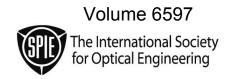
# PROCEEDINGS OF SPIE

# Nanodesign, Technology, and Computer Simulations

Alexander I. Melker Teodor Breczko Editors

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# **Contents**

ix xi xiii	Introduction 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)

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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 a-superdislocation core structures and microcrack formation in basal plane In Ti <sub>3</sub> AI [6597-13] L. I. Yakovenkova, L. E. Karkina, Institute of Metal Physics (Russia)
65970F	Molecular dynamic simulation of Ti <sub>3</sub> Al 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. Zolotorevsky, P. A. Golikov, Y. F. Titovets, St. Petersburg State Polytechnical Univ. (Russia)
SESSION 3	LASER, OPTICAL, X-RAY, AND OTHER TECHNOLOGIES
659701	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 pinduced 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 Gd <sub>2</sub> O <sub>2</sub> S:Tb, Y <sub>2</sub> O <sub>2</sub> S:Tb phosphors [6597-19] B. V. Mikhitaryan, 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. Konstantino 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)				
659700	Diffractometric measurement of the temperature dependence of piezoelectric tensor in GMO monocrystal [6597-23]  T. Breczko, 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 Fe <sub>95</sub> Si <sub>5</sub> 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 Ti <sub>50</sub> Ni <sub>25</sub> Cu <sub>25</sub> [6597-26] T. Breczko, J. Szczepanek, Univ. of Warmia and Mazury in Olsztyn (Poland)				
65970\$	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. Wierzba, 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 weaking 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 straunder 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. Breczko, 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)				

- 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

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## 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 nanoto 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)