PROCEEDINGS OF SPIE

SPIDigitalLibrary.org/conference-proceedings-of-spie

Front Matter: Volume 6597

, "Front Matter: Volume 6597," Proc. SPIE 6597, Nanodesign, Technology, and Computer Simulations, 659701 (10 April 2007); doi: 10.1117/12.739289

SPIE.

Event: Nanodesign, Technology, and Computer Simulations, 2006, Olsztyn, Poland

PROCEEDINGS OF SPIE

Nanodesign, Technology, and Computer Simulations

Alexander I. Melker
Teodor Breczko
Editors

19–25 June 2006
Olsztyn, Poland

Sponsored by
SPIE Poland Chapter
SPIE Russia Chapter

Proceedings of SPIE—The International Society for Optical Engineering, 9780819467331, v. 6597

SPIE is an international technical society dedicated to advancing engineering and scientific applications of optical, photonic, imaging, electronic, and optoelectronic technologies.

The papers included in this volume were part of the technical conference cited on the cover and title page. Papers were selected and subject to review by the editors and conference program committee. Some conference presentations may not be available for publication. The papers published in these proceedings reflect the work and thoughts of the authors and are published herein as submitted. The publisher is not responsible for the validity of the information or for any outcomes resulting from reliance thereon.

Please use the following format to cite material from this book:

Author(s), "Title of Paper," in *Nanodesign, Technology, and Computer Simulations*, edited by Alexander I. Melker, Teodor Breczko, Proceedings of SPIE Vol. 6597 (SPIE, Bellingham, WA, 2007) Article CID Number.

ISSN 0277-786X
ISBN 9780819467331

Published by
SPIE—The International Society for Optical Engineering
P.O. Box 10, Bellingham, Washington 98227-0010 USA
Telephone 1 360/676-3290 (Pacific Time) · Fax 1 360/647-1445
<http://www.spie.org>

Copyright © 2007, The Society of Photo-Optical Instrumentation Engineers

Copying of material in this book for internal or personal use, or for the internal or personal use of specific clients, beyond the fair use provisions granted by the U.S. Copyright Law is authorized by SPIE subject to payment of copying fees. The Transactional Reporting Service base fee for this volume is \$18.00 per article (or portion thereof), which should be paid directly to the Copyright Clearance Center (CCC), 222 Rosewood Drive, Danvers, MA 01923. Payment may also be made electronically through CCC Online at <http://www.copyright.com>. Other copying for republication, resale, advertising or promotion, or any form of systematic or multiple reproduction of any material in this book is prohibited except with permission in writing from the publisher. The CCC fee code is 0277-786X/07/\$18.00.

Printed in the United States of America.

Contents

ix	Conference Committees
xi	Introduction
xiii	Related Publications

659702	Fiftieth anniversary of molecular dynamics [6597-01] A. I. Melker, St. Petersburg State Polytechnical Univ. (Russia)
--------	--

SESSION 1 ELECTRONIC AND ATOMIC DYNAMICS

659703	Path integral representation of the evolution operator for the Dirac equation [6597-02] A. S. Lukyanenko, St. Petersburg State Polytechnical Univ. (Russia); I. A. Lukyanenko, St. Petersburg State Univ. (Russia)
659704	Influence of dissipation on quantum wave dynamics in confined potential systems [6597-03] A. A. Smirnovsky, A. L. Sanin, St. Petersburg State Polytechnical Univ. (Russia)
659705	Motion, tunneling, and quantum revivals of wave packets into systems with distributed potential and boundary walls [6597-04] A. L. Sanin, A. A. Smirnovsky, A. T. Bagmanov, St. Petersburg State Polytechnical Univ. (Russia)
659706	A-dependence of nuclear deep inelastic scattering [6597-05] Y. A. Berdnikov, M. M. Ryzhinskiy, St. Petersburg State Polytechnical Univ. (Russia); Y. M. Shabelski, Petersburg Nuclear Physics Institute (Russia)
659707	Modeling of Co overlayers on Pd (111) from first principles [6597-06] S. Uba, L. Uba, Univ. of Bialystok (Poland); V. N. Antonov, Institute of Metal Physics (Ukraine)

Pagination: Proceedings of SPIE follow an e-First publication model, with papers published first online and then in print and on CD-ROM. Papers are published as they are submitted and meet publication criteria. A unique, consistent, permanent citation identifier (CID) number is assigned to each article at the time of the first publication. Utilization of CIDs allows articles to be fully citable as soon they are published online, and connects the same identifier to all online, print, and electronic versions of the publication.

