Multiscale modeling of complex physical systems

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A number of important physical phenomena can only be addressed properly by models across several length or time scales. A typical example is the fracture of materials, which involves the breaking of interatomic bonds at the micorscopic level and the ensuing large deformation of the physical system at macroscopic scales. A different class of systems where multiscale modeling must be invoked because of the coupling between molecular motions and the larger scale environmental conditions, are biological macromolecules such as nucleic acids and proteins.

In the last few years we have been developing methods for studying such phenomena across several length scales, and applying these methods to representative systems. This presentation will review some examples of the methods and the systems we have considered. The methods will include the development of variational phenomenological theories [PRL **78**, 4221 (1997)] which apply to the macroscopic scale but use as input information calculated at the microscopic scale from first-principles quantum mechanical calculations and can thus address realistic problems of practical importance [PRL **87**, 095501 (2001)]; and the use use of a quasi-continuum approach for complex crystals [PRB **59**, 235 (1999)] to describe large scale deformation [PRL **84**, 1260 (2000)] or the competition between external fields [Act.Mat. **50**, 2989 (2002)]. Finally, we will also describe on-going work on extended biological macromolecules, which also require multiscale models. The examples which will be considered are: the electronic states in overstretched DNA and the implications for its conductivity [PRB **66**, 241104 (2003)]; and the microscopic motions responsible for the rotary motion in the enzyme ATP-synthase, which catalyzes the synthesis of the molecular unit of energy in all forms of life. Due to the rather complex nature of these systems, the present studies are only a first step toward their understanding and point to important unresolved issues which will require the further extension of multiscale modeling tools.

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