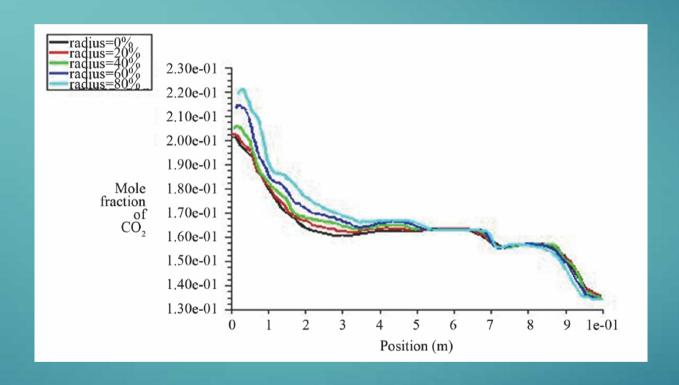


MODELING AND NUMERICAL SIMULATION OF MATERIAL SCIENCE





Journal Editorial Board

ISSN: 2164-5345 (Print) ISSN: 2164-5353 (Online)

http://www.scirp.org/journal/mnsms

.....

Honorary Editor in Chief

Prof. Kiet Tieu University of Wollongong, Australia

Executive Editor in Chief

Prof. Hai-Liang Yu Shenyang University, China

Editorial Board

Dr. Jean-Pierre Badiali Research Director of Exceptional Class, France

Dr. François Barthelat McGill University, Canada

Prof. Giuseppe Bonifazi Università di Roma, Italy

Prof. Roberto Brighenti University of Parma, Italy

Prof. Zhenshan Cui Shanghai Jiao Tong University, China

Dr. Shaogang Hao Iowa State University, USA

Dr. Chen Huang Theoretical Division, Los Alamos National Laboratory, NM, USA

Dr. Ayhan Ince General Dynamics Land Systems, Canada

Dr. Jinwu Kang Tsinghua University, China

Prof. Alexandre Ksenofontov National Research Nuclear University, Russia

Prof. Xianghua Liu Northeastern University, China

Dr. Yingtao Liu Arizona State University, USA

Dr. Jane Weizhen LuCity University of Hong Kong, ChinaProf. Gilles LubineauCOHMAS Laboratory, Saudi Arabia

Dr. Scott T. Miller Applied Research Laboratory at Penn State, USA

Dr. Qing PengRensselaer Polytechnic Institute, USA

Dr. Hai Qing Siemens Wind Power, Denmark

Prof. Hou-Fa Shen Tsinghua University, China

Prof. Ashok Srvastava Louisiana State University, USA

Dr. Baolin Wang The University of New South Wales, Australia

Dr. Huanan Yu Washington State University, USA

Prof. Hamit Yurtseven Middle East Technical University, Turkey

Prof. Shi-Hong Zhang Chinese Academy of Sciences, China



Table of Contents

Volume 4	Number 2	April 2014
Comparison o	of Functionals for Metal Hexaboride Band Structure Calculations	
J. A. Alarco,	P. C. Talbot, I. D. R. Mackinnon	53
Performance	Prediction of a Pressurized Entrained Flow Ultra-Fine Coal Gasifier	
P. P. Mashing	go, G. R. John, C. F. Mhilu	70

Modeling and Numerical Simulation of Material Science (MNSMS)

Journal Information

SUBSCRIPTIONS

The *Modeling and Numerical Simulation of Material Science* (Online at Scientific Research Publishing, www.SciRP.org) is published quarterly by Scientific Research Publishing, Inc., USA.

Subscription rates:

Print: \$69 per issue.

To subscribe, please contact Journals Subscriptions Department, E-mail: sub@scirp.org

SERVICES

Advertisements

Advertisement Sales Department, E-mail: service@scirp.org

Reprints (minimum quantity 100 copies)

Reprints Co-ordinator, Scientific Research Publishing, Inc., USA.

E-mail: sub@scirp.org

COPYRIGHT

COPYRIGHT AND REUSE RIGHTS FOR THE FRONT MATTER OF THE JOURNAL:

Copyright © 2014 by Scientific Research Publishing Inc.

This work is licensed under the Creative Commons Attribution International License (CC BY). http://creativecommons.org/licenses/by/4.0/

COPYRIGHT FOR INDIVIDUAL PAPERS OF THE JOURNAL:

Copyright © 2014 by author(s) and Scientific Research Publishing Inc.

REUSE RIGHTS FOR INDIVIDUAL PAPERS:

Note: At SCIRP authors can choose between CC BY and CC BY-NC. Please consult each paper for its reuse rights.

DISCLAIMER OF LIABILITY

Statements and opinions expressed in the articles and communications are those of the individual contributors and not the statements and opinion of Scientific Research Publishing, Inc. We assume no responsibility or liability for any damage or injury to persons or property arising out of the use of any materials, instructions, methods or ideas contained herein. We expressly disclaim any implied warranties of merchantability or fitness for a particular purpose. If expert assistance is required, the services of a competent professional person should be sought.

PRODUCTION INFORMATION

For manuscripts that have been accepted for publication, please contact:

E-mail: mnsms@scirp.org



Modeling and Numerical Simulation of Material Science

ISSN 2164-5345 (print) ISSN 2164-5353 (online)

http://www.scirp.org/journal/mnsms

Modeling and Numerical Simulation of Material Science (MNSMS) is an international peer-reviewed, open access journal publishing in English original research studies, reviews and case reports in all aspects of Material Science. Symposia or workshop papers may be published as supplements.

Honorary Editor in Chief

Prof. Kiet Tieu University of Wollongong, Australia

Executive Editor in Chief

Prof. Hai-Liang Yu Shenyang University, China

Subject Coverage

All the manuscripts must be prepared in English, and are subject to a rigorous and fair peer-review process. Accepted papers will immediately appear online followed by printed hard copies. The journal publishes original papers including but not limited to the following fields:

- Application of modeling and numerical simulation methods in analysis of solidification, forming, welding, heat treatment, surface engineering, process of materials, include, ferrous metals and alloys, non-ferrous metals and alloys, biomaterials, carbons, ceramic materials, polymer, composites, and other advanced materials.
- New development of modeling and numerical simulations methods for analysis material processes, such as finite element method, finite difference method, boundary element method, slab method, crystal finite element method, CA, MD, statistical methods, artificial intelligence method.

Notes for Intending Authors

Submitted papers should not have been previously published nor be currently under consideration for publication elsewhere. Paper submission will be handled electronically through the website. All papers are refereed through a peer review process. For more details about the submissions, please access the website.

E-mail: mnsms@scirp.org

Website and E-Mail

http://www.scirp.org/journal/mnsms

What is SCIRP?

Scientific Research Publishing (SCIRP) is one of the largest Open Access journal publishers. It is currently publishing more than 200 open access, online, peer-reviewed journals covering a wide range of academic disciplines. SCIRP serves the worldwide academic communities and contributes to the progress and application of science, by delivering superior scientific publications and scientific information solution provider that enable advancement in scientific research.

What is Open Access?

All original research papers published by SCIRP are made freely and permanently accessible online immediately upon publication. To be able to provide open access journals, SCIRP defrays operation costs from authors and subscription charges only for its printed version. Open access publishing allows an immediate, world-wide, barrier-free, open access to the full text of research papers, which is in the best interests of the scientific community.

- •High visibility for maximum global exposure with open access publishing model
- •Rigorous peer review of research papers
- Prompt faster publication with less cost
- •Guaranteed targeted, multidisciplinary audience





Website: http://www.scirp.org Subscription: sub@scirp.org Advertisement: service@scirp.org