

PAPER REF: 6782

## **FINITE ELEMENT APPROACH TO SIMULATE CNT-REINFORCED CALCIUM-SILICATE-HYDRATE (C-S-H) COMPOSITE**

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### **ABSTRACT**

Concrete is an old and reliable material for construction. Its mechanical behavior has been widely studied and is well known. It is common to use reinforcements such as steel to improve the ductility of concrete under tension. Recently, nanomaterials have become an interesting solution to improve concrete's mechanical behavior, creating a totally new kind of reinforced composites. As the name may suggest, the understanding of the concrete at the nanoscale then become crucial. From all components of concrete, cement plays a significant role in the mechanical behavior. In particular, cement is controlled by the formation of Calcium-Silicate-Hydrate (CSH). Several authors have proposed different crystalline structure for CSH such as Tobermorit. Molecular dynamics (MD) is the traditional tool to simulate the behavior of the crystalline structure. In this work, a novel approach is used. Following the methodology proposed by Li and Chou, (2003), the interatomic bonds and potentials are simulated using structural finite elements. The finite element (FE) method is faster than MD and extensively used by engineers. This approach is tested by comparing the elastic modulus of both methods. Overall, the new methodology gives promising results.

**Keywords:** Molecular Dynamics, Finite Element Method, Calcium-Silicate-Hydrate.

### **INTRODUCTION**

Concrete is certainly one of the most reliable construction materials. It has been widely used by humanity throughout his history because of its versatility and affordable cost. Concrete has a multiscale composition with different amorphous phases (Eftekhari and Mohammadi, 2016a). Cement is the structural component, determining most of the mechanical properties of concrete. It is brittle in tension and compression, lacking tensile strength compared to compressive strength. This behavior can be improved using reinforced steel bars or polymeric fibers. A new approach consists in using nanomaterials, such as Carbon Nanotubes (CNT). This allows an improved tensile and compressive strength (Eftekhari et al., 2013), creep behavior, resistance to impact (Eftekhari and Mohammadi, 2016b) and fracture toughness (Eftekhari et al., 2014). In order to improve the mechanical properties using CNTs, it is necessary to understand the structure and behavior of cement at the nanoscale.

Cement is made of hydrated and unhydrated products. The Calcium-Silicate-Hydrate (CSH) is the principal product coming from the hydration reaction of calcium silicates. It acts as a binding phase and determines the mechanical properties of cement. The basic hypothesis is that the improvement of concrete properties is directly related with the optimization of the CSH properties. In general, CSH can be considered as a degenerated clay (layered) structure,

composed of silico-aluminates stacked in specific orientations and glued with weak interaction of metal ions and water molecules (Manzano et al., 2012). Water can vary widely so the composition of CSH can only be approximated. Because of these characteristics, CSH is a challenging structure. It is believed that the local atomic structure in the CSH gel is similar to crystalline minerals such as tobermorite (Selvam et al., 2011). Hence, this crystal structure is often used as a starting point to simulate the atomic structure of CSH.

CSH has been traditionally modeled using molecular dynamics (MD) simulations. MD is a calculation method for statistical mechanics, which allows to represent the motion and interactions of atoms and molecules. The potential energy of the interaction's force is represented through interatomic potentials or molecular force fields. The main purpose of MD simulations of CSH is the validation of the molecular structure and the study of the mechanical properties. For instance, Pellenq et al., (2009) constructed a CSH structure based on the 11 Å model of tobermorite proposed by Hamid, (1981). This molecular structure was later used by Abdolhosseini Qomi et al., (2014) to study molecular structure defects (C/S ratio and correlation distances) and mechanical properties (indentation modulus and hardness ratio).

The MD approach is useful to study the mechanical behavior of CSH and it is a powerful tool to gain insight into the molecular structure. Nevertheless, the CPU requirements are usually very high even for a relative small number of atoms. Moreover, the formalism behind the atomic interactions is often outside the basic knowledge of most of engineers. On the other hand, the finite element (FE) method is a widespread and robust tool. Several FE codes are available, both for academic and industrial purposes. The theory of FEs is part of almost every engineering school nowadays. Hence, is interesting to study the feasibility of reproducing MD simulations results using the FE approach. The approach is inspired in the one developed by Li and Chou, (2003) to simulate Carbon Nanotubes (CNT). This approach assumes that the carbon atoms and their interactions within the nanotube can be represented as a frame-like structure. Thus, the bonds among neighboring atoms are assumed to behave like structural beam elements. This is done by linking interatomic potential energies of to the strain energies of an equivalent beam element representing the C-C bond.

In this paper, the methodology developed by Li and Chou, (2003) is used to simulate the CSH molecule. The representation of interatomic interactions is discussed and the results of a tensile test are analyzed.

## **NUMERICAL MODELING**

The FE approach still relies on the atomistic simulations, from which the molecular structure is retrieved. Once the structure is defined and validated as a representative volume element (RVE), the atom coordinates and their connections are exported as nodes and finite elements, respectively. Depending on the type of interaction among atoms (or molecules), the interatomic potential can be represented through the element stiffness and/or a constitutive model. By defining certain boundary conditions, the FE method can be used to obtain elastic parameters or other mechanical properties of the RVE.