SPIE uses a six-digit CID article numbering system in which:

- The first four digits correspond to the SPIE volume number.
- The last two digits indicate publication order within the volume using a Base 36 numbering system employing both numerals and letters. These two-number sets start with 00, 01, 02, 03, 04, 05, 06, 07, 08, 09, 0A, 0B ... 0Z, followed by 10-1Z, 20-2Z, etc.

The CID number appears on each page of the manuscript. The complete citation is used on the first page, and an abbreviated version on subsequent pages.

- 659708 **Vibrations of tetra-atomic bent symmetric molecules** [6597-07]
A. I. Melker, M. A. Vorobyeva, St. Petersburg State Polytechnical Univ. (Russia)
- 659709 **Integration of quantum hydrodynamical equation** [6597-08]
V. G. Ulyanova, A. L. Sanin, St. Petersburg State Polytechnical Univ. (Russia)
- 65970A **Generation function method in the dynamics of an adiabatically loaded anharmonic oscillator** [6597-09]
N. N. Gorobey, A. S. Lukyanenko, St. Petersburg State Polytechnical Univ. (Russia)
- 65970B **Self-organization of chaos in mythology from a scientific point of view** [6597-10]
A. I. Melker, St. Petersburg State Polytechnical Univ. (Russia)

SESSION 2 MOLECULAR DYNAMICS

- 65970C **Torsion of single-wall carbon nanotubes: molecular dynamics study** [6597-11]
A. I. Melker, K. I. Zhaldybin, St. Petersburg State Polytechnical Univ. (Russia)
- 65970D **Mutual reaction between interstitial clusters in bcc Fe** [6597-12]
D. Terentyev, SCK-CEN (Belgium) and St. Petersburg State Polytechnical Univ. (Russia);
L. Malerba, SCK-CEN (Belgium)
- 65970E **Atomistic study of the α -superdislocation core structures and microcrack formation in basal plane in Ti_3Al** [6597-13]
L. I. Yakovenkova, L. E. Karkina, Institute of Metal Physics (Russia)
- 65970F **Molecular dynamic simulation of Ti_3Al brittle fracture behavior** [6597-14]
L. I. Yakovenkova, L. E. Karkina, Institute of Metal Physics (Russia)
- 65970G **Molecular dynamics study of $\alpha \leftrightarrow \gamma$ transformations in Fe-Ni nanoparticles** [6597-15]
L. E. Karkina, I. N. Karkin, Institute of Metal Physics (Russia)
- 65970H **Modeling kinetics of $\alpha \rightarrow \gamma$ transformation in steels** [6597-16]
N. Y. Zolotarevsky, P. A. Golikov, Y. F. Titovets, St. Petersburg State Polytechnical Univ. (Russia)

SESSION 3 LASER, OPTICAL, X-RAY, AND OTHER TECHNOLOGIES

- 65970I **Thermodynamic approach to experimental research of functional crystalline materials** [6597-17]
T. Breczko, Univ. of Bialystok (Poland)
- 65970J **Manifestation of microinhomogenous structure of doped fluorophosphate glasses in γ -induced optical spectra** [6597-18]
T. V. Bocharova, G. O. Karapetyan, St. Petersburg State Polytechnical Univ. (Russia);
N. O. Tagil'tseva, St. Petersburg State Technological Institute (Russia); A. N. Vlasova, St. Petersburg State Polytechnical Univ. (Russia)
- 65970K **Heat treatments of $\text{Gd}_2\text{O}_3\text{:Sb}$, $\text{Y}_2\text{O}_3\text{:Sb}$ phosphors** [6597-19]
B. V. Mikhitarian, North Caucasian State Technical Univ. (Russia); O. Y. Manashirov, SPF Luminophor (Russia); S. B. Mikhrin, St. Petersburg State Polytechnical Univ. (Russia)

