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Modeling of viscoplastic deformation in geomaterials with a polycrystalline approach

T. Zeng [a,b], J.F. Shao [a,b,*], W.Y. Xu [a]

[a] HOHAI University, Nanjing 210098, China
[b] LML, UMR CNRS 8107, University of Lille, Cité Scientifique, 59655 Villeneuve d'Ascq, France

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ABSTRACT

A micromechanical model is proposed to describe the viscoplastic deformation of cohesive frictional geomaterials with a granular texture. Inspired by the widely used polycrystalline theory, the macroscopic viscoplastic deformation is attributed to the subcritical sliding along a number of oriented weakness planes, which are assimilated to the crystallographic planes in single crystals. Main features of geomaterials, such as pressure sensitivity and plastic compressibility/dilatancy, are taken into account by introducing an appropriate yield criterion and a non-associated plastic potential for each weakness plane. A simple interaction law is adopted to relate the local stress and strain fields to the macroscopic ones of the representative elementary volume. Computational aspects about the implementation of constitutive equations of both single crystal and polycrystal are discussed in detail. The performance of proposed model is checked through the comparisons between numerical results and experimental data on both triaxial compression tests and creep tests performed on a typical rock - granite.

1. Introduction

In various engineering applications with quasi-brittle rocks, for instance the long-term stability of underground cavities and slopes and long-term performance of facilities for the geological storage of nuclear wastes, the time-dependent deformation plays an essential role. For a large class of rocks like granite, sandstone, etc., it is recognized that the inelastic deformation is mainly related to frictional sliding on the weakness planes [1,2]. Generally, two families of constitutive models have been developed for modeling their mechanical behaviors: phenomenology models and micromechanical approaches. The phenomenology models, which are based on experimental data and formulated within the framework of thermodynamics of irreversible process, possess certain advantages, e.g. good reproduction of macroscopic experimental data, easy implementation for structural analysis. However, such kind of models do not establish the relationships between macroscopic responses and physical mechanisms at microscopic scales. Further, it is not possible to explicitly take into account the effects of microstructural evolutions, e.g. the variations of mineralogical compositions and porosity, on the macroscopic responses.

During recent decades, various micromechanical approaches have been developed to enrich and complete the phenomenological models. One class of them is developed by using a proper homogenization procedure, based on the extension of Eshelby's solution for the elastic inclusion problem [3]. According to author's knowledge, most existing micromechanical models for geomaterials are based on the "matrix-inclusion" morphology, i.e. heterogeneous defects (crack, void, mineral grains, etc.) are considered as either a spherical or a penny shaped inclusions embedded in a homogeneous matrix. Such morphology is acceptable only when certain phase is dominant with respect to others. However, some geomaterials, like granite [4,5], sandstone, limestone, have a granular morphology. Their microstructure is represented by an assembly of cemented mineral grains. The choice of a matrix phase is not possible and therefore a new morphology has to be specified.

A micromechanical approach based on the physical considerations assumes that constitutive models for the constituents at microscopic scale have been established on the basis of physical mechanisms relevant at this scale, and the macroscopic behavior is then deduced from these physical models and the interaction between constituents. In the case of geomaterials with granular texture, complex physical mechanisms at different scales should be taken into account. For example, for a typical granite which is

* Corresponding author at: LML, UMR CNRS 8107, University of Lille, 59655 Villeneuve d'ascq, France. Tel.: +33 320434626.
E-mail address: jian-fu.shao@polytech-lille.fr (J.F. Shao).

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mainly composed of quartz grains, one of the deformation mechanism is the plastic sliding along weakness planes. According to [6], the weakness planes inside the quartz are quite similar to the crystallographic planes in CFC crystal. On the other hand, considering typical clayey rocks, at the microscopic scale, the clay matrix can be considered as a polycrystal aggregate composed of clay particles as single crystals. The main inelastic deformation mechanism is the plastic sliding along parallel inter-layers inside the clay particle. The similar microstructure is also observed in cement matrix [7]. The plastic sliding along such weakness planes can be described by an appropriate plastic model. The interactions between mineral grains are generally taken into account by using a suitable interaction law. The macroscopic behavior of heterogeneous geomaterials is finally determined by a homogenization procedure. As a first stage study, the present work is rather devoted to theoretical and numerical development rather experimental investigation. The basic concept of the widely used polycrystalline models has been also used for modeling some geomaterials. For instance, Pouya proposed a micro–macro approach for the crack initiation and inelastic deformation in rock salt using a polycrystalline approach [8,9]. In this work, we proposed to extend these previous works by considering some specific features of geomaterials as mentioned below. A generalized interpretation of the weakness planes is also introduced and is not restricted to crystallographic slip planes. This work should be completed by further experimental investigations for the identification of material microstructure, in particular the distribution of weakness planes. However, the micromechanical approach proposed in this work can be easily applied to various geomaterials with different distributions of weakness planes. Compared with the existing models for pressure-independent metal materials [10–13], the specific properties of geomaterials are taken into account, in particular, the dependency on confining pressure and plastic volumetric compressibility/dilatancy. Moreover, the elastic deformation is not negligible for geomaterials and then taken into account in the model. Based on the previous works [14–16], a generalized interaction law taking into account the effects of plastic volumetric deformation, is proposed. As an example of application, we consider that the system of weakness planes inside quartz grain can be approximated by that of CFC crystal. Moreover, some improvements of numerical algorithm for the implementation of polycrystalline models are also proposed in the present work, in particular the determination of actually active slip systems in the local constitutive model of single crystal.

