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Stress-induced crystal preferred orientation in the poromechanics of in-pore crystallization

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ABSTRACT

A non-hydrostatic stress field affects the orientation of crystals growing in the pore network of an elastic porous medium. The hypothesis of a hydrostatic state of stress within the crystal has been implicitly made in the recent extension of poromechanics to in-pore crystalization (Coussy, 2006). This underlying hypothesis is revisited on a small-scale conceptual model based on Eshelby's problem and shows that chemo-mechanical equilibrium requires that the crystal adapts its shape and orientation to the far-field stress, therefore resulting at equilibrium in a hydrostatic state of stress within the crystal. The optimum crystal shape as a function of the far-field stress is consistently investigated, highlighting limiting cases. The small scale model allows to understand the macroscopic effects associated with deviatoric stresses in the poromechanics of in-pore crystallization. Moreover, it provides the building block for an up-scaling of the macroscopic tangent poroelastic properties, which depend on both the current crystal saturation and the state of stress. A dilute micromechanical scheme illustrates the variation of the macroscopic Biot's coefficient tensor as a function of deviatoric stresses. A simple configuration akin to a potential laboratory experiment finally illustrates the strong induced anisotropy of the crystallization induced macroscopic strain when deviatoric stresses are applied to the material prior to crystallization.

1. Introduction

The mechanism of crystallization in porous materials (stone, cement, etc.) has received attention due to the observed detrimental effect (e.g. cracking) associated with frost action in cold climate (Pingeon and Pleau, 1995) and salt precipitation in coastal environments (see the special issue of Environmental Geology, 2007 for example). Most of the proposed models focus on a "small-scale" configuration—typically a single crystal and a single pore with a simplified geometry—where physico-chemical mechanisms can be elegantly highlighted (Scherer, 1999). The prediction of such small-scale models have, however, little applicability due to the intrinsic heterogeneity and complexity of the material in terms of pore geometries, connective channels between pores, solid grain properties, etc. Recently, proper constitutive relations at a continuum scale have emerged (Coussy, 2005, 2006; Coussy and Monteiro, 2007), which take into account the physico-chemical phenomena identified at smaller scale. By continuum scale, we mean the scale at which the complex pore network of the material can be grasped by the concepts of porosity and representative pore-size distribution. These models, based on an extension of Biot's theory of poromechanics, have been successfully used to analyze experiments on limestone (Espinosa-Marzal and Scherer, 2009).

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The effects of in-pore crystallization have also important applications in the oil-field. A typical example is related to the use of delayed expanding agents in well cementing. These cement expanding additives crystallize in the late stage of cement hydration (Chatterji, 1995). The resulting crystallization pressure creates a compressive stress at the cement/rock and cement/steel casing interfaces, therefore ensuring a good seal between producing layers and shallow aquifers (Baumgarte et al., 1999). Another example is the precipitation of calcite during cement carbonation when exposed to CO_2 which may lead to micro-cracking (Fabbri et al., 2009). A notable difference between these problems and the case of salt precipitation, for example, is the fact that oil-wells are subjected to pressure much larger than the ambient one. Moreover, the state of stress in the cement and the surrounding rock formations is not hydrostatic. It will be shown that this difference with surface conditions will turn out to have a great importance in the way crystallization pressure stresses the material macroscopically.

The fact that a non-hydrostatic far-field stress orients the growth of a crystal is a familiar feature in geology. Crystal growth at mineral grain contacts, which may be viewed as a reverse mechanism to pressure-solution at grains contact, is strongly affected by non-hydrostatic far-field stress and crystals tend to orient themselves in the direction of the least compressive stress (Durney, 1976). Such mechanisms have been extensively investigated in the geological community following the pioneering works of Kamb (1959) and Weyl (1959) (see also Paterson, 1973). Nevertheless, in the case of crystallization, there has been no attempt, to our knowledge, to reach the level of a continuum. Our aim is to include consistently these effects within the scope of in-pore crystallization at the level of a representative volume element of the porous medium. The main hypothesis underlying the development of a macroscopic Biot-like constitutive law is the occurrence of a hydrostatic state of stress within the neo-formed crystal. We will revisit such a hypothesis highlighting its necessary implication on the shape of the formed crystal in the presence of a non-hydrostatic far-field stress. Such an analysis will be performed at the micro-scale using the well-known solution of an ellipsoid inclusion in an infinite elastic matrix (Eshelby, 1957). A macroscopic incremental constitutive law—following the work of Coussy (2006, 2007)—will then be derived taking into account the constraints on the crystal shape and orientation identified from the small-scale equilibrium. An up-scaling scheme based on a simple dilute approximation will provide the evolution law for the tangent properties as a function of the macroscopic stresses. The resulting macroscopic model is potentially amenable to experimental studies. A simple configuration that could be reproduced experimentally is therefore investigated.

Boldface is used for tensors (lower case for second order and upper case for fourth order tensors), and scalars are denoted by lightface letters. Double contraction is assumed throughout, i.e. $\mathbb{L}\boldsymbol{\varepsilon} = \mathbb{L}_{ijkl}\varepsilon_{kl}$.

2. Equilibrium of a single crystal in a pore

We first revisit the equilibrium of a single crystal filling a pore of the material (see Fig. 1) while a stress field $\boldsymbol{\sigma}_\infty$, possibly anisotropic, acts in the far-field of the matrix. Such a simple configuration—similar to the classical Eshelby problem—can be viewed as a small-scale conceptual model statistically representative of the effect of in-pore crystallization. The crystal is supposed here to grow due to the supersaturation of the pore solution. For simplicity, we consider a simple chemical system made of an ideal binary solution (solvent and solute of component k) and a crystal (solid phase of component k). Such a simple chemical system does not however restrict in any means the following developments. Multiple components solution, chemical activity coefficients, etc. could also be taken into account only at the expense of heavier derivations. Although no connecting channels are depicted in Fig. 1, the crystal is in indeed in connection with the surrounding solution via a pore-throat of negligible diameter compared to the crystal size at least for mechanical purpose. On the other hand, it is worthwhile to note that such a connecting pore-throat will come into play

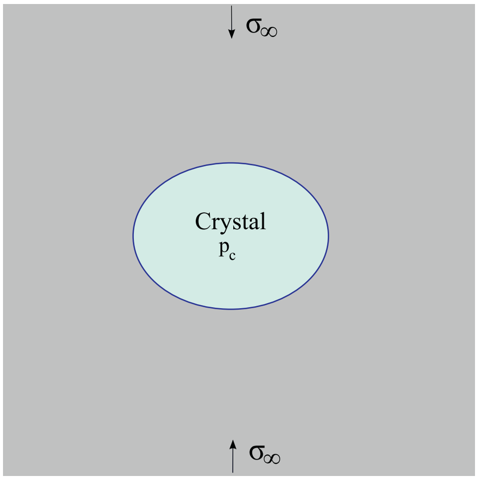

Fig. 1. A crystal filled pore in an infinite solid matrix under a given far-field stress $\boldsymbol{\sigma}_\infty$ highlighting the thin-film of fluid at the interface.