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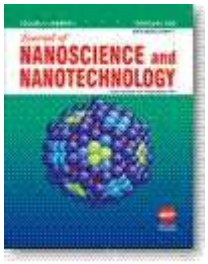

Mathematical and Computational Models for Transport and Coupled Processes in Micro- and Nanotechnology

Authors: Melnik, Roderick; Povitsky, Alex; Srivastava, Deepak
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This special issue contains refereed papers based on invited presentations at the workshop on "Transport and Coupled Processes in Micro- and Nanotechnology" of the 7thWorld Congress on Computational Mechanics held in Los Angeles, California, USA, July 16 - 22, 2006.

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A SPECIAL SECTION

Mathematical and Computational Models for Transport and Coupled Processes in Micro- and Nanotechnology

As the range of applications of micro- and nanostructures continues to grow, the role of mathematical models and computational experiments in this field becomes increasingly important. Designing of and working with structures and devices on scales between a nanometer and a micron bring new fundamental challenges that can be addressed by combined efforts of researchers working in chemical kinetics, micro-scale fluid dynamics, heat-transfer, mathematical modeling, micro-scale solid mechanics and solid-state physics.

A number of talks along these directions were presented at the VII-th World Congress on Computational Mechanics in Los Angeles, in particular at the workshop on "Transport and Coupled Processes in Micro- and Nanotechnology" organized by the Guest Editors of this special issue. The workshop brought together engineers, mathematicians, and scientists working in this rapidly evolving field in order to discuss state-of-the-art models, procedures, and algorithms for the analysis of transport and coupled processes and phenomena encountered in micro- and nanotechnological applications. Such processes and phenomena are of increasing importance due to extreme sensitivity of nanomaterials and devices to mechanical, thermal and other effects that can lead to complete or partial failure. Several selected papers written by the authors who presented their talks in other sessions of WCCM-7 are also included in this special issue. We thank all our referees for their time and efforts in providing an important keystone for a high standard special issue.

The original contributions to this special issue covered a range of topics from micro-fluidics applications, thermo-fluids aspects of synthesis of macromolecules including carbon nanotubes to the analysis of semiconductor heterostructures, sensor and actuator control schemes on micro- and nano-levels, as well as biotechnological applications. Much of the discussion at the workshop was devoted to a hierarchical modeling approach as we welcomed contributions that discussed all aspects of modeling matter at the molecular/atomistic level and life at the cellular level, as well as contributions dealing with continuum mechanics methodologies in particular when the authors discussed the validity of these methods for micro- and nano-scale phenomena. Among other application areas, we would like to mention contributions in modeling of high-energy phenomena in a small scale range such as a short-pulse laser ablation as well as contributions in applications, stability and accuracy of combined atomistic and continuum simulations. Many presentations discussed multi-scale modeling techniques in the context of transport and coupled phenomena and processes encountered in micro- and nanotechnology. This issue included 16 papers covering some of the above topics.

We hope that this special issue will become a useful reference for researchers studying coupled and transport processes at micro- and nano-scale and will help strengthen interdisciplinary collaboration in this important field of nanoscience and nanotechnology.

Roderick Melnik
Wilfrid Laurier University
Waterloo, ON, Canada

Alex Povitsky
University of Akron, Akron, OH, USA

Deepak Srivastava
NASA Ames Research Center, Moffett Field, CA, USA

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ABOUT THE GUEST EDITORS

Dr. Roderick Melnik is Full Professor in the Faculty of Science at the Wilfrid Laurier University, the older of the two universities in Waterloo Canada where he holds Tier I Canada Research Chair, Canada's most prestigious academic position. He is Head of the M2NeT Lab. He is also an adjunct professor in the Department of Physics and Astronomy of the University of Waterloo. He received his Ph.D. in 1989 from Kiev State University. Since 1998 he is an elected Fellow of the Institute of Mathematics and its Applications in the United Kingdom. Before moving to Canada in 2004, Professor Melnik held full professorships in the USA and Denmark and was senior scientist at the Commonwealth Scientific and Industrial Research Organisation (CSIRO) in Sydney, Australia. He was a Visiting Fellow at the Isaac Newton Institute, University of Cambridge in England and was honored with Hans Christian Andersen Academy Fellowship, awarded world-wide to only one researcher a year in all academic fields. Dr. Melnik has published extensively, as a sole author and with his collaborators from around the world. Professor Melnik's major areas of research are centered around mathematical modelling for new technologies, including the analysis of low dimensional semiconductor nanostructures.

Dr. Alex Povitsky is an Associate Professor at the Department of Mechanical Engineering, The University of Akron, Akron, Ohio, USA. He has been a Summer Faculty Fellow at US Air Force Research Laboratory in 2005–2007. He studied applied mathematics, computational science and metallurgical engineering in Moscow Institute for Steel and Alloys (Technical University). He did his Ph.D. in mechanical engineering specializing in computational fluid dynamics (CFD). He was a postdoctoral fellow at the Department of Aerospace Engineering at the Technion-Israel Institute of Technology (1991–1994) where he became involved in parallel computing for CFD. He was the lecturer at the Technion (1994–1997), Senior Scientist for Institute of Computer Applications (ICASE) at NASA Langley Research Center (1997–2001), Associate Professor at Concordia University (Montreal) (2001–2003). His publications are in thermo-fluid modeling of synthesis of nanotubes, parallel computing for CFD, aeroacoustics, and modeling of industrial applications of chemically reacting flows. His current research focuses on simulation of microfluids using combined molecular and continuum flow approach, and on coupled thermal and gas dynamic approach to ablation.

Deepak Srivastava has been a Lead Scientist and Manager of computational materials design and nanotechnology related activities at NASA Ames Center for Nanotechnology for last ten years. In recent years he has given more than 100 invited talks on computational materials design, nanotechnology, and aerospace and defense related materials applications in USA and abroad. His recent award and honors include winner of Feynman Prize in Nanotechnology (Theory) in 1997, Veridian Medal Paper (1999), The Eric Reissener Medal (2002), and CSC Award for Technical Excellence (2003). Dr. Srivastava has served as Associate Editor of two peer reviewed nanotechnology and computational materials sciences related journals and sits on the editorial boards of two other journals. Dr. Srivastava co-founded and served as CTO of a computational materials design company Junius Tech, which was acquired by a nanomaterials rational design and fabrication company—Nanostellar in the automotive catalysis sector. At Nanostellar he served as a technical advisor for two years helping to build and advice the technical team, investigate future new product and technology areas, and technology development consulting on a regular basis. Since the beginning of 2007, Dr. Srivastava has also become the CTO of Nanoexa, a clean energy company focused on quantum simulation based design, performance optimization, and product development for the next generation of Li-Ion battery and Solar PV materials, devices and applications.