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Computational materials: Multi-scale modeling and simulation of nanostructured materials

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Abstract

The paper provides details on the current approach to multi-scale modeling and simulation of advanced materials for structural applications. Examples are given that illustrate the suggested approaches to predicting the behavior and influencing the design of nanostructured materials such as high-performance polymers, composites, and nanotube-reinforced polymers. Primary simulation and measurement methods applicable to multi-scale modeling are outlined. Key challenges including verification and validation are highlighted and discussed.

Keywords: Multi-scale modeling; Computational materials; Nanotechnology

1. Introduction

"I have not failed. I've just found 10,000 ways that don't work" – Thomas Alva Edison (1847–1931).

Each distinct age in the development of humankind has been associated with advances in materials technology. Some historians have linked key technological and societal events with the materials technology that was prevalent during the "stone age," "bronze age," and so forth. The description of our current age and culture will be up to future historians, but the last 350 years have seen many advances in materials technology that have helped shape our world today. Much of this groundbreaking work (Table 1) was because of perseverant research scientists and engineers finding solutions after long periods of experimentation and development.

Within the last 20 years, many research institutions have recognized the need for a more systematic approach to new materials development that employs a multi-scale modeling approach. This approach was one that would combine interdisciplinary research, new advances in computational modeling and simulation, and critical laboratory experiments to rapidly reduce the time from concept to end product. The general consensus is that this new paradigm by which all future materials research would be conducted and has come to be known simply as "Computational Materials."

Traditionally, research institutions have relied on a discipline-oriented approach to material development and design with new materials. It is recognized, however, that within the scope of materials and structures research, the breadth of length and time scales may range more than 12 orders of magnitude, and different scientific and engineering disciplines are involved at each level. To help address this wide-ranging interdisciplinary research, Computational Materials programs have been formulated with the specific goal of exploiting the

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Table 1
Significant events in materials development over the last 350 years

1665 – Robert Hooke … material microstructure
1808 – John Dalton … atomic theory
1824 – Portland cement
1839 – Vulcanization
1856 – Large-scale steel production
1869 – Mendeleev and Meyer … Periodic Table of the Chemical Elements
1886 – Aluminum
1900 – Max Planck …. quantum mechanics
1909 – Bakelite
1921 – A.A. Griffith …. fracture strength
1928 – Staudinger… polymers (small molecules that link to form chains)
1955 – Synthetic diamond
1970 – Optical fibers
1985 – First university initiatives attempt computational materials design
1985 – Bucky balls (C_{60}) discovered at Rice University
1991 – *Carbon nanotubes* discovered by Sumio Iijima

tremendous physical and mechanical properties of new nano-materials by understanding materials at atomic, molecular, and supramolecular levels.

Computational Materials draws from physics and chemistry, but focuses on constitutive descriptions of materials that are useful in formulating macroscopic models of material performance. The objective of this paper is to describe in some detail how convergent technologies have facilitated multiscale modeling of novel nanostructured materials and to outline the Computational Materials approach for materials and structures research. In particular, the paper discusses how the Computational Materials approach utilizes multi-scale analysis methods, as illustrated in Fig. 1 and critical experiments or measurements, illustrated in Fig. 2, to establish the technology for the scale-up of nanostructured materials into engineering level, multifunctional materials for advanced applications such as next generation aircraft and spacecraft.

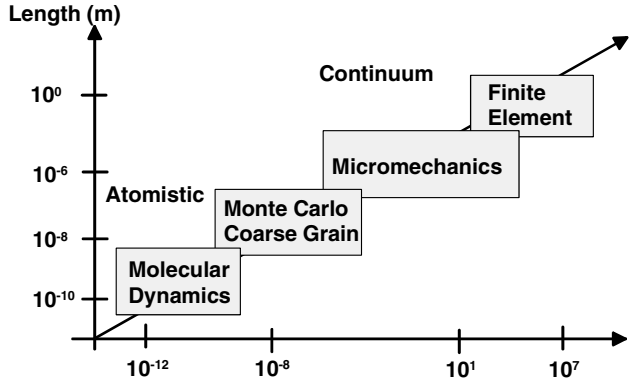

Fig. 1. Range of length and time scales of the key simulation methods.

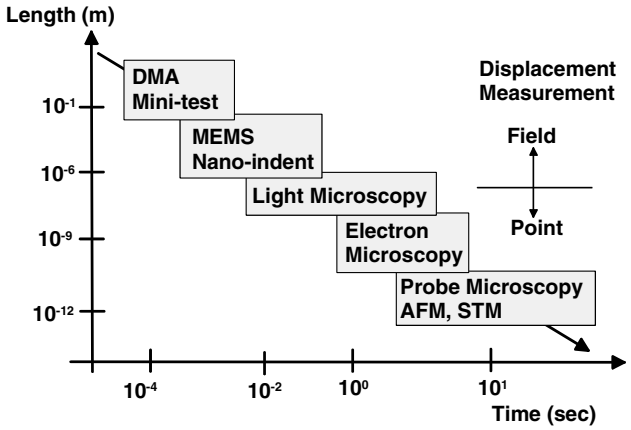

Fig. 2. Range of length and time scales associated with key measurement methods.

The benefits of the Computational Materials approach are threefold. First, it encourages a reduced reliance on costly trial and error, or serendipity, of the "Edisonian" approach to materials research. Second, it increases the confidence that new materials will possess the desired properties when scaled up from the laboratory level, so that lead-time for the introduction of new technologies is reduced. Third, the Computational Materials approach lowers the likelihood of conservative or compromised designs that might have resulted from reliance on less-than-perfect materials.

The paper is organized as follows. Key challenges are discussed, contributions from convergent technologies: measurement science, and information technology, are presented, details of the primary simulation methods are outlined, and the issues of method verification and validation are explained.

2. Key challenges

For aerospace applications, the most notable design challenges are directly related to enhancing the performance of advanced aircraft and spacecraft by increasing: size per mass, strength per mass, function per mass and power, and intelligence per mass and power. In terms of multi-scale modeling and the application of advanced nanostructured materials, these challenges translate into more specific requirements that include high-strength-per-mass smart materials for vehicles and large space structures, materials with designed-in mechanical/thermal/electrical properties, materials for high-efficiency energy conversion, and materials with embedded sensing/compensating systems for reliability and safety.

3. Computational materials

In order to address these goals and challenges, Computational Materials programs have developed schemes