

This article was downloaded by: [Indian Institute of Technology Kharagpur]

On: 23 October 2008

Access details: Access Details: [subscription number 901727275]

Publisher Taylor & Francis

Informa Ltd Registered in England and Wales Registered Number: 1072954 Registered office: Mortimer House, 37-41 Mortimer Street, London W1T 3JH, UK



Materials and Manufacturing Processes

Publication details, including instructions for authors and subscription information:

<http://www.informaworld.com/smpp/title-content=t713597284>

A Review of: "Multiscale Simulation Methods for Nanomaterials, R.B. Ross and S. Mohanty (editors)"

Baidurya Bhattacharya^a

^a Department of Civil Engineering, Indian Institute of Technology, Kharagpur 721302, India

Online Publication Date: 01 October 2008

To cite this Article Bhattacharya, Baidurya(2008)'A Review of: "Multiscale Simulation Methods for Nanomaterials, R.B. Ross and S. Mohanty (editors)"',Materials and Manufacturing Processes,23:8,893 — 894

To link to this Article: DOI: 10.1080/10426910802385141

URL: <http://dx.doi.org/10.1080/10426910802385141>

PLEASE SCROLL DOWN FOR ARTICLE

Full terms and conditions of use: <http://www.informaworld.com/terms-and-conditions-of-access.pdf>

This article may be used for research, teaching and private study purposes. Any substantial or systematic reproduction, re-distribution, re-selling, loan or sub-licensing, systematic supply or distribution in any form to anyone is expressly forbidden.

The publisher does not give any warranty express or implied or make any representation that the contents will be complete or accurate or up to date. The accuracy of any instructions, formulae and drug doses should be independently verified with primary sources. The publisher shall not be liable for any loss, actions, claims, proceedings, demand or costs or damages whatsoever or howsoever caused arising directly or indirectly in connection with or arising out of the use of this material.

Book Review

Multiscale Simulation Methods for Nanomaterials, R.B. Ross and S. Mohanty (editors), John Wiley & Sons, Inc., Hoboken, New Jersey, 275 pages, Wiley-Interscience, 2008, ISBN: 978-0-470-10528-3.

Wiley has recently published a book of 14 chapters. Each of these chapters is an expanded version of the presentation made at the National American Chemical Society Meeting in Washington, DC, in the fall of 2005, on large scale molecular dynamics, nanoscale, and mesoscale modeling and simulation. The title of this book, *Multiscale Simulation Methods for Nanomaterials*, is ambitious and should have reflected the stated focus on “mesoscale” modeling instead of the appealing lead word in the title, more so since not all the chapters use multiscale modeling, but merely allude to the possibility. The chapters are all self-contained, and several of them are very well written. This collection is more for the advanced reader and less for the uninitiated.

The first chapter written by the editors of the book gives a nice overview of multiscale simulations and what is to come in the rest of the book. They introduce the term “mesoscale phenomena” as distinct from atomistic and continuum phenomena, give examples, and stress the need of multiscale modeling (both in time and space). Two kinds of multiscale modeling are identified: *hierarchical*, in which there is one-way scale bridging, and *handshake*, in which there is two-way information exchange between different scales.

The next chapter performs quantum mechanical modeling of the self-assembly and charge transfer in a photosynthetic minimal protocell attempting to provide a perspective of the requirements for success in the synthesis of potentially new living organisms in the presence of water and fatty acid molecules. The minimal protocell contains of the order of 1000 atoms and can be considered to be a self-assembling molecular electronics device (according to quantum-based electron interaction potential) that absorbs light and carries out its metabolism according to quantum electron excitation and tunneling equations.

Chapter three is about doping single walled carbon nanotubes (SWNTs) by encapsulating organic molecules. SWNTs, which are obtained by rolling sp² hybridized 2D graphene, can act both as quantum wave guides and quantum dots, and can possibly be used as molecular wires and field effect transistors. The authors investigate the charge transport processes and quantum conductance in (10, 10) SWNTs doped with organic molecules (F4-TCNQ, TTF, or TDAE) by large scale quantum electronic structure

calculations coupled with a Green’s function formulation. They find that even though a molecule can induce *n*- or *p*-type doping, it has a rather small (and desirable) effect on the transport properties of the doped tube compared to the parent SWNT.

Chapter four describes both computational and experimental work aimed at two seemingly conflicting properties of PPVs: their conductance and their luminescence. Working on CN-PPV and MEH-PPV, the authors suggest that more so than *aggregates* of these chains (which enhance carrier mobility by adding to the polymer’s standard interchain conductance), it is the *order* in these chains that cause the conductance/luminescence tradeoff. The authors obtain evidence of order by observing orientation of the nanostructures through high resolution fluorescent imaging and tapping mode AFM.

An algorithm for mapping (and validating) a coarse grained (CG) model to the underlying molecular description is described in the next chapter. The algorithm uses SO(3) optimization to align molecular fragments positioned at CG sites, rotated to minimize an energy function consisting of both intra- and intermolecular terms. The authors show how such an algorithm can be advantageous in a hybrid dual resolution MD. Bulk liquid dodecane is used as an example.