- 65970L **Laser fluorescence fluctuation excesses in molecular immunology experiments** [6597-20]
N. E. Galich, St. Petersburg State Polytechnical Univ. (Russia); M. V. Filatov, B.P. Konstantinov
Petersburg Nuclear Physics Institute (Russia)
- 65970M **Differential dynamic and integral static light scattering for nondestructive testing of 3D
disperse systems with nanoparticles** [6597-21]
A. Bezrukova, St. Petersburg State Polytechnical Univ. (Russia); M. Lubomska, P. Magri,
M. Rogalski, Univ. of Metz (France)
- 65970N **Nondestructive method for determining the service life of polymer insulation** [6597-22]
E. M. Kostenko, St. Petersburg State Polytechnic Univ. (Russia)
- 65970O **Diffraction measurement of the temperature dependence of piezoelectric tensor in
GMO monocrystal** [6597-23]
T. Breczek, A. Lempaszek, Univ. of Warmia and Mazury in Olsztyn (Poland)
- 65970P **Revealing of qualitative correlation between mechanical properties and structure of
amorphous-nanocrystalline metallic alloy 82K3XCP by microindentation on substrates and
x-ray powder diffraction** [6597-24]
A. E. Kalabushkin, St. Petersburg State Polytechnical Univ. (Russia); I. V. Ushakov, Derzhavin
Tambov State Univ. (Russia); V. M. Polikarpov, Tambov State Technical Univ. (Russia);
Y. F. Titovets, St. Petersburg State Polytechnical Univ. (Russia)
- 65970Q **Investigation of selected structural parameters in Fe₉₅Si₅ amorphous alloy during
crystallization process** [6597-25]
A. Fronczyk, Univ. of Warmia and Mazury in Olsztyn (Poland)
- 65970R **Observations of crystalline structures occurring in the tape obtained with the melt-spinning
method from the alloy with elastic memory Ti₅₀Ni₂₅Cu₂₅** [6597-26]
T. Breczek, J. Szczepanek, Univ. of Warmia and Mazury in Olsztyn (Poland)
- 65970S **X-ray diffraction analysis of oxidized Zr-based alloys** [6597-27]
G. Gosmanová, I. Kraus, Czech Technical Univ. (Czech Republic); M. Kolega, NTC, West
Czech Univ. (Czech Republic); V. Vrtílková, UJP Praha, Inc. (Czech Republic)

SESSION 4 NANO, MICRO, AND MACRO MECHANICS

- 65970T **Micromechanics of screw dislocations in elastic solids with inner and outer cylindrical
boundaries** [6597-28]
P. S. Gusev, St. Petersburg State Polytechnical Univ. (Russia); M. Yu. Gutkin, St. Petersburg
State Polytechnical Univ. (Russia) and Institute of Problems of Mechanical Engineering
(Russia); A. G. Sheinerman, Institute of Problems of Mechanical Engineering (Russia);
M. A. Smirnov, St. Petersburg State Polytechnical Univ. (Russia)
- 65970U **Plastic deformation at the top of a stopped crack** [6597-29]
Yu. I. Tyalin, V. A. Tyalina, D. V. Zolotova, A. A. Butyagin, Derzhavin Tambov State Univ.
(Russia)
- 65970V **Influence of electromagnetic radiation on the movement of dislocations in ionic crystals**
[6597-30]
V. A. Feodorov, T. N. Plushnikova, A. V. Chivanov, M. V. Chemerkina, R. A. Kirillov, Derzhavin
Tambov State Univ. (Russia)

