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A discrete element thermo-mechanical modelling of diffuse damage induced by thermal expansion mismatch of two-phase materials

Damien André[a,*], Bertrand Levraut[a], Nicolas Tessier-Doyen[b], Marc Huger[a]

[a] *ENSCI, SPCTS, UMR 7315, F-87000 Limoges, France*
[b] *Univ. Limoges, SPCTS, UMR 7315, F-87000 Limoges, France*

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Highlights

- A discrete element model for bi-phase material is proposed.
- A robust method for modeling thermal expansion is proposed.
- Thermal expansion mismatch induces damage.
- The amount of damages may be predicted by the proposed method.
- Results are reliable compared with experimental observations.

Abstract

At the macroscopic scale, brittle media such as rocks, concretes or ceramics can be seen as homogeneous continua. However, at the microscopic scale, these materials involve sophisticated microstructures that mix several phases. Generally, these microstructures are composed of a large amount of inclusions embedded in a brittle matrix that ensures the cohesion of the material. These materials generally exhibit complex mechanical behaviors resulting from the interactions between the different phases of the microstructure.

As a result, the macroscopic behavior of these media may be predicted considering an accurate knowledge of their microstructures. This paper proposes a model to study the impact of diffuse damage resulting from thermal expansion mismatch between the mixed phases. This type of damage (which is not catastrophic for the integrity of two-phase materials) may appear when heterogeneous materials are subjected to thermal cycles.

This phenomenon involves a high amount of discontinuities and can not be tackled easily with the Finite Element Method (FEM). The Discrete Element Method (DEM) naturally accounts for discontinuities and is therefore a good alternative to the continuum approaches. However, the difficulty with DEM is to perform quantitative simulations because the mechanical quantities

* Corresponding author.
E-mail address: damien.andre@unilim.fr (D. André).

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are not described in terms of the classical continuum theory. This study describes the approach used here to tackle this fundamental difficulty. The results given by the proposed approach are finally compared to experimental observations.

Keywords: Discrete element method; Thermal expansion; Damages; Young's modulus; Coefficient of thermal expansion

1. Introduction

Rocks, concretes or ceramics are heterogeneous materials exhibiting multi-phase compositions involving different sizes of aggregates, various bonding phases and additives. Description and prediction of thermo-mechanical behavior of such materials present a real difficulty due to their complex microstructure. Hashin & Shtrikman (H&S) have developed an analytic method to predict thermo-mechanical properties of perfectly cohesive (free of damage) multi-phase materials [1]. However, most of these materials present numerous micro-cracks at room temperature. These micro-cracks result from thermal expansion mismatches between their different phases. These local defects highly influence thermo-mechanical properties and may have a great influence on materials lifetime in service conditions.

For instance, Young's modulus is strongly affected by the presence of micro-cracks and the measured values are often in disagreement with H&S's prediction [2,3]. The study proposed here focuses on a numerical method able to predict the occurrence of these defects and their overall influence on macroscopic properties such as Young's modulus and Coefficient of Thermal Expansion (CTE). Any materials that exhibit coarse aggregates such as concretes, rocks or ceramics may be addressed by the presented method.

Various numerical approaches can be distinguished. In the mechanical engineering field, the most used is the Finite Element Method (FEM). FEM, which is the most widespread technique is well suitable for materials characterized by reliable stress–strain laws. However, at the microscopic scale, this method is not adapted to describe discontinuities [4] without assumptions on their localization, their paths, their growths and their coalescences. Alternative methods to FEM exist such as X-FEM (Extended Finite Element Method) that keeps the rate of convergence towards singularities (micro-cracks) thanks to form functions. However, this method is adapted to describe the crack propagation in quasi-static mode but is not suitable for the management of opening and closure of numerous micro-cracks simultaneously.

The DEM is an interesting alternative way to study multi-damaged materials because it takes naturally into account discontinuities. The DEM implements a group of distinct elements (also named *discrete element*) which are in interaction through contacts or cohesive laws. This model consists in an assembly of discrete elements, deformable or not, linked by simple mechanical laws. The advantage is the natural description of crack initiation, crack propagation and coalescence. Researchers have used this method to study damages in solids, such as concretes [5], rocks [6] or ceramics [7]. However, the main difficulty is to get quantitative predictions. This is due to the necessity to find relations between microscopic laws, at the discrete element scale, and the macroscopic properties, at the structure scale. In this study the considered macroscopic properties are Young's modulus, Poisson's ratio, coefficient of thermal expansion and failure strength.

In this study, only the thermo-mechanical effects are taken into account. To avoid complex physico-chemical interactions, a model material is preferred in place of an industrial one. The phases of this model material have been chosen to ensure chemical neutrality and to avoid the presence of interphases. This model material is composed of two phases: spherical alumina inclusions embedded in a borosilicate glass matrix. The selected model material exhibits a positive CTE mismatch between the glass matrix and the alumina inclusions.

A short first section is dedicated to model material processing. The second section focuses on the H&S analytic model whose limits are highlighted. The third and fourth section introduces the DEM model. In this part, the method to model thermal expansion with DEM, that presents an innovative feature, is focused. As a preliminary validation, the next section proposes the implementation of the DEM model without cracks. The numerical results are compared to the H&S predictions. In the last part, the micro-cracks are implemented and the given numerical results are compared to the experimental data in terms of macroscopic Young's modulus and CTE. The capability of the presented method to simulate, understand and predict qualitatively and quantitatively the impact of the micro-crack density on thermo-mechanical properties is finally discussed.