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Coupled thermomechanical response of gradient plasticity

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ABSTRACT

The coupled thermo-mechanical strain gradient plasticity theory that accounts for micro-structure based size effects is outlined within this work. This incorporates spatial gradients of selected micro-structural fields based on length-scales that describe the evolving dissipative mechanisms. In the mechanical part, the model problem of von Mises plasticity with gradient-extended hardening/softening response is considered as discussed in Miehe et al. (2013, 2014a). In the thermal part, we follow the investigations of Simó and Miehe (1992) that demonstrate the effect of temperature on the mechanical fields resulting in a thermal expansion. To this end, two classes of solution schemes for the coupled problem are considered: (i) *Global product formula algorithm* arising from operator split which leads to a two step solution procedure, and (ii) an *implicit coupled algorithm* which employs simultaneous solution of the coupled system of equations. In the product formula algorithm, the mechanical and thermal problems are solved separately, resulting in a symmetric problem. However, in the implicit coupled algorithm, a simultaneous solution of the coupled system of equations for gradient thermo-plasticity is employed. A noteworthy drawback of this solution scheme arises from the high computational efforts in comparison with the product formula algorithm. From the computational viewpoint, the standard Galerkin finite element method fails in the context of isochoric plastic flow due to the over-constrained pressure field. To circumvent these difficulties, we extend the well-known Q1P0-type and MINI-type mixed finite elements design of gradient plasticity to account for thermal effects. The performance of the formulation is demonstrated by means of some representative examples.

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1. Introduction

With the recent developments of micro- and nano-technology that have a wide spectrum of engineering applications such as in automotive industry and medical fields, the predictive modeling of the mechanical behavior at small dimensions like on the micro-scale has been a topic of intensive research during the last years. In this context, the term *size effects* is used to describe the influence of the structure-size on the mechanical response during inelastic deformations. In *conventional theories* of local continuum mechanics, no size effects are predicted. As a result, micro-structure interactions are not involved in the constitutive formulation. One significant limitation of these conventional theories that arises in the computation of localized inelastic deformations in softening materials using finite element techniques is the pathological mesh dependency that leads

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to loss of ellipticity of the governing equations. To overcome this non-physical behavior, *extended continuum theories* of inelasticity have been proposed in literature, which incorporate length scales. Hereby, additional internal variables and their nonlocal counterparts can be introduced to reflect the micro-structural response. The non-locality is obtained by weighted averaging over a spatial neighborhood of a local quantity. Furthermore the gradient-enhanced models are naturally rooted in the micro-mechanical descriptions of the dislocation flow in crystals, where the *plastic length scale* is related to the lattice spacing. Associated models of gradient crystal plasticity are proposed by many authors, e.g. Evers et al. (2004), Gurtin (2008, 2010), Svendsen and Bargmann (2010), Clayton (2011), Wulfinghoff and Böhlke (2012, 2015), Klusemann and Yalcinkaya (2013) and Miehe et al. (2014b). In contrast, pure phenomenologically-based theories of gradient plasticity often use plastic length scales as limiters of localized zones determined by macroscopic experiments, see for example Gurtin (2003), Gudmundson (2004), Anand et al. (2005, 2012), Reddy et al. (2008), Fleck and Willis (2009a, 2009b), Lele and Anand (2009), Polizzotto (2009, 2014), Voyiadjis et al. (2010), Kuroda and Tvergaard (2010), Miehe et al. (2013; 2014a; 2016a).