- 65970W **Interdiffusion: mechano-chemical problem in three dimensions** [6597-31]
M. Danielewski, B. Wierzb, AGH Univ. of Science and Technology (Poland)
- 65970X **Influence of the dispersion in the laws of continuum mechanics** [6597-32]
E. V. Prozorova, St. Petersburg State Univ. (Russia)
- 65970Y **Computer simulation of electrohydraulic sheet metal forming** [6597-33]
A. V. Mamutov, V. S. Mamutov, St. Petersburg State Polytechnical Univ. (Russia)
- 65970Z **Numerical modeling of cyclic strengthening and weakening of material** [6597-34]
W. Dudda, Univ. of Warmia and Mazury in Olsztyn (Poland)
- 659710 **Prevention of cyclic instability at the modeling of elasto-plastic deformation at large strains under proportional and non-proportional loading** [6597-35]
A. S. Semenov, B. E. Melnikov, M. Yu. Gorokhov, St. Petersburg State Polytechnical Univ. (Russia); V. Ulbricht, Dresden Univ. of Technology (Germany)
- 659711 **Finite element of a rod in an immovable coordinate system** [6597-36]
Y. Kharchenko, Univ. of Warmia and Mazury in Olsztyn (Poland)
- 659712 **On the measurement of recovery strains of thermo-mechanically cycled Ni-Ti memory alloy** [6597-37]
K. Kus, P. Chwiedziewicz, Univ. of Warmia and Mazury in Olsztyn (Poland)
- 659713 **Changes of thermal hysteresis during homogenisation process of Ni-Mn-Ga polycrystalline alloy** [6597-38]
T. Brezko, M. Bramowicz, Univ. of Warmia and Mazury in Olsztyn (Poland)
- 659714 **Method of mechanical testing of laser treated metallic glass by indenters with different geometry** [6597-39]
I. V. Ushakov, Derzhavin Tambov State Univ. (Russia)
- 659715 **Mechanical behavior of metallic glasses at the viscous-brittle transition** [6597-40]
A. M. Glezer, I. E. Permyakova, G. V. Kurdyumov Institute for Physical Metallurgy (Russia); V. A. Feodorov, Derzhavin Tambov State Univ. (Russia)
- 659716 **On physical and mathematical representation of the determining functions for the macroscopic equations of rheological complex media** [6597-41]
G. D. Fedorovsky, St. Petersburg State Univ. (Russia)

SESSION 5 COMPUTER TECHNOLOGIES AND VISUALIZATION

- 659717 **Visualization of four-variable algebraic equations representing form and coloration simultaneously** [6597-42]
T. S. Tarasova, V. M. Degtyarev, St. Petersburg State Telecommunications Univ. (Russia)
- 659718 **Nokia Lifeblog: a mobile diary that writes itself** [6597-43]
I. Kuznetsov, Nokia Corp. (Finland)
- 659719 **Automatic sound signals quality estimation** [6597-44]
M. N. Gusev, V. M. Degtyarev, St. Petersburg State Telecommunications Univ. (Russia); V. A. Smirnov, O. B. Bolotova, St. Petersburg State Univ. (Russia)

- 65971A **Setting up a system and an algorithm of adaptive control in regime of real time with electrolyte flows during formation of oxide-ceramic coatings** [6597-45]
N. M. Chigrinova, Powder Metallurgy Institute (Belarus)
- 65971B **Computer simulation of the scaled power bipolar SHF transistor structures** [6597-46]
V. V. Nelayev, V. A. Efremov, Yu. P. Snitovsky, Belarusian State Univ. of Informatics and Radioelectronics (Belarus)

Author Index

Conference Committees

Organizing Committee Chairs

Alexander I. Melker, St. Petersburg State Polytechnical University (Russia)
Teodor Breczko, University of Warmia and Mazury in Olsztyn (Poland) and
University of Bialystok (Poland)

Organizing Committee

Anna Bien, University of Warmia and Mazury in Olsztyn (Poland)
Adam Froczyk, University of Warmia and Mazury in Olsztyn (Poland)
Krzysztof Kus, University of Warmia and Mazury in Olsztyn (Poland)
Sergei Starovoitov, St. Petersburg State Polytechnic University (Russia)
Tatiana Vorobyeva, St. Petersburg State Polytechnic University (Russia)

