Foreword

Toward Computational Materials Science and Engineering

Organic Materials Lab.

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In the 20th century, a man at a Plexiglas plant is typing at the keyboard of a computer. Several images are displayed on the monitor. Finally, the man shows an image of a molecular model rotating on the screen to the plant manager. The plant manager is surprised because the model demonstrates transparent aluminum. This is one scene from "STARTREK IV: the Voyage Home," a science fiction movie released in 1986. The man at the keyboard is Scotty, chief engineer aboard the U.S.S. Enterprise. In 2286, Earth is threatened by a deep-space probe that has drained all power from the planet and is vaporizing the oceans. This destruction is due to signals transmitted by the probe in an attempt to communicate with whales, which have become extinct. To save Earth, Admiral Kirk and his crew time-warp back to the 20th century and return with a pair of whales. Scotty and McCoy make a trade information of the transparent aluminum for Plexiglas to build a whale tank in the ship.

Since the mid 1980's, when this movie was released, the creation of novel materials via computer has been an interesting dream of physicists, chemists, materials researchers and materials engineers. Computational materials science has received considerable attention to guide us toward new materials with unique properties. This science uses computers to model and predict materials properties. The basic phenomena of materials are modeled at the atomistic scale by molecular calculation. Recently, in our laboratories, a new visible-light photocatalyst was actually synthesized according to molecular calculation. This is one successful application of atomistic simulation.

Understanding the practical or macroscopic material properties from atomistic simulation alone is difficult. There is a large difference in scale between atomistic and macroscopic scales. Moreover, macroscopic properties strongly depend on the material microstructure which is affected by the manufacturing process. Computational materials science is now focused on multi-scale simulations, which work as a bridge between atomistic phenomena and macroscopic behavior. A multi-scale simulation software package, OCTA, has been developed for polymer modeling as part of a national project and has been freely downloadable over the Internet since last year.

One of our frontier groups has actively studied multi-scale simulations for materials science and engineering over the last three years. The results of these studies are described in this issue. Multi-scale simulation will proceed in conjunction with experimental studies on the acceleration of materials research and development.