Despite the fact that temperature distribution during heat accumulation has a strong influence on the mechanical properties, thermal effects were not included in the constitutive formulation of most of the recently developed strain gradient theories. Lehmann and Blix (1985) and Wriggers et al. (1992) investigate the thermo-mechanical behavior of the necking problem in classical elasto-plasticity. Here the authors observed that, the development of a neck in a uniaxial tension test is influenced by the heat production due to inelastic deformation. Anand et al. (2009) proposed a coupled thermo-mechanical elasto-viscoplasticity theory to model strain rate and temperature dependent large-deformation response of amorphous polymeric materials. A variational formulation for the thermo-mechanical coupling in finite strain plasticity theory with nonlinear kinematic hardening is outlined in Canadija and Mosler (2011) based on the works Yang et al. (2006) and Stainier and Ortiz (2010). However no size effects were involved in the constitutive formulation. This has motivated Voyiadjis and Faghihi (2012) and Faghihi et al. (2013) to propose a nonlocal thermodynamic consistent framework with energetic and dissipative gradient length scales that addressing the coupled thermal and mechanical responses of materials in small scales and fast transient process. In this context, Forest (2014) and Forest and Aifantis (2010) introduced some links between recent gradient thermo-elasto-plasticity theories and the thermo-mechanics of generalized continua based on the micromorphic approach. Extensions to an anisotropic model for gradient thermo-plasticity can be seen in the work of Bertram and Forest (2014). Recently Wcislo and Pamin (2016) developed a gradient-enhanced thermomechanical model that is strictly related to the phenomenon of thermal softening. It incorporates higher order gradients of the temperature field. In this work, we extend the above mentioned gradient plasticity model introduced in Miehe et al. (2013, 2014a) to account for thermal effects under small strain deformations and its extension towards finite deformations in the logarithmic strain space.

From the numerical implementation aspects, two global solution procedures for the thermo-mechanically coupled problem are introduced, namely the *global product formula algorithm* and the *implicit coupled algorithm* in line with the work of Simó and Miehe (1992). In the product formula algorithm, the mechanical and thermal problems are solved separately, see Miehe et al. (2011). The idea here is to decompose the coupled field equations of gradient thermo-plasticity into an elasto-plastic problem with frozen temperature, followed by a heat conduction problem at fixed updated mechanical configuration. These two sub-problems are then coupled via the plastic structural heating and the mechanical dissipation. Due to the two steps solution procedure, we end up with a *symmetric structure* for each sub-problem. Alternatively, in the implicit coupled algorithm, there is no separation between the mechanical and thermal parts. The temperature field is no longer kept constant in the mechanical step. All the components of the problem are computed simultaneously using the same time-stepping scheme. This approach has proven to be *computationally more intensive* than the product formula algorithm and leads to a *non-symmetric structure* of the problem as discussed in Simó and Miehe (1992).

On the computational side, a variety of numerical strategies has been proposed in the literature for finite element design of the coupled problem. With regard to strain gradient plasticity theories, de Borst and Mühlhaus (1992) propose a rather numerical expensive C^1-continuous two-field formulation that allows the computation of second derivatives for the Laplacian of the incremental plastic parameter in the yield function. The follow-up work of de Borst and Pamin (1996) suggested a C^0-continuous three-field formulation based on an additional penalty constraint that introduces a new field variable for the gradient of the incremental plastic parameter. In the work of Liebe and Steinmann (2001), a global active set strategy of gradient plasticity was considered, where Kuhn-Tucker-type loading/unloading conditions were checked in weak form via finite element residuals at the nodes. Such a formulation needs a non-standard global active set search, which is not robust when applied to complex inhomogeneous response. Numerical implementations of gradient plasticity at small strains in terms of discontinuous Galerkin methods are outlined in Djoko et al. (2007a, 2007b). Nevertheless, many problems arise in all of these numerical strategies, such as the observation of spurious oscillations of the plastic variables near the elastic-plastic-boundaries (EPBs), see, e.g. de Borst and Pamin (1996) and Liebe and Steinmann (2001). This has encouraged Engelen et al. (2003) and Geers (2004) to propose a gradient plasticity model based on an accompanying PDE of the modified Helmholtz type, that defines the nonlocal plastic strain in terms of its local counterpart. In this regard, we develop a *mixed finite element design* for the gradient thermo-plasticity problem in line with our recent works Miehe et al. (2013, 2014a). This allows a straightforward local definition of plastic loading-unloading driven by the global fields. The proposed procedure includes a rational method for the definition of elastic-plastic-boundaries in gradient thermo-plasticity along with a post-processor that defines the plastic variables in the elastic range. Additionally, we extend the well-known Q1P0-type and MINI-type mixed finite element design to describe the thermo-mechanical coupling, including a local-global update strategy. The corresponding model guarantees from the computational side a mesh-objective response in the post-critical ranges of softening materials. To account for large strains, the constitutive model is extended towards finite deformations in the logarithmic

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