International Scientific Advisory Committee

Joaquim Teixeira de Assis, Universidade do Estado do Rio de Janeiro (Brazil)
Kurt Aulenbacher, Johannes Gutenberg Universität Mainz (Germany)
Gerhardt Betz, Technische Universität Wien (Austria)
Vladimir Brailovski, École Polytechnique de Montréal (Canada)
Teodor Breczko, University of Warmia and Mazury in Olsztyn (Poland) and
University of Bialystok (Poland)
Jean-Louis Bretonnet, Université de Metz (France)
Johan Claes, Limburg Universitair Centrum (Belgium)
Vladimir M. Degtyarev, St. Petersburg State Telecommunications University
(Russia)
Henri-Jean Drouhin, École Polytechnique (France)
Padraig Dunne, University College Dublin (Ireland)
Arnljot Elgsaeter, Universitetet i Trondheim (Norway)
Victor A. Feodorov, Derzhavin Tambov State University (Russia)
Sergei Fomin, California State University, Chico (USA)
Jorge Eduardo Fiscina, Centro Atómico Bariloche (Argentina)
Tachishige Hirose, Tokyo Metropolitan University (Japan)
Marc Hou, Université Libre de Bruxelles (Belgium)
Alexander Glamazdin, Kharkov Institute of Physics and Technology (Ukraine)
Noel Jakse, Université de Metz (France)
Ivo Kraus, Czech Technical University (Czech Republic)
Cheng-Tzu Kuo, National Chiao Tung University (Taiwan)
Wieslaw Kuzmicz, Politechnika Warszawska (Poland)
Boris E. Melnikov, St. Petersburg State Polytechnical University (Russia)
Mattias Militzer, University of British Columbia (Canada)
Vladimir Monin, Universidade do Estado do Rio de Janeiro (Brazil)

Vladislav V. Nelayev, Belrusian State University of Informatics and
Radioelectronics (Belarus)
Sergio de Nicola, Istituto di Cibernetica del CNR (Italy)
Albrecht Ott, Universität Bayreuth (Germany)
Vladimir Palmov, St. Petersburg State Polytechnical University (Russia)
Jörg Pezoldt, Technische Universität Ilmenau (Germany)
Dimitri Popov, State University of New York (USA)
Andrey L. Sanin, St. Petersburg State Polytechnical University (Russia)
Bernhard Schrefler, University of Padua (Italy)
Igor Shturtz, St. Petersburg State Polytechnical University (Russia)
Yuri F. Titovets, St. Petersburg State Polytechnical University (Russia)
Stanisław Uba, University of Białystok (Poland)
Ludmila I. Yakovenkova, Institute of Metal Physics (Russia)

Introduction

The Tenth International Workshop on Nanodesign, Technology, and Computer Simulations, NDTCS-2006 took place 5-8 July 2006 in Olsztyn, Poland. Roughly 70 scientists and graduate students attended representing Belgium, Belarus, Czech Republic, Finland, France, Germany, Poland, Russia and Ukraine. The workshop incorporated a set of all-union specialized symposia that were established by St. Petersburg State Polytechnical University. The previous nine workshops took place in St. Petersburg, Russia, and had the name "Nondestructive Testing and Computer Simulations in Science and Engineering." These conferences have created strong base for the wide 'cross-links' between the different fields of science that allows consideration of important, common problems from different angles. However, the focus of investigations is tending to move with the passage of time gradually toward nanoscience and nanotechnology, this new active area of research. To support this tendency, it was decided to change the name, but to conserve the abbreviation which became a brand of those annual workshops. The current name, "International Workshop on Nanodesign, Technology, and Computer Simulations," reflects better the profile of the conference.

Since nanoscience and nanotechnology play active role in modern industry, the tenth workshop has focused on the quest for improved technology, specifically, progress in nanodesign and technology (NDT) and computer simulations (CSs). These two distinct areas now have much in common and make the quest for improved technology easier. Today, due to the great improvements in experimental and computational methods, it is possible to solve a variety of complex practical problems accurately and efficiently. The wide participation of scientists from Central and Eastern Europe provided useful insight into the beneficial ideas generated in the many geographically diverse scientific schools.

