Accepted Manuscript

Cracking and damage from crystallization in pores: Coupled chemo-hydro-mechanics and phase-field modeling

Jinhyun Choo, WaiChing Sun

PII: S0045-7825(18)30051-3
DOI: https://doi.org/10.1016/j.cma.2018.01.044
Reference: CMA 11764

To appear in: *Comput. Methods Appl. Mech. Engrg.*

Received date : 16 August 2017
Revised date : 18 November 2017
Accepted date : 24 January 2018

Cracking and damage from crystallization in pores: Coupled chemo-hydro-mechanics and phase-field modeling

Jinhyun Choo[a,b,*], WaiChing Sun[a]

[a] Department of Civil Engineering and Engineering Mechanics, Columbia University, New Work, NY 10027, USA
[b] Department of Civil Engineering, The University of Hong Kong, Pokfulam, Hong Kong

Abstract

Cracking and damage from crystallization of minerals in pores center on a wide range of problems, from weathering and deterioration of structures to storage of CO_2 via in situ carbonation. Here we develop a theoretical and computational framework for modeling these crystallization-induced deformation and fracture in fluid-infiltrated porous materials. Conservation laws are formulated for coupled chemo-hydro-mechanical processes in a multiphase material composed of the solid matrix, liquid solution, gas, and crystals. We then derive an expression for the effective stress tensor that is energy-conjugate to the strain rate of a porous material containing crystals growing in pores. This form of effective stress incorporates the excess pore pressure exerted by crystal growth—the crystallization pressure—which has been recognized as the direct cause of deformation and fracture during crystallization in pores. Continuum thermodynamics is further exploited to formalize a constitutive framework for porous media subject to crystal growth. The chemo-hydro-mechanical model is then coupled with a phase-field approach to fracture which enables simulation of complex fractures without explicitly tracking their geometry. For robust and efficient solution of the initial-boundary value problem at hand, we utilize a combination of finite element and finite volume methods and devise a block-partitioned preconditioning strategy. Through numerical examples we demonstrate the capability of the proposed framework for simulating complex interactions among unsaturated flow, crystallization kinetics, and cracking in the solid matrix.

Keywords: in-pore crystallization, chemo-hydro-mechanics, fracture, phase field, effective stress, reactive transport

1. Introduction

Growth of mineral crystals in pores can give rise to severe damage and cracks in the host material. These coupled chemo-hydro-mechanical processes are now central to a number of problems in our society. A well-known example is weathering and deterioration of historic and building structures due to salt crystallization. Many of these structures are comprised of materials prone to invasion of salt water (e.g., stone), so they can be severely damaged when salt minerals grow inside the pores. See Fig. 1 for example. Preventing this type of damage has been a critical element of conservation of cultural heritage and structures around the world [1–6]. Also, crystallization of minerals in

*Corresponding Author
Email addresses: jchoo@hku.hk (Jinhyun Choo), wsun@columbia.edu (WaiChing Sun)