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Scale transition of a higher order plasticity model – A consistent homogenization theory from meso to macro

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ABSTRACT

Standard plasticity models cannot capture the microstructural size effect associated with grain sizes, as well as structural size effects induced by external boundaries and overall gradients. Many higher-order plasticity models introduce a length scale parameter to resolve the latter limitation – microstructural influences are not explicitly account for. This paper adopts two distinct length scales in the formulation, i.e. an intrinsic length scale (l) governing micro-processes such as dislocation pile-up at internal boundaries, as well as the characteristic grain size (L), and aims to unravel the interaction between these two length scales and the characteristic specimen size (H) at the macro level. At the meso-scale, we adopt the strain gradient plasticity model developed in Gurtin (2004) [Gurtin, M. E., 2004. A gradient theory of small-deformation isotropic plasticity that accounts for the Burgers vector and for dissipation due to plastic spin. J. Mech. Phys. Solids 52, 2545–2568] which accounts for the direct influence of grain boundaries. Through a novel homogenization theory, the plasticity model is translated consistently from meso to macro. The two length scale parameters (l and L) manifest themselves naturally at the macro scale, hence capturing both types of size effects in an average sense. The resulting (macro) higher-order model is thermodynamically consistent to the meso model, and has the same structure as a micromorphic continuum. Finally, we consider a bending example for the two limiting cases – microhard and microfree conditions at grain boundaries – and illustrate the excellent match between the meso and homogenized solutions.

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1. Introduction

Classical models are scale independent and thus cannot predict any of the size effects observed experimentally – the (microstructural) grain size dependent behavior commonly known as the Hall–Petch effect; the (structural) "smaller is stronger" phenomenon when a structure deforms non-uniformly, e.g. in bending (Stölken and Evans, 1998) or in torsion (Fleck et al., 1994). Since the plastic strain gradients are related to the geometrically necessary dislocations (GNDs) required for the compatibility of deformation (Ashby, 1970), many higher-order plasticity models have incorporated these gradient terms to account for the size effects (e.g. Aifantis, 1987; Fleck and Hutchinson, 2001; Gudmundson, 2004; Niordson and Hutchinson, 2003; Voyiadjis and Deliktas, 2009). "Conventional" higher-order plasticity models typically focus on the latter

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size effect, disregarding the microstructural influences and are imprecise on the physical interpretations on their length scale(s). We address this issue through three distinct length scales – an intrinsic length scale (l) governing micro-processes such as dislocation pile-up at internal and external boundaries, the grain size (L) characterizing the amount of internal boundaries, and a characteristic specimen size (H) – and aim to unravel the interaction of these length scales in the resulting (macro) homogenized plasticity model for polycrystals.

Another broad class of higher-order formulations, termed as the "micromorphic" continuum, incorporates additional kinematic fields to characterize the underlying micro-processes. The work done (and associated size effects) due to the rapidly fluctuating microscopic deformation, otherwise not picked up in a standard model, is captured through the introduction of micro-deformation directors (e.g. Zhang et al., 2011). Based on the generalized micromorphic framework by Forest (2009), a morphic-plasticity continuum characterizing the micro-plasticity process with additional plastic field was developed by Poh et al. (2011). In the limiting case, the morphic-plasticity theory recovers the gradient plasticity formulation in the preceding paragraph (Forest, 2009; Forest and Aifantis, 2010). In general, however, the physical interpretation of the morphic kinematic fields is so far elusive.

Many of these higher-order plasticity/micromorphic continuum models are adopted at the (macro) structural level, where the higher-order boundary conditions characterize the resistance to plastic flow/micro-process at the external surfaces of the specimen. They are thus continuous formulations that do not explicitly solve for the responses at grain boundaries. In these applications, the length scale parameter associated with the gradient term is a collective measure of the underlying micro-processes and structural influences. It is thus unclear what physical length scales constitute the (macro) modeling length scale parameter – an issue we address in our homogenization framework through the consistent propagation of two well-defined length scales (l and L) from meso to macro, resulting in a macro model that captures both types of size effects in an average sense.

To account for the direct influence of grain boundaries on the material response, we adopt in this paper the isotropic gradient plasticity theory by Gurtin (2004). At the granular level, the defect energy associated with GNDs is characterized with the norm of the Burgers tensor and its associated length scale parameter, while the Burgers-vector flow across grain boundaries is captured via the higher order boundary conditions. Though its isotropy assumption neglects the underlying crystallography, by incorporating the plastic spin into the formulation, its predictions resemble those from an analogous gradient crystal plasticity model with many slip systems, in which the most efficient ones become active (Bardella, 2009; Bardella and Giacomini, 2008). A similar theory called the "microcurl" formulation has also been proposed by Cordero et al. (2010) based on the generalized micromorphic framework. While the underlying crystal mechanics can be gleaned through these enhanced formulations which are implemented at the meso-scale, a major drawback is the high computational cost resulting from the sub-granular discretization in a generic problem.

In view of the potential prohibitive computational demands, Okumura et al. (2007) has proposed a *computational* homogenization framework for gradient plasticity models, albeit only in tensile loading. The extension to a generic case is likely to be rather involved – see the gradient enhanced computational homogenization framework by Kouznetsova et al. (2002). Motivated by the need for a more effective approach and yet capturing the crystal mechanics adequately through well-defined length scale parameters, Poh et al. (2013a) have proposed an *analytical* homogenization theory for gradient plasticity models in simple shear, and later extending it to an idealized bending problem with symmetric double slip system (Poh et al., 2013b). These problems reduce to a one-dimensional setting and are solved analytically, allowing the predictive capabilities of the homogenized plasticity model to be illustrated in a clear and transparent manner. It was also demonstrated in Poh et al. (2013b) that the homogenized solution can be understood as the ensemble average over all possible phases of the microstructural arrangement.

In this paper, we reformulate the analytical homogenization theory for a general setting by adopting the gradient plasticity formulation in Gurtin (2004) at the meso level. Through a consistent coarse graining procedure, the homogenized model resembles a continuous micromorphic continuum, such as those presented by Poh et al. (2011) and Vernerey et al. (2007, 2008). A distinct difference between the two frameworks is highlighted: the micromorphic theory generally follows a "top-down" approach whereby macro energy/dissipation potentials are postulated *a priori*. In contrast, the proposed homogenized formulation is developed based on the consistent propagation of fine-scale thermodynamics to the coarse scale – a "bottom-up" approach – leading to a transparent (modeling) length scale parameter, as well as a clear physical interpretation of the additional kinematic fields. It is furthermore highlighted that while the homogenization theory assumes a clear separation of scale between meso and macro, an excellent prediction is achievable even when the scale separation is low – see the bending problem in Section 10 where the film thickness is just one order larger than the grain size.

Note also the departure from the (bottom-up) variational principle by Smyshlyaev and Fleck (1996), where the (macro) effective material response is determined through the minimization of functionals incorporating gradient effects at the meso-scale. The variational theory was later reformulated in Fleck and Willis (2004) based on the gradient plasticity model by Fleck and Hutchinson (2001), and further extended in Aifantis and Willis (2005) to account for the interfacial resistance. Since the variational framework considers a uniform macroscopic deformation, the extracted effective response captures only the microstructural size effect. Our homogenization theory, on the other hand, recovers a morphic-type formulation. For a generic loading, both microstructural and structural size effects are captured through a balance equation. In the absence of macroscopic gradient, e.g. the simple shear problem in Poh et al. (2013a), the balance equation governs the interaction among the applied stress, the bulk material resistance and the interfacial resistance.

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