Fact Sheet: South East Regional Research Initiative, Department of Homeland Security

Research Project: Nano particle reinforced composites for critical infrastructure protection

Research Topic: Molecular dynamic simulation

Problem

Multi-scale research, starting from molecular dynamics simulation to developing continuum theory of nano-composite material systems and develop material database for nano-particle reinforced composites and other low-cost, high-strength, innovative materials, such as fly ash and polymer enhanced concrete.

A critical issue for nanotechnology is the ability to understand, model, and simulate the behavior of small structures and to make the connection between structure properties and functions.

Approach

In this study it is proposed to use computational tools (molecular dynamics (MD) simulations) to predict mechanical properties of nano-reinforced polymers.
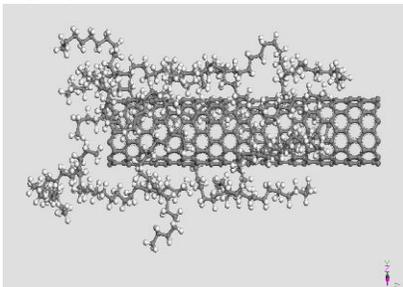
Bulk amorphous polymer structures (in case of polymer based composites) or hydration products (e.g. Calcium Silicate Hydrates (C-S-H) in case of cement-based materials) will be generated by constructing chains in a periodic cell, taking into account bond torsion probabilities and bulk packing requirements. The models will be equilibrated by a series of energy minimization and molecular dynamics runs. The crystal structures for the semi-crystalline polymers will be generated and the simulated bulk structures will be subjected to three different methods for evaluating their mechanical behavior: the static method; the fluctuation method; and the dynamic method. In the static method, each structure will be subjected to a number of successive deformations followed by a re-minimization in order to map out the energy hyper-surface and subsequently to determine the elastic moduli. The dynamic method involves using constant stress molecular dynamics to measure the stress-strain behavior of a material subjected to an applied load. For the dynamic method, a force field (united atoms) can be used. The fluctuation method makes use of the fact that the elastic constants, which appear in the fluctuation formulae, can be obtained from statistical ensembles of the simulations.

The materials that will be studied include:

- Low cost matrices : Nylon-6 thermoplastics, vinyl ester thermosets, hydrated cement, and pozolanic materials (e.g. silica fume or fly ash)
- Nano-particle reinforcement: different types of clay, graphite platelets, carbon nanotubes with a range of volume fractions.

Findings

The work is in progress. A 128-node parallel processing license of Accelrys, a molecular dynamics simulation software, was purchased. Negotiation has been conducted with the Mississippi Center for Supercomputing Research to house and maintain the software, and to allow the simultaneous use of up to 128 SGI and Linux based computers at the Supercomputing Center. Simulation of single and multi-wall carbon nanotubes as well as nylon-6 thermoplastic. The results will be used as a bench mark for simulation of other polymeric matrices and nano reinforcements.

Building nanocomposite polymeric and cement based materials is almost completed and initial runs were submitted for further evaluation.
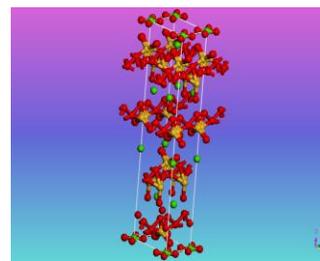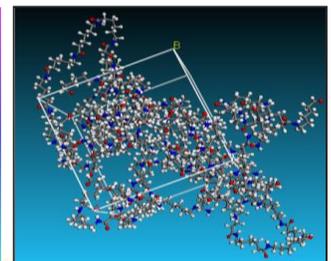
C-S-H (cement)   *Nylon-6*

Impact

Whereas traditional construction material database (e.g. concrete, reinforced concrete, steel, masonry, timber, polymer concrete, and fiber reinforced polymers) can be easily generated from available literature, material database of emerging new materials (e.g. nano-structured materials) is yet to be developed.

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