Throughout the paper, the following conventions and notations will be adopted: all formulae and numerical calculations are carried out under a fixed coordinate system. Lower case letters and capital letters are introduced to represent the local and overall fields, respectively. With the first-order, second-order, and forth-order tensors denoted as $\underline{a}$, $\underline{\underline{a}}$, and $\mathbb{A}$, we perform the following tensor operations: simple contraction $\underline{a} \cdot \underline{b} = a_i b_i$; double contraction $\underline{\underline{a}} : \underline{\underline{b}} = a_{ij} b_{ij}$, $\mathbb{A} : \underline{\underline{b}} = A_{ijkl} b_{kl}$; dyadic products $\underline{a} \otimes \underline{b} = a_i b_j$. With the second-order identity tensor $\underline{\underline{\delta}}$, two classical isotropic fourth-order projectors $\mathbb{I}$ and $\mathbb{K}$ are expressed as $I_{ijkl} = \frac{1}{2}(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk})$, $K_{ijkl} = \frac{1}{3}\delta_{ij}\delta_{kl}$. The fourth-order deviatoric projector $\mathbb{J}$ is given by $\mathbb{J} = \mathbb{I} - \mathbb{K}$.

2. A polycrystalline model for granite

2.1. Micromechanical background

The micromechanical model contains three scales: the macroscopic scale corresponds to the Representative Element Volume (REV) of heterogeneous rocks, the REV being an aggregate of randomly distributed grains; the mesoscopic scale relates to any single granular; and the microscopic scale is where the plastic deformation generates. For clarity, those three scales are briefly shown in Fig. 1.

Within the elastic range, each grain is assumed to be isotropic with the elastic stiffness tensor $\mathbb{C}$. Therefore, the REV is also elastically isotropic and characterized by the same elastic stiffness as that for every grain, i.e. $\mathbb{C}^{hom} = \mathbb{C}$. Concerning the inelastic range, the weakness planes in each granular can be considered to be equivalent to the crystallographic planes in single crystal. Granite is mainly composed of quartz grains. According to [6], although quartz lacks the center of symmetry, in some deformation studies of quartz with diffraction methods, high crystal symmetry can be used by adding a center of symmetry. Therefore, as a first approximation, the quartz here is assigned with the high symmetry crystal structure and we use the crystallographic planes of FCC crystal as weakness planes. Further, the viscoplastic deformation of granite entirely comes from the time-dependent sliding on these planes. Other mechanisms such as micro-cracking, grain interfaces degradation or even debonding will be considered in our future work.

2.2. Grain-matrix generalized interaction law

The interaction law is necessary to establish the relationship between mesoscopic fields in each grain and the macroscopic ones prescribed at the remote boundary of REV. In general, the mesoscopic fields are not uniform and it is impossible to obtain their exact distribution. Therefore, for the sake of simplicity and to enable the homogenization process, a plausible assumption is usually made that the mesoscopic fields are uniform throughout each grain.

There are different approaches developed for the estimation of local mesoscopic fields. For polycrystalline materials, the Eshelby's solution based on self-consistent method is the most suitable one, which allows a good description of interaction among grains. In this paper, the model is a little different from "Kröner–Weng" model [14,15] since the effect of volumetric plastic deformation is involved. A generalized interaction law is firstly briefed. Recasting

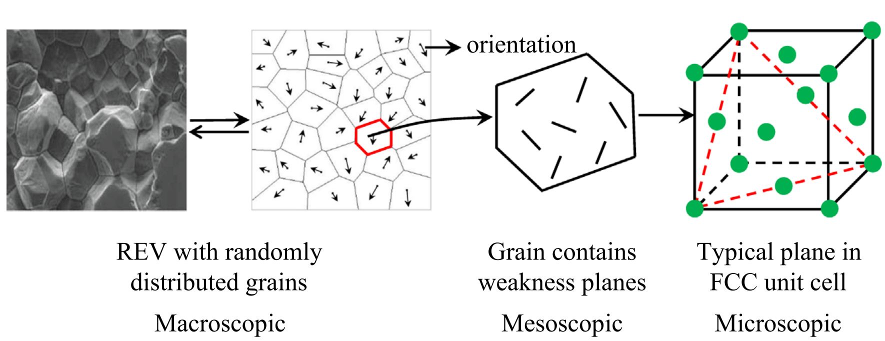

Fig. 1. Schematic representations of REV, weakness planes and typical crystallographical plane in FCC unit cell. The microscopic photograph of granite is from [4].