend of miniaturization and nanotechnology, the predictive modeling of these effects play an increasingly important role. Non-standard modeling approaches to solids, which include independent variables accounting for length scales and long range effects of a material microstructure, can be traced back to the work Cosserat and Cosserat [1] on *micropolar theories*, Mindlin [2] and Toupin [3] on *micromorphic theories* and Capriz et al. [4] on *continua with affine*

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micro-structure. The book Capriz [5] outlines a general framework suitable for establishing order parameter-based models of continua with micro-structures. Recent comprehensive treatments in this spirit are the works of Svendsen [6] and Mariano [7]. General *gradient-type dissipative solids* were considered in Maugin [8] and Maugin & Muschik [9,10] by an extension of the classical local theory of internal variables, governed by the method of virtual power as reviewed in Maugin [11]. The monograph of Frémond [12] outlines a treatment of first-order gradient-type dissipative solids in the full thermodynamic context. Forest [13] suggests a unified concept for the extension of standard local to generalized micromorphic theories. In all of these treatments, a critical aspect is to define the *working of microstructural processes* of the material. We refer to the works Gurtin [14–16] for a rigorous account of this viewpoint. These processes are described by the micro-structural fields (order parameters or generalized internal variables). Hence, substructural interactions are accompanied by explicit power expressions in the rate of the micro-structural variables, yielding *additional balance-type partial differential equations* associated with the micro-structure. As a consequence, standard macro-balances of mass and momentum are coupled with additional micro-balance equations, which govern micro-force-systems associated with the order parameters. Typical examples of these theoretical frameworks are the treatments of Gurtin [14], Fried & Gurtin [17], Hildebrand & Miehe [18] on diffusive *phase transformations*, the formulations Frémond & Nedjar [19], Peerlings et al. [20,21] of *gradient damage models* and the approach of Bourdin et al. [22], Miehe et al. [23,24] and Borden et al. [25] to *diffusive fracture*. They all consider scalar fraction fields as micro-structural field variables and provide length scales such as finite widths of interfaces or localized zones. The incorporation of size effects is of particular importance when plastic deformations are modeled at small scales. Over the last two decades, several micromechanically-based approaches to *gradient plasticity* were developed. Here, size effects can be traced back to lattice-curvature-based dislocation densities as outlined in Nye [26], Kröner [27], Ashby [28], Fleck et al. [29], Fleck & Hutchinson [30], Nix & Gao [31] and Arzt [32]. Strain-gradient theories for single crystal plasticity based on micro-force balances are proposed by Gurtin [15,33], Menzel & Steinmann [34], Svendsen [35] and Evers et al. [36]. Purely phenomenologically-based theories of gradient plasticity with micro-structural field variables are considered in the works of Aifantis [37], Mühlhaus & Aifantis [38], Gurtin [16], Gurtin & Anand [39], Geers [40], Reddy et al. [41] and Fleck & Willis [42,43]. However, a unified framework of finite gradient plasticity based on mixed variational principles is missing in the literature.

The field equations of dissipative solids may be related to *rate-type incremental variational formulations*. We refer to the contributions on *local plasticity* by Hill [44], Martin [45], Han & Reddy [46], Simó & Honein [47], Simó & Hughes [48], Ortiz & Stainier [49], Miehe [50] and Carstensen et al. [51]. These variational principles may be considered as the canonically compact formulations of the boundary value problem for standard dissipative solids defined in Biot [52], Ziegler [53] and Halphen & Nguyen [54]. Though restricted to the so-called associative theory of plasticity governed by *normality rules* for the evolution of the internal variables, which are related to dissipation functions, they cover the most important models for engineering application. However, the above mentioned treatments are restricted to *local* theories, where the evolution of the order parameters is described by ordinary differential equations. The recent work of Miehe [55] outlines a generalization towards a unified variational framework with mixed multi-field representations, which provides an embedding of those model problems under the category of gradient-enhanced standard dissipative media. A central aspect is the construction of *rate-type continuous and incremental algorithmic potentials*, which govern the evolution problem of those solids.

In this work, we extend this formulation to the large-strain format with a focus on gradient plasticity and develop characteristic types of multi-field variational principles, which are of practical importance and well suited for numerical implementation. We focus on gradient-extended dissipative solids, whose local constitutive state depends on a *macro-motion* $\boldsymbol{\varphi}$ and a *micro-motion* $\mathfrak{q}$ through

$$\mathfrak{c} := \{\boldsymbol{\varphi}, \nabla\boldsymbol{\varphi}, \nabla^2\boldsymbol{\varphi}, \ldots, \mathfrak{q}, \nabla\mathfrak{q}, \nabla^2\mathfrak{q}, \ldots\}.$$

We develop *two-field minimization principles* for quasi-static applications, governed by *rate-type potentials* based on constitutive energy storage and dissipation functions ψ and ϕ,

$$\{\dot{\boldsymbol{\varphi}}, \dot{\mathfrak{q}}\} = \arg\left\{\inf_{\boldsymbol{\varphi}}\inf_{\dot{\mathfrak{q}}} \int_{\mathcal{B}} \left\{\frac{d}{dt}\psi(\mathfrak{c}) + \phi(\dot{\mathfrak{c}};\mathfrak{c})\right\} dV\right\},$$

which are shown to fully determine the micro- and macro-balances of gradient-extended dissipative solids. They are extended to *three-field saddle point principles*, incorporating the dissipative driving force $\mathfrak{b}$ as a third field, e.g.

$$\{\dot{\boldsymbol{\varphi}}, \dot{\mathfrak{q}}, \mathfrak{b}\} = \arg\left\{\inf_{\boldsymbol{\varphi}},\inf_{\dot{\mathfrak{q}}}\sup_{\mathfrak{b}} \int_{\mathcal{B}} \left\{\frac{d}{dt}\psi(\mathfrak{c}) + \mathfrak{b}\cdot\dot{\mathfrak{c}} - \phi^*(\mathfrak{b};\mathfrak{c})\right\} dV\right\}$$

in order to cover problems with dual dissipation functions ϕ^* formulated in terms of the driving forces $\mathfrak{b}$ dual to constitutive state $\mathfrak{c}$. Finally, we outline *four-field saddle point principles* based on energy and threshold functions ψ and f

$$\{\dot{\boldsymbol{\varphi}}, \dot{\mathfrak{q}}, \mathfrak{b}, \lambda\} = \arg\left\{\inf_{\dot{\boldsymbol{\varphi}},\dot{\mathfrak{q}}}\sup_{\mathfrak{b},\lambda\geqslant 0} \int_{\mathcal{B}} \left\{\frac{d}{dt}\psi(\mathfrak{c}) + \mathfrak{b}\cdot\dot{\mathfrak{c}} - \lambda f(\mathfrak{b};\mathfrak{c})\right\} dV\right\}$$

with a Lagrange parameter λ as the fourth field. The kernels π, π^* and π^*_λ of the above integrals, extracted in the three Boxes 1, 2 and 3 below, provide *rate-type potentials per unit volume* whose functional or variational derivatives fully determine all continuum field equations of gradient-extended dissipative solids as the Euler equations of the above variational principles. These potentials provide the most compact representations of those complex material models, and are the cornerstones of a