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Structural solution using molecular dynamics: Fundamentals and a case study of epoxy-silica interface

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ABSTRACT

In this paper, the molecular dynamics (MD) simulation technique is described in the context of structural mechanics applications, providing a fundamental understanding of the atomistic approach, and demonstrating its applicability. Atomistic models provide a bottom-up description of material properties and processes, and MD simulation is capable of solving the dynamic evolution of equilibrium and non-equilibrium processes. The applicability of the technique to structural engineering problems is demonstrated through an interface debonding problem in a multi-layered material system usually encountered in composite structures. Interface debonding may lead to a possible premature failure of fiber reinforced polymer (FRP) bonded reinforced concrete (RC) structural elements subjected to moisture. Existing knowledge on meso-scale fracture mechanics may not fully explain the weakening of the interface between concrete and epoxy, when the interface is under moisture; there is a need to study the moisture affected debonding of the interface using a more fundamental approach that incorporates chemistry in the description of materials. The results of the atomistic modeling presented in this paper show that the adhesive strength (in terms of energy) between epoxy and silica is weakened in the presence of water through its interaction with epoxy. This is correlated with the existing meso-scale experimental data. This example demonstrates that MD simulation can be effectively used in studying the durability of the system through an understanding of how materials interact with the environment at the molecular level. In view of the limitation of MD simulation on both length- and time-scales, future research may focus on the development of a bridging technique between MD and finite element modeling (FEM) to be able to correlate the results from the nano- to the macro-scale.

1. Introduction

Some of the earliest developments of molecular dynamics (MD) simulation were reported in 1957 (Alder and Wainwright, 1957) for studies on the dynamics of a hard sphere system consisting of several hundreds of particles. Since then, advancement of MD simulation has been observed with the evolution of computational power in the last few decades. MD simulation represents a powerful tool for potential applications in various research fields including physics, chemistry, biology, bio-engineering and medicine (Allen and Tildesley, 1989; Rapaport, 1997). Recently, efforts have been made towards applying the method to structural mechanics and engineering. Traditionally, the classical continuum mechanics theories have been the basis for most computational methods used in various engineering fields including civil and mechanical engineering; examples are finite elements, finite difference, finite volume and boundary element methods. The capability of the continuum approach is limited when structural solution at a small length scale is of concern, or if predictions about material behavior should be made from a fundamental bottom-up perspective.

MD simulation is based on modeling at atomistic level when the discrete nature of the matter at that level is explicitly considered. In an atomistic model the atomic distance provides a natural measure for the spatial discretization. The smallest unit in the atomistic model is an atom; the motion of each in the material is modeled over the course of a simulation time span. Collective behavior of the atoms allows one to understand how the material undergoes structural deformation. Atomistic models provide a fundamental chemistry-based description of material properties and processes, and MD simulation is capable of solving the dynamic evolution of equilibrium and non-equilibrium processes. Thus, a particular and detailed insight into the physics of fundamental processes can be obtained. The atomistic approach has been shown to be powerful in obtaining solutions for small scale structural mechanics problems such as, localized fracture processes in materials (see, for example (Buehler and Ackbarow, 2007) and references therein).

The objective of this paper is first to describe the MD simulation in the context of structural mechanics through a fundamental

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