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# Surface effects, boundary conditions and evolution laws within second strain gradient plasticity

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ABSTRACT

The principle of the virtual power (PVP) is used in conjunction with the concepts of "energy residual" and "insulation condition" to address second strain gradient plasticity. The *energy residual* with its typical divergence format is an extra stress power playing the role of basic state variable to describe the gradient effects, whereas the *insulation condition* constitutes a global energy characterization of the body as part of the body/environment system. The microstructure of a second strain gradient material (but not of a first strain gradient one) is shown to exhibit surface effects with the formation of a thin boundary layer. This boundary layer is in local (and global) equilibrium according to the principles of the material surface mechanics and supports the boundary microtractions, except a part (Cauchy-like traction) transmitted to the bulk microstructure; it works as a structured two-dimensional manifold replacing the conventional purely geometrical concept of boundary surface. By the insulation condition the higher order boundary conditions are determined (for first and second strain gradient plasticity), including those for the moving elastic/plastic interface. Besides the usual continuity boundary conditions, some extra (at most three) "rest" boundary conditions are required to fix the current location of the interface. The restrictions on the constitutive equations and the evolution laws are also addressed, whereby a mixed modeling scheme is used to model the dissipative stresses. An application to an elastic-softening bar in extension shows the ability of the proposed model to capture and describe the formation of a multi-waved deformation pattern within the localization band.



## 1. Introduction

Second strain gradient plasticity models are here defined as elastic–plastic material models featured by a free energy function whose arguments include the gradients of one or more plastic strain measures up to the second order. The latter models have attracted relatively little attention within the wide literature. A brief review of the available literature on this subject and related issues is given hereafter.

Basing on previous studies on basic features of the underlying microstructure (Aifantis, 1984, 1987), Zbib and Aifantis (1988, 1989) addressed the shear banding analysis for metal and soil plasticity models featured by a yield strength depending on the effective plastic strain, as well as on its second and fourth order gradients which, according to the definition above, amounts to a second strain gradient plasticity model. The latter research line was further pursued in a paper by Mühlhaus

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and Aifantis (1991a) whereby a (non-local) integral strain model is shown—through a Taylor series expansion technique—to be equivalent to a series of strain gradient models of increasing (even) order up to infinite, which however was approximated by retaining only the contributions up to the fourth order. The obtained model was used for shear banding analysis, as well as to address the related boundary-value rate problem through a variational total potential energy principle. Besides the relevant governing field equations, the standard and the higher order (h.o.) boundary conditions were provided. Mühlhaus and Aifantis (1991b) addressed the strain localization problem by a mixed-type method whereby the lower order gradient of both the effective plastic strain and the effective stress are employed, which indeed amounts to a h.o. strain gradient approach. Mühlhaus (1994) elaborated further the h.o. strain gradient plasticity by Mühlhaus and Aifantis (1991a) to address geological materials sensitive to the mean pressure and obeying a Drucker–Prager yielding law, and to study the conditions for the formation of multiple shear bands within the softening region. Jirásek et al. (2010) addressed the strain localization problem in the case a non-uniform stress distribution along a bar (of variable cross-section). For this purpose, both explicit and implicit (Engelen et al., 2003, 2006; Peerlings, 2007) formulations of strain gradient plasticity were employed with second and fourth order enhancement of the yield stress in the explicit case whereby the gradient plasticity theory by Mühlhaus and Aifantis (1991a) was used. Menzel and Steinmamm (2000) formulated a h.o. gradient plasticity theory for polycrystals by introducing a free energy function of the elastic strain and of a special fourth order gradient (i.e. the curl of the curl) of the plastic strain, therein used for strain localization analysis.

The second strain gradient plasticity theory emerging from the above literature does constitute an alternative to the ancillary first gradient model, to which one has to resort whenever the material response must be evaluated at a lower microscale. This makes it possible to capture and describe a richer amount of salient features of the material behavior than with the common first strain gradient plasticity (e.g. preferred wavelengths and multi-waved profiles of the localized deformation patterns, accommodation of the equilibrium conditions at an edge of the boundary surface), but obviously at the cost of a heavier computational burden. As a matter of facts, the research work has paid little attention to the h.o. gradient plasticity theory in question, which in fact still exhibits some deficiencies, namely

- The surface effects that accompany a h.o. gradient plasticity theory are nowhere mentioned and discussed.
- The boundary conditions for the moving elastic/plastic interface are not exhaustively addressed.
- No evolution laws for the dissipation mechanisms associated to the plastic strain gradients are formulated.

Therefore, it appears that there is enough motivation for a reconsideration of this subject in the primary purpose to improve the understanding of its theoretical framework, then to develop suitable computational methods for applications to the engineering practice. In the present paper, second strain gradient plasticity is addressed with a particular concern to some related issues as the surface effects, the h.o. boundary conditions and the evolutions laws.

Some *surface effects*, similar to those exhibited by higher-grade elastic materials (see Polizzotto (2012) related to second grade elasticity, and Polizzotto (2013) related to third grade elasticity), do manifest themselves within the microstructure of a second strain gradient plasticity model. Indeed, the material particles of any subdomain, located close to the circumventing boundary surface where a cut has been made, coalesce to form up a structured membrane-like boundary layer behaving according to the principles of material surface mechanics (Gurtin and Murdoch, 1975, 1978). This thin boundary layer finds itself in local (and global) equilibrium under some specific surface stresses and all the external tractions, except for a part (called Cauchy-like traction) which instead is supported by the bulk microstructure. No such surface effects are exhibited by a first strain gradient plasticity model, although in both the first and second strain gradient models the microstructure behaves as a structured continuum with specific balance equations. (Surface effects as grain boundary effects that manifest themselves also within a first strain gradient model (see e.g. Ma et al. (2006) and the literature therein) are not considered in the present paper.)

The above surface effects may be qualified as *non-energetic*, meaning that they are featured by the absence of any specific surface energy density and thus of any concomitant surface constitutive equations. Indeed, the motion of the surface particles is guided by the embedding bulk material, which means that the boundary layer may be considered as *infinitely soft* against any change of configuration tending to preserve the continuity (either of the displacement at the macroscopic level, or of the plastic strain at the microscopic one) between the boundary layer and the adjacent bulk material; or *infinitely rigid* against any change of configuration tending to destroy the mentioned continuity.

The above kind of surface effects were investigated in the pioneering work by Toupin and Gazis (1963) concerning with the so-called "puckering phenomenon" detected by low-energy electron-diffraction experimental studies of the clean surface of crystals (Germer et al., 1961). The latter phenomenon consists in the different lattice spacing normal to the surface of the first few atomic layers with respect to the normal spacing of the deep layers as a consequence of a non-uniform stress state. By discrete lattice models, Toupin and Gazis (1963) showed that the mentioned phenomenon can be described taking into account both the nearest and next-nearest neighbor interactions. These authors also considered an infinite slab of cubic crystals and, using the second grade elasticity theory by Toupin (1962), found that the transverse displacement across the thickness is enhanced at the points close to the free faces of the slab, the more the closer is the point, with the formation of two thin boundary layers. Mindlin (1965) and Wu (1992) elaborated a third grade elasticity theory and showed that the material cohesion and the surface tension can be accounted for by means of a bulk strain energy contribution proportional to the Laplacian of the volumetric strain. Mindlin (1965) also showed that a third grade elasticity theory is a continuum counterpart of a