Synopsis

Thesis Title : Evaluation of Engineering Properties of Cement Clinkers Using Molecular Dynamics

Student Name: Aleena Alex

Roll Number : 30EE12A41003

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Thesis supervisor : Dr. Saptarshi Sasmal, Senior Scientist, CSIR- SERC.

Various cementitious composites are extensively used in construction industry. Their properties vary in a large scale and incorporation of desirable properties in cementitious composites has been an active area of interest for research. Such a study not only helps to attain higher efficient materials but also helps to improve upon already existing ones. Identifying and modeling the atomistic structure and simulating the material response are hence relevant and futuristic. There exist various methods for simulating materials and minerals, mainly homogeneous metal like materials, at nano-micro level and thus studying their engineering properties. In the nano level, atomistic properties are simulated by methods such as Monte Carlo Simulation and Molecular Dynamics using empirical inter atomic potential and ab initio quantum mechanical methods. These properties can then be extended to micro level. The results of such simulations have become as valid as theoretical and experimental results. Also simulations based on reasonable physical models can provide experimentalists with guidance. Simulation of atomistic properties of heterogeneous materials like cement and concrete is yet another challenge that has not been entirely addressed.

The strength of concrete originates from the strength of the hardened cement paste, which in turn originates from the hydration products (Murray 2010). The major portion of the hydration products is in the form of a rigid gel, called Calcium Silicate Hydrate (C-S-H). It is believed that C-S-H gel is responsible for strength and cohesion of concrete structures. Currently, there is not an adequate theory for describing the source of the strength or cohesion in C-S-H gel.

Linking the nanostructure of cement clinkers to their micro properties and evaluation of their mechanical behavior is an active area of research. Development of molecular models of amorphous and inhomogeneous nanoparticles will give a better understanding of the cohesive property of cement paste and its tensile behavior. Molecular Dynamic simulations enable to model interactions at a length scale of nanometers over a time scale of femtoseconds which is difficult to obtain through experimental or analytical investigations. The present work is aimed at stimulating the molecular structures of the cement clinkers, such as Tri Calcium Silicate (C3S), Tri Dicalcium

Silicate (C2S) to evaluate the mechanical properties such as Young's modulus. Energy of the system is minimized by adjusting the atomic coordinates. The parameters of Buckingham and Stillinger Weber force fields are used in the simulation are valance, bond and van der Waals terms. The system is brought down to NPT conditions of temperature and pressure. Applying a suitable strain rate, simulation is carried out to evaluate the

load-deformation behavior of the clinkers. The properties of the cement clinkers evaluated in the present study will be further used for molecular modelling of hydrated cement paste, i.e., Calcium Silicate Hydrate (C-S-H) which is the major strength providing composite developed during hydration process of cementitious composites. This study will provide the important information for multi-scale modelling of cementitious composite.