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# A comparative molecular dynamics-phase-field modeling approach to brittle fracture

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## Highlights

- A link between molecular and continuum models for brittle fracture is proposed.
- Parameters obtained from the molecular scale are used in the continuum approach.
- Under this approach, the phase-field parameters acquire an entirely physical meaning.
- This approach can assist multi-scale modeling of materials.

## Abstract

In this work, a novel comparative method for highly brittle materials such as aragonite crystals is proposed, which provides an efficient and accurate in-sight understanding for multi-scale fracture modeling. In particular, physically-motivated molecular dynamics (MD) simulations are performed to model quasi-static brittle crack propagation on the nano-scale and followingly compared to macroscopic modeling of fracture using the phase-field modeling (PFM) technique. A link between the two modeling schemes is later proposed by deriving PFM parameters from the MD atomistic simulations. Thus, in this combined approach, MD simulations provide a more realistic meaning and physical estimation of the PFM parameters. The proposed computational approach, that encompasses mechanics on discrete and continuum levels, can assist multi-scale modeling and easing, for instance, the simulation of biological materials and the design of new materials.


*Keywords:* Molecular dynamics; Phase-field modeling; Fracture; Aragonite

## 1. Introduction

In engineering and material science, much attention has been given in recent years to the prediction of material failure. One of the most interesting and challenging problems in fundamental fracture research is how to improve the

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understanding of brittle fracture processes, which occur primarily in high-strength materials with poor ductility and toughness. By definition, brittle fracture is the breakage of interatomic bonds without noticeable plastic deformation. This type of fracture occurs when the local strain energy becomes larger than the energy necessary to pull the atom layers apart. In order to be able to predict and study this fracture behavior, a wide diversity of experimental, mathematical, and most recently, computational methods have been proposed for different (length) scale levels, such as nano-, micro- and meso-scale. For each of these groups, the main focus is still efficiency and accuracy of the models.

At the atomistic level, molecular dynamics (MD) simulations are increasingly becoming powerful tools to investigate crack initiation and propagation. Due to their real time scales (pico seconds), MD methods are perfectly suited to study the very high-speed crack propagation of highly brittle materials. All-atom MD simulations have been extensively used to study crack propagation [1] for a variety of inorganic crystals, such as $Si_3N_4$ [2], $SiO_2$ [3], 3C-SiC [4], and GaAs [5]. Although these studies have provided valuable in-sights into crack dynamics, a systematic analysis of mechanical properties at an atomistic scale, as well as a link to the macroscopic continuum mechanical approaches is still not well established.

Although MD simulations are efficient to study material on the nano-scale, they become impractical when the investigated systems have significantly larger dimensions, i.e., huge number of molecules, or if the considered time range is relatively long. Nowadays, typical MD simulations can be performed on systems containing hundreds of thousands, or perhaps, a few millions of atoms for simulation times ranging from a few hundred nanoseconds up to a millisecond. These numbers are certainly respectable, but one may run into conditions where size and/or time limitations become important. The challenges related to the limited dimensions or time scales can be tackled using continuum mechanical methods, where atomic details of the material are disregarded. In fact, as it has been shown in numerous other studies [6–9], the mechanical behavior of a given continuous material can be reproduced in a different scale by using mechanical parameters derived directly from atomistic MD simulations.

Due to its versatility, the phase-field modeling (PFM) has emerged as a powerful tool in continuum mechanics to model fracture and many other multi-phase material evolutions. Although phenomenological, PFM has proven to offer a good trade-off between numerical treatment, accuracy, and computational costs. The pioneering works of Griffith [10] and Irwin [11], as well as the variational formulations presented in [12,13], have helped to build a well-established energy-based framework for brittle fracture, which has continued to be developed and enhanced during the past decades.

In order to provide for a robust numerical implementation of this approach in typical finite element codes, a phenomenological phase-field variable, which approximates the crack–material sharp interface by a diffusive transition zone, needs to be incorporated. The idea of diffusive interfaces stems from physics and has been used by, e.g., Cahn and Hilliard [14] to describe interfaces in a heterogeneous system by a partial differential evolution equation. Crack propagation models for quasi-static, dynamic and cohesive brittle fracture have successfully been established in [15–20], to mention some. Nevertheless, it is seldom to find a thorough physical explanation or validation of the phase-field parameters. Moreover, there have not been any attempts to implement the PFM for brittle fracture into an atomistic scale level, neither have there been material properties derived from all-atom simulations, which could help to illuminate a physical explanation to the PFM parameters.

The aim of this research work is to create a link between the understanding of brittle fracture of a highly brittle material at an atomistic scale and its macroscopic mechanical features. Therefore, the fracture behavior of an aragonite ($CaCO_3$) tablet, under quasi-static assumptions, is studied using MD simulations and PFM. To this end, the key mechanical properties, e.g., Lamé constants ($\lambda_e$, $\mu_e$), phase-field transition width ($\epsilon$), and the mechanical energy release rate ($G$) of aragonite crystals, are obtained from MD simulations. Subsequently, these physical properties are used to reproduce the nano-scale model with a continuous PFM approach. The combination of these methods gives a deeper understanding of brittle fracture at a discrete atomistic level, whilst concurrently helping to establish a link to continuum mechanical fracture models.

In this work, Sections 2 and 3 briefly describe the molecular dynamics, as well as the employed phase-field modeling for brittle fracture. Although it does not aim to deepen in any of both theories, the explanation of the MD approach is somewhat broaden so to help the reader to understand the basics behind all-atom simulations. For the PFM, no new method is proposed in this work, and instead, the numerical experiments are conducted considering already existing and well accepted models for brittle fracture. In Section 4, a thorough description and brief evaluation of the numerical experiments in MD as well as PFM are presented. The comparison between these two approaches

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