Thermodynamic framework for variance-based non-local constitutive models: Application to polycrystalline plasticity

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Abstract

Many constitutive models used for thermo-mechanical applications rely on the internal variable concept to represent the effect of microstructural transformations (e.g., hardening, damage, phase transitions) on the behavior of solid materials. For the majority of constitutive models, the evolution equations associated with the different internal variables are purely local. Specifically, the evolution of the internal state of a material point solely depends on the current state of that material point. However, there are some situations for which it is needed to include some information regarding the spatial distribution of state variables. As discussed by Bazant and Jiràsek (2002), there are different motivations for such constitutive models, which are often referred to as non-local. Indeed, non-local models allow (i) considering deviations from locality due to material heterogeneity at small scales, (ii) limiting strain localization resulting from softening, which is largely used in the context of damage mechanics, and (iii) capturing size effects associated with metal plasticity or fracture of ceramic materials.

Non-local constitutive models can be classified as either gradient-type or integral-type model. Gradient-type models treat the spatial gradients of internal variables as additional state variables. The consequence is that the evolution of internal variables is governed by a set of equilibrium equations and some boundary conditions. Such equations and boundary conditions are generally derived from an extended principle of virtual power. Gradient-type models have been largely used in the context of conventional plasticity, either to capture size effects or to limit strain localization associated with softening. Also, the role of Geometrically Necessary Dislocations (GND) on strain hardening can be incorporated in the framework of crystal plasticity by considering the spatial gradients of plastic shear strains as state variables. The phase-field method, which is widely used for solving interfacial problems, also relies on the spatial gradients of some order parameters to evaluate surface energy. Many applications of the phase-field method to either brittle or ductile fracture have been proposed. When applied to fracture, the phase-field method allows circumventing the difficulties associated with excessive damage localization and considering the increase of surface energy resulting from crack nucleation and crack growth.

In contrast with gradient-type models, integral-type models use some non-local variables obtained after spatial integration of their local counterparts. Generally speaking, such non-local variables can be interpreted as the spatial averages of the corresponding local variables over the neighborhood of the material point of interest. Integral-type models have been largely used in the context of brittle or ductile fracture, mostly to limit damage localization.

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Integral-type models for plasticity-induced softening have also been developed. A common approach consists of introducing the spatial average, i.e., the zeroth moment, of either the plastic strain tensor or the hardening variable in constitutive relations.

The present work aims at enriching integral-type constitutive models by incorporating not only the spatial average, but also the spatial variance of internal variables in constitutive relations. The objective is to include additional information regarding the spatial distribution of internal variables when constructing integral-type constitutive models. The proposed framework is developed in the context of continuum thermodynamics and can be applied to different types of problems, including plasticity and damage. In the first part of this presentation, the definitions of the average and the variance of an internal variable will be introduced. The general form of constitutive equations, which relies on continuum thermodynamics, will be detailed in the second part. Particular attention will be given to the treatment of near-boundary regions for which different options will be proposed.
For the purpose of illustration, a crystal plasticity-based model developed within the proposed framework will be exposed in the final part of this presentation. Such a model treats the average and the variance of the plastic deformation gradient tensor as additional variables. For the treatment of near-boundary regions, two different options, referred to as the " hard " or " soft " surrounding assumptions, are evaluated. For a given material point, the former option assumes that each crystallite is surrounded by a fictitious elastic medium while the latter option considers that the fictitious surrounding experiences the same plastic deformation as the material point of interest. The numerical examples indicate that, when the soft surrounding assumption is adopted, the effect of non-locality is limited to the diffusion of plastic strains, no size dependency of the macroscopic behavior being observed. At the opposite, when the hard surrounding assumption is used, the macroscopic hardening rate is found to depend on the mean grain size. Such a size-effect is related to the role of non-locality on the development of internal stresses, which provide an additional contribution to kinematic hardening.