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Multiscale modeling of cohesive geomaterials with a polycrystalline approach

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ABSTRACT

The main objective of this paper is to investigate the macroscopic elastic–plastic behaviors of a class of cohesive geomaterials with the aid of classical polycrystalline schemes. Specific local constitutive equations are proposed to describe the typical features of geomaterials. The local yield criterion for crystallographic sliding systems takes into account the pressure sensitivity and a non-associated plastic potential is introduced to properly describe the plastic dilatancy. Consequently, the concentration law is also modified in order to establish the relationship between the macroscopic stress tensor and the local stress tensor in each mineral grain. Computational aspects associated with the numerical implementation of polycrystalline model are revisited and discussed. The proposed model is applied to a typical polycrystalline rock, granite. After the identification of material parameters, its validity is verified through comparisons between model's predictions and experimental data on both conventional and true triaxial compression tests.

1. Introduction

In many engineering applications, it is necessary to describe mechanical behaviors of various geomaterials (soils, rocks and concretes) by appropriate constitutive models. Phenomenological models, generally formulated within the framework of thermodynamics of irreversible processes, have been largely developed and applied, including plastic models, viscoplastic models, damage models and coupled models. A number of models are able to correctly reproduce main features of mechanical behaviors of geomaterials under different loading conditions. However, such models generally do not properly take into account physical mechanisms involved at pertinent material scales and their consequences on material macroscopic responses. Indeed, most geomaterials contain different kinds of heterogeneities at different material scales, for instance, mineral grains, voids, micro-cracks and interfaces. The macroscopic responses of these materials are inherently related to their heterogeneous microstructure. In particular, the inelastic deformation and failure process of geomaterials are directly related to the evolution of their microstructure, e.g., debonding of interfaces, microcrack growth, pore expansion and collapse, frictional sliding along microcracks, plastic sliding along crystallographic planes. Therefore, the formulation of constitutive models should reflect these various physical phenomena. For this purpose, significant advances have been made during the last decades on the development of micro-mechanical models. Generally, two families of micro-mechanical models have been proposed, respectively for plastic deformation in ductile porous materials (Gurson, 1977; Maghous et al., 2009; Monchiet et al., 2008; Guo et al., 2008; Shen et al., 2012) and micro-crack induced damage in brittle ones (Gambarotta and Lagomarsino, 1993; Pensée et al., 2002; Zhu et al., 2008a,b), just to mention a few. These models are formulated using either limit analysis technique, linear fracture mechanics theory or homogenization

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procedures based on Eshelby's inclusion solution (Eshelby, 1957). The micro-mechanical models provide a completely new way to describe the inelastic responses of geomaterials. Some of them are successfully applied in numerical analysis of engineering structures.

However, in most micro-mechanical models developed so far, the geomaterials are generally represented by a matrix-inclusion system. This kind of description is indeed representative for a number of materials such as concretes with the cement paste as the matrix phase, hard clayey rocks with a dominant clay matrix, etc. However, many other geomaterials, for instance granite, sandstone and limestone, cannot be represented by such a matrix-inclusion system. Their micro-structures are generally constituted by cemented randomly distributed mineral grains. Therefore, there is a need to consider a new microstructural description for micro-mechanical modeling of this kind of materials.

For these materials, the macroscopic plastic deformation and damage are mostly generated by the degradation of cementation interfaces and frictional sliding along crystallographic and weakness planes. The well-established polycrystalline theory for metal materials provides a feasible framework to develop such micro-mechanical models. However, for the sake of simplicity and as a first stage of development, we consider here only the plastic deformation due to the sliding along crystallographic or weakness planes, while the effect of grain interfaces degradation will be taken into account in future works.

Concerning the modeling of inelastic deformation in relation with the sliding in weakness planes, some original models have been proposed, in particular the so-called multi-laminate models (Zienkiewicz and Pande, 1977) and micro-plane models (Bazant and Oh, 1983). In these models, the overall inelastic strains are related to the local ones due to the sliding and degradation of weakness planes in some orientations. The relationship between the local and overall stresses and strains is established through static or kinematic constraints and energy conditions.

As the fundamental difference with these models, the formulation of micro-mechanical models based on a homogenization procedure is performed in three steps: the definition of a representative elementary volume (REV), the determination of concentration law establishing the relationship between the microscopic and macroscopic stresses or strains, the homogenization averaging to find the macroscopic properties. The determination of the concentration law should take into account the morphology of material microstructure such as granular geometry and orientation, texture, voids, etc. Further, through an appropriate concentration law, it is possible to account for interactions between grains and effects of spatial distribution of grains. It is also possible to consider effects of mineral compositions in multi-phase materials. Therefore, the homogenization-based micro-mechanical approach provides a more general framework than the multi-laminate and micro-plane models.

As mentioned above, one essential requirement for the homogenization-based micro-mechanical models lies in establishing the relationship between local stress and strain in the individual crystals and the overall stress and strain of the polycrystal, namely the so-called concentration law which is usually called the interaction law in polycrystalline materials. Various laws have been proposed so far, for instance (Taylor, 1938; Budiansky and Wu, 1962; Hill, 1965), just to mention some basic ones here. Among these models, the model suggested by Kröner, Budiansky and Wu (KBW model), which takes into account the interaction between slipping crystals, is extensively used due to its simplicity. Still based on Eshelby's solution, the strains or stresses in a single crystal are approximately obtained by solving a spherical single crystal embedded in a uniform infinite plastically deformed matrix. The macroscopic properties of the matrix, also named Homogeneous Equivalent medium (HEM), are unknown and taken as identical to those of the polycrystalline materail. In this paper, without losing the assumptions and simplifications made in KBW model and at the same time, taking into account the specific features of geomaterials, a generalized form of KBW model is proposed. This model can physically relate the macroscopic volumetric dilatancy to the microscopic normal aperture caused by the sliding of slip systems.

Another requirement is the complete description of the behavior of each single crystal inside the REV. Since our study is restricted to infinitesimal deformation, elastic lattice distortion is therefore neglected. The plastic deformation of the single crystal is the sum of contributions from all active slip systems. To reflect the effect of confining pressure on each slip system, the classical Schmid's law for each crystallographic plane is replaced by a Mohr–Coulomb type yield criterion. A general hardening law is adopted to depict the self-hardening and cross-hardening behavior of each slip system. Furthermore, a non-associate plastic flow rule is proposed in order to properly describe the volumetric deformation observed in experimental investigations.

The present paper is organized as follows: The scale decomposition is firstly introduced and the representative elementary volume of studied materials is defined. Before introducing the specific yield criterion and plastic potential for a single crystal, a general form of interaction law is proposed. The stress update algorithm for rate form of constitutive relations, both at local and macro levels, are described in detail. After the determination of model's parameters from laboratory tests, performance of the proposed model is evaluated by conducting the comparisons between numerical results and experiment data for a typical polycrystalline rock.

2. Notation

Unless otherwise specified, the formulae and numerical calculations are expressed and carried out with respect to a fixed coordinate system. The local fields (in each single crystal) are denoted by lower case letters, and the overall ones (in polycrystalline REV) by capital letters. The following tensor notations and operations are adopted: first-order tensor (vector) $\underline{a}$; second-order tensor $\underline{\underline{a}}$; fourth-order tensor $\mathbb{A}$; and simple contraction $\underline{a}\cdot\underline{b}=a_ib_i,(i=1,2,3)$; double contraction $\underline{\underline{a}}:\underline{\underline{b}}=a_{ij}b_{ij}$, $\mathbb{A}:\underline{\underline{b}}=A_{ijkl}b_{kl}$; dyadic