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Engineer Research and
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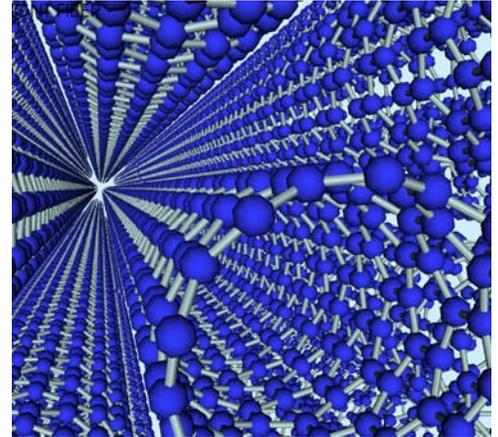
Ongoing Research

Molecular Dynamics Guided Design of Carbon Nanotube-Based Super Construction Materials

Problem

Carbon nanotube (CNT) technology has the potential of producing composite construction materials vastly stronger and lighter than current materials. A barrier to realizing the potential of these materials is developing appropriate molecular designs for CNT composite materials.

These molecular designs must be based on molecular dynamics (MD) simulations. However, MD simulations on the scale needed challenge even the most powerful computers available. Determining the behavior of CNT materials from MD calculations is the subject of state-of-the-art research. These methods are being developed as they are being used.



Description

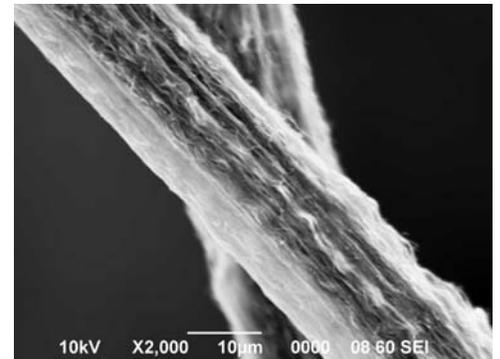
The purpose of this research is to develop a theoretical approach to predicting the response of CNT-based composite materials before they are fabricated. The traditional approach to developing a new material is to create the material first, then test its properties. Using the approach produced by this research, a model of a CNT material is being created using computer software and the engineering material properties of the material are being determined by analyzing the computer model. The resultant molecular designs will then be synthesized.

Existing MD simulation codes will be modified, as necessary, and methods for modeling molecular defects inside the MD simulations will be developed. The MD simulations will be performed on the ERDC Major Shared Resource Center's new Cray XT3. Methods to interpret macroscopic constitutive properties from MD simulations will be further developed, and the accuracy of these methods will be determined by validating the results against existing laboratory data.

Expected Products

A molecular-based method that can predict the applicable constitutive properties of theoretical CNT-composite engineered materials as a function of:

- Molecular configuration of CNT structures.
- Molecular defects.
- Molecular interaction of the different materials composing the composites.



Potential Users

This research lays part of the basic foundation necessary for the efficient development of CNT composite construction materials by making it possible for molecular designers to

predict the properties of the materials before the methods to produce those materials are developed.

Projected Benefits

CNT composite construction materials offer 1 to 2 orders of magnitude strength and weight improvements over current materials. Recent advances in high-performance computing now make it possible to predict the bulk mechanical properties of engineered CNT-composite materials based on molecular dynamics. Over the next 2 to 3 decades, CNT materials have the potential to offer:

- 50- to 150-fold increase in strength over that of steel.
- Order-of-magnitude decrease in weight.

Program Manager

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