Accepted Manuscript

Computational thermomechanics of crystalline rock, Part I: A combined multi-phase-field/crystal plasticity approach for single crystal simulations

SeonHong Na, WaiChing Sun

PII: S0045-7825(17)30772-7
DOI: https://doi.org/10.1016/j.cma.2017.12.022
Reference: CMA 11714

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

Computer Methods in Applied Mechanics and Engineering manuscript No.
(will be inserted by the editor)

Computational thermomechanics of crystalline rock. Part I: a combined multi-phase-field/crystal plasticity approach for single crystal simulations

SeonHong Na · WaiChing Sun

Received: January 3, 2018/ Accepted: date

Abstract Rock salt is one of the major materials used for nuclear waste geological disposal. The desired characteristics of rock salt, i.e., high thermal conductivity, low permeability, and self-healing are highly related to its crystalline microstructure. Conventionally, this microstructural effect is often incorporated phenomenologically in macroscopic damage models. Nevertheless, the thermo-mechanical behavior of a crystalline material is dictated by the nature of crystal lattice and micromechanics (i.e., the slip-system). This paper presents a model proposed to examine these fundamental mechanisms at the grain scale level. We employ a crystal plasticity framework in which single-crystal halite is modeled as a face-centered cubic (FCC) structure with the secondary atoms in its octahedral holes, where a pair of Na^{+} and Cl^{-} ions forms the bond basis. Utilizing the crystal plasticity framework, we capture the existence of an elastic region in the stress space and the sequence of slip system activation of single-crystal halite under different temperature ranges. To capture the anisotropic nature of the intragranular fracture, we couple a crystal plasticity model with a multi-phase-field formulation that does not require high-order terms for the phase field. Numerical examples demonstrate that the proposed model is able to capture the anisotropy of inelastic and damage behavior under various loading rates and temperature conditions.

Keywords halite; rock salt; thermo-mechanics; crystal plasticity; anisotropic damage

1 Introduction

The demands for safe and permanent disposal of nuclear waste in geologic formations date back over decades. Natural rock salt, found in domal and bedded formations and the re-consolidated counterpart formed in a high-pressure and high-temperature environment, has been used for geological repositories of nuclear waste disposal in the United States and Germany [1]. Two operating facilities include the Waste Isolation Pilot Plant (WIPP) in Carlsbad (New Mexico, USA), and the Endlager für radioaktive Abfälle Morsleben (ERAM) site in Morsleben, Germany [2].

The decision to use salt formation for storage and disposal of radioactive wastes is attributed to its desirable thermo-hydro-mechanical-chemical characteristics, i.e., (1) high thermal conductivity, (2) low permeability, (3) self-healing mechanism and, (4) biologically inactivity of rock salt (as compared with clay). Firstly, the heat generated from nuclear wastes can be dissipated to the surrounding area much faster in salt than in other materials since the host salt rock exhibits high thermal conductivity [3]. In addition, the permeability of rock salt is sufficiently low that it is often idealized as impermeable. Therefore, it may function as a secured barrier for radioactive wastes [4]. Finally, the creeping property of salt enables microcracks or damage under mechanical load to be self-sealed, which may also naturally guarantee the necessary geological barrier function (e.g., von Berlepsch and Haverkamp [2], Chan et al. [5]).

Corresponding author: WaiChing Sun
Assistant Professor, Department of Civil Engineering and Engineering Mechanics, Fu Foundation School of Engineering and Applied Science Columbia University in the City of New York , 614 SW Mudd, Mail Code: 4709, New York, NY 10027 Tel.: 212-851-4371, Fax: 212-854-6267, E-mail: wsun@columbia.edu