The CSH molecule is taken from the MD model of Eftekhari and Mohammadi, (2016a), which is based on the one proposed by Abdolhosseini Qomi et al., (2014). The numerical model is shown in Fig. 1a). In the CSH molecule model, there are intra-molecular covalent bonds and intra-atomic electromagnetic and van der Waals forces. Each one is modeled using a different interaction model i.e., a potential describing the force evolution in space. Intra-

molecular covalent bonds are represented by bond stretching, bond angle and bond torsion models using a harmonic model. Inter-atomic van der Waals forces act in attraction at long distances and repulsion in short distances and can be modeled using the Lennard-Jones, (1924) potential. Electromagnetic force is represented by the Coulomb relation for atomic charges. Hence, the total potential energy of the system is given by the summation of energies due to all interactions:

$$E = \sum E_R + \sum E_\theta + \sum E_\phi + \sum E_{vdw} + \sum E_{el}$$

where  $E_R$  is related to the bond stretch,  $E_\theta$  the bond angle bending,  $E_\phi$  the angle torsion,  $E_{vdw}$  the energy van der Waals force and  $E_{el}$ , the electromagnetic force. In the FE model, the mechanical behavior of the covalent bonds is better represented using beam elements, while van der Waals and electromagnetic forces are modeled using springs. The energy of the FE system must equal that of the MD system, from which the stiffness of the FEs is obtained (Li and Chou, 2003).

A tensile test is simulated by applying certain boundary conditions. One end is fixed in all three directions (clamped), while in the other end is pulled with a small displacement. The material (beam) is assumed to behave as linear-elastic. All the FE simulations are performed using the FE software ANSYS® Academic Research, Release 16.1, (2015). The covalent bonds are represented using the 3D 2-node BEAM188 element, while the electromagnetic and van der Waals forces are represented through the linear spring LINK11. The CSH molecule, showing the covalents bond and the atoms, is depicted in Fig. 1b).

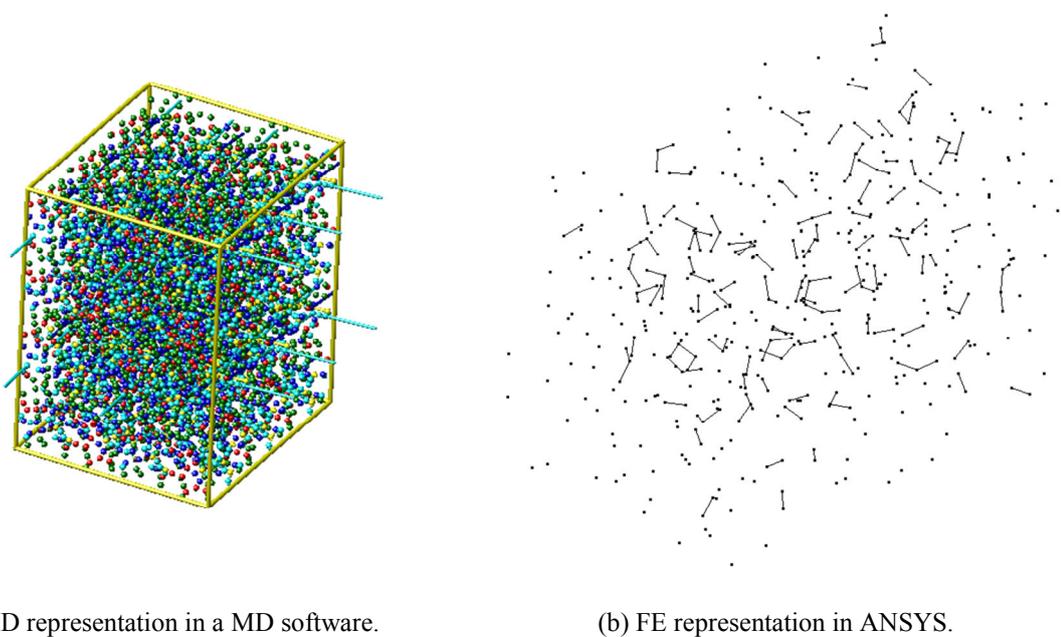


Fig.1 - CSH molecule representation.

## RESULTS

The obtained elastic modulus is shown in Table 1. Compared with the MD results from Eftekhari and Mohammadi, (2016a), the FE results is higher but falls within an acceptable range. The difference can be explained in the terms of the stiffness of the van der Waals spring element, which is assumed to behave linearly even if the Lennard-Jones, (1924) potential is highly non-linear. The elastic modulus chosen for the beam elements is also important in the overall behavior of the molecule. The difference can also be explained by the periodic boundary conditions of the MD simulations, which are not exactly replicated in the FE simulations.

Table 1 - Uniaxial tensile simulations results.

	<b>MD</b>	<b>FE</b>	<b>Difference [%]</b>
<b>Young Modulus [Gpa]</b>	40.97	49.57	20.99

## CONCLUSION

This study presents a novel methodology for simulations at the nanoscopic scale, based on FE simulations. In this approach, interatomic potentials are replaced with structural finite elements. The simulated elastic modulus of the FE simulations is higher than the one predicted from MD simulations, but still within an acceptable range. Further work is being devoted to improve the stiffness of the FEs and to replicate the boundary conditions of the MD simulations.

## ACKNOWLEDGMENTS

The authors acknowledge the support from the Chilean National Commission for Scientific and Technological Research (CONICYT), through grant “FONDECYT REGULAR No.1160691” and “Proyectos Basales USA1555 USACH-MECESUP”. The authors also acknowledge Prof. Mehdi Eftekhari for providing molecular dynamics simulations files.

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