There were a total of 62 contributions to the workshop program that were organized into five oral/poster sessions:

1. Electronic and Atomic Dynamics
2. Molecular Dynamics
3. Laser, Optical, X-Ray and other Technologies
4. Nano, Micro, and Macro Mechanics
5. Computer Technologies and Visualization.

Papers at the workshop discussed these topics, with particular emphasis on the application of advanced theories, experimental techniques, and computational methods. The basic idea was to offer new approaches in many areas, from nano- to macro-scale science and technology. Invited tutorial lectures preceded the

special sessions at the plenary session. Forty-six papers were accepted for publication in these proceedings.

Session 1 deals mainly with theoretical aspects of interactions in atomic systems and is related to interactions between external fields, electrons, and phonons in solids and molecules.

Applications of computer simulations have continued to grow in the last few years and Session 2 has acted as a focus for major advances. Considerable advances have also been made in the solution of complex structural dynamics problems of materials science. The methods of computer simulations, especially molecular dynamics, are successfully used for their study. Laser, optical, x-ray and other techniques and measurements, are discussed in Session 3.

Much important research presented in Session 4 relates to structure and properties relations, especially mechanical properties. In addition, new experimental and theoretical methods, characterizing structure of real materials at the microscopic and the macroscopic level, are considered. This session also has a direct relationship to engineering applications.

Session 5 focuses on the problems of developing new algorithms of computer simulation for complex systems that permit an increased calculation rate. In addition, considerable attention is given to visualization. Practicing engineers, on the other hand, envisage the implementation of the computer techniques as an analysis and design tool.

The scientific exchange continued informally during a series of social events, which included a sightseeing tour July 5 to Olsztyn Castle, among which administrators was famous Nicolaus Copernicus, a party July 6 on the shore of Kortowo Lake in the park of the University of Warmia and Mazury, and a day excursion on July 8 to Malbork, a very beautiful and powerful castle of the Teutonic Knights, and to Gdansk, an ancient Hansestadt.

The next international workshop on Nanodesign, Technology, and Computer Simulations, NDTCS-2007 is planned for 17–21 September 2007, in Bayreuth, Germany.

The workshop web page can be found at:
<http://www.spbstu.ru/conference/ndtcs.html>.
<http://www.ep1.uni-bayreuth.de>

Alexander I. Melker
Teodor Breczko

Related Publications

Modelling and Computer Simulation in Materials Science and Engineering, Vol. 6, No. 4 (1998).

International Workshop on New Approaches to High-Tech Materials: Nondestructive Testing and Computer Simulations in Materials Science and Engineering, Alexander I. Melker, Editor, Proceedings of SPIE, Vol. 3345 (1998)

International Workshop on Nondestructive Testing and Computer Simulations in Science and Engineering, Alexander I. Melker, Editor, Proceedings of SPIE, Vol. 3687 (1999)

Third International Workshop on Nondestructive Testing and Computer Simulations in Science and Engineering, Alexander I. Melker, Editor, Proceedings of SPIE Vol. 4064 (2000)

Fourth International Workshop on Nondestructive Testing and Computer Simulations in Science and Engineering, Alexander I. Melker, Editor, Proceedings of SPIE Vol. 4348 (2001)

Fifth International Workshop on Nondestructive Testing and Computer Simulations in Science and Engineering, Alexander I. Melker, Editor, Proceedings of SPIE Vol. 4627 (2002)

Sixth International Workshop on Nondestructive Testing and Computer Simulations in Science and Engineering, Alexander I. Melker, Editor, Proceedings of SPIE Vol. 5127 (2003)

Seventh International Workshop on Nondestructive Testing and Computer Simulations in Science and Engineering, Alexander I. Melker, Editor, Proceedings of SPIE Vol. 5400 (2004)

Eighth International Workshop on Nondestructive Testing and Computer Simulations in Science and Engineering, Alexander I. Melker, Editor, Proceedings of SPIE Vol. 5831 (2005)

Ninth International Workshop on Nondestructive Testing and Computer Simulations, Alexander I. Melker, Editor, Proceedings of SPIE Vol. 6253 (2006)