Chapter six talks about protein dynamics, stability, and conformational denaturation of proteins in biopreservative solution, and focuses on the interaction of protein and solvent through molecular dynamics (using AMBER package). The subject protein is lysozyme and the candidate solvents are glycerol and trehalose. The authors hypothesize that suppression of rapid (of the order of pico- to nanoseconds) atomic scale fluctuations may prevent longer time scale motion of the protein molecule and increase its conformational stability. They zero in on the coupling of protein and solvent dynamics, and focus on the protein-solvent interface. They conclude that the solvent dynamics influences the protein surface through hydrogen bond interactions (the dynamics of the hydrogen bond network between the protein surface and the first shell of the solvent control the structural relaxation of the protein), which in turn influences the core atoms through intramolecular interactions (van der Waals, electrostatic, bonded etc.).

An exclusive chapter deals with nanoparticles dispersed in solvents. To help dispersion, these nanoparticles are surface-coated with simple organic functional groups. The interaction of the functional groups and the solvent occurs over a few Angstrom, while those between the nanoparticles occur over a distance of 10–30 nm. The author attempts

to develop a coarse grained model of the behavior of these nanoparticles. The energy of interaction between two surfaces of functional groups is determined first. This gives the interaction energy between two nanoparticles and force fields can be derived. Once this is complete, the nanoparticle-surface modifier-solvent system reduces to a simple box of interacting particles which can be studied with standard means to determine the standard aggregate equilibrium quantities.

Chapter eight describes an ad hoc scheme for coupling continuum and atomistic simulations that can compensate for deficiencies in the interatomic potential, notably those arising from electronic effects, through the use of average macroscopic quantities, by stepwise feedback of common parameters between the two domains. A list of unresolved issues in the ad hoc scheme is included. The authors first present the implementation of a continuum thermostat in which the solution of the continuum heat equation in a region at the beginning of a time-step uses the average kinetic energy of the atoms in that region as initial condition, the macroscopic diffusivity, and the rate of heat generated to determine the temperature at the next time step. The atomistic simulation uses this new temperature to rescale the velocities. This thermostat scheme is used next to model Joule heating due to current flow in which a virtual network of resistors connects adjacent regions of the grid. Finally, the authors present simulation of electrically hot and cold metal to metal contacts that represent an asperity contact in a MEMS device. The authors also discuss the possibility of applying the ad hoc scheme in diffusion and chemical kinetics-controlled processes.

Chapter nine presents a fully analytic implementation of the density functional theory that uses analytic atom-centered localized Gaussian basis sets. The exchange correlation part of the Kohn–Sham potential, representing the quantal contributions, is obtained from Slater’s exchange functional, parameterized by appropriate scaling factors. The authors study the electronic and structural properties of large carbon fullerenes (up to C_{2160}) and fullerene-like cages of AlN and BN containing a few hundred atoms and optimize their geometries.

Chapter ten develops interatomic potential functions for Al (from molecules, nanoclusters, and nanoparticles to bulk crystals) based on density functional theory (DFT) that can take into account size dependence. The size dependence of atomization energy for Al is used for the fit. The authors

study size dependence of density, thermal expansion, and particle shape of Al nanodroplets.

The next chapter is a review article providing five examples of large scale Monte Carlo simulations (MCS) involving: (i) structure and retention in reversed-phase liquid chromatography (using efficient configurational bias MCS in isobaric isothermal Gibbs ensemble), (ii) solubility of helium in *n*-hexadecane (using configurational bias MCS in constant pressure Gibbs ensemble), (iii) structure and solubility in supercritical carbon dioxide (using constant pressure Gibbs ensemble MCS), (iv) interfacial properties of an aqueous solution containing ions with a range of sizes (using Gibbs ensemble MCS), and (v) first principles MCS of the vapor liquid coexistence curve of water (using Kohn–Sham density functional theory).

Studies related to phosphoryl transfer reactions in solution through quantum mechanical/molecular mechanical simulations are described in this chapter. A new semi-empirical quantum model integrated with a linear-scaling Ewald method (to calculate long range electrostatic interactions) is integrated into CHARMM molecular simulation package. The authors study the relative hydrolysis rates of cyclic and acyclic phosphates, and compare with available experimental data.

Chapter thirteen extends the classical force field based molecular dynamics to the simulation of chemical reactions involving large molecules and nanostructures in order to capture time scales that are too large for quantum chemical methods. The authors describe the “reactive molecular dynamics” scheme in which chemically active atoms are identified at the end of each MD step by comparing each covalently bonded atom pair’s fractional bond order to a preset bond dissociation criterion. The authors study the thermal decomposition of polymethyl methacrylate, polybisphenol A carbonate, and polyisobutylene.

The last chapter describes simulation-based methods, with special emphasis on dissipative particle dynamics, to predict dynamic behavior and nonequilibrium structures of surfactants. The author looks at both ionic and nonionic surfactant solutions as well as mixed surfactant systems.

Baidurya Bhattacharya
Department of Civil Engineering,
Indian Institute of Technology,
Kharagpur 721302, India