

Nondestructive Testing and Computer
Simulations in Science and Engineering
Volume 3687

PROCEEDINGS OF SPIE



SPIE—The International Society for Optical Engineering

International Workshop on

Nondestructive Testing and Computer Simulations in Science and Engineering

Alexander I. Melker
Chair/Editor

8–12 June 1998
St. Petersburg, Russia

Organized by
St. Petersburg State Technical University (Russia)
St. Petersburg Academy of Sciences on Strength Problems (Russia)

Sponsored by
NPO Special Materials (Russia)
SPIE Russia Chapter

Published by
SPIE—The International Society for Optical Engineering



Volume 3687

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



The papers appearing in this book comprise the proceedings of the meeting mentioned on the cover and title page. They reflect the authors' opinions and are published as presented and without change, in the interests of timely dissemination. Their inclusion in this publication does not necessarily constitute endorsement by the editors or by SPIE.

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

Author(s), "Title of paper," in *International Workshop on Nondestructive Testing and Computer Simulations in Science and Engineering*, Alexander I. Melker, Editor, Proceedings of SPIE Vol. 3687, page numbers (1999).

ISSN 0277-786X
ISBN 0-8194-3161-3

Published by
SPIE—The International Society for Optical Engineering
P.O. Box 10, Bellingham, Washington 98227-0010 USA
Telephone 360/676-3290 (Pacific Time) • Fax 360/647-1445

Copyright ©1999, 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 \$10.00 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.directory.net/copyright/>. 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/99/\$10.00.

Printed in the United States of America.

Conference Committees

Organizing Committee

Chair

Alexander Melker, St. Petersburg State Technical University (Russia)

Vice-Chair

Vadim Privalov, Baltic State Technical University (Russia)

Members

Serguey Romanov, St. Petersburg State Technical University (Russia)

Tatiana Vorobyeva, St. Petersburg State Technical University (Russia)

International Scientific Advisory Committee

Gerhardt Betz, Technische Universitaet Wien (Austria)

Vitaly Boronin, St. Petersburg State Technical University (Russia)

Alexei Borovkov, St. Petersburg State Technical University (Russia)

Teodor Breczko, Academy of Agriculture and Technology/Olsztyn (Poland)

Arnljot Elgsaeter, University of Trondheim (Norway)

Andre Gorbunov, Technische Universitaet Dresden (FRG)

Tachishige Hirose, Tokyo Metropolitan University (Japan)

Vadim Ivanov, St. Petersburg State Technical University (Russia)

Noel Jakse, Universite de Metz (France)

Paul van Kampen, Dublin City University (Ireland)

Arnold Kiv, South Ukrainian Pedagogical University (Ukraine)

Ivo Kraus, Czech Technical University/Prague

Boris Melnikov, St. Petersburg State Technical University (Russia)

Vladislav Nelayev, Belorussian State University/Minsk

Vladimir Palmov, St. Petersburg State Technical University (Russia)

Bernhard Schrefler, University of Padua (Italy)

Lothar Schuelke, Universtaet-GH Siegen (FRG)

Erwin Stein, Hannover Universitaet (FRG)

Igor Shturtz, St. Petersburg State Technical University (Russia)

Yuri Titovets, St. Petersburg State Technical University (Russia)

Yuri Trushin, A.F. Ioffe Physical Technical Institute (Russia)

Gonzalo Velez Jahn, Universidad Central de Venezuela/Caracas

Ludmila Yakovenkova, Institute of Metal Physics/Ekaterinburg (Russia)

Introduction

The second International Workshop on Nondestructive Testing and Computer Simulations in Science and Engineering, NDTCS-98, took place 8-12 June 1998 in St. Petersburg. Roughly 150 scientists and graduate students representing Austria, Belarus, Brazil, Canada, Czech Republic, France, Germany, Ireland, Italy, Japan, Mexico, Norway, Poland, Romania, Russia, Sweden, Switzerland, Ukraine, United States, Uzbekistan and Venezuela attended. The workshop continues a set of All-Union specialized symposia in this active area of research. The symposia were established by St. Petersburg State Technical University and quickly expanded throughout the former Soviet Union. These migrating symposia operated with success from March 1976, when the first symposium on Computer Simulation of Radiation Damage in Solids began, until 1991, when most of them ceased all activity with the splitting of the Soviet Union. The first International Workshop, NDTCS-97, gave impetus to the reconstruction of the science of CIS with wide international participation.

The second International Workshop, NDTCS-98, has continued this tradition and focused on the quest for improved technology, specifically, progress in nondestructive testing (NDT) and computer simulations (CSs). The quest for improved technology has recently become easier, this larger due to progress in two distinct areas: nondestructive testing (NDT) and computer simulations (CSs). Today, due to the great improvements in experimental and computational methods, it is possible to solve variety complex practical problems accurately and efficiently.

There were a total of 167 contributions to the second Workshop program that were organized into eight oral/poster sessions:

1. Laser, Optical, and X-Ray Technologies
2. Electronic Structure and Physical Properties of Condensed Matter
3. Molecular and Brownian Dynamics of Condensed Matter
4. Computer Technologies and Visualization
5. Beams and Nanotechnologies
6. Phase Transitions
7. Defects and Mechanical Properties of Solids
8. Methods of Continuum and Computational Mechanics

The Workshop discussed papers on these topics, with particular emphasis on the application of advanced theories, experimental techniques and computational methods. The basic idea was to offer new approaches from nano- to macroscale science and technology. Most of the sessions were supplemented with an invited tutorial lecture. A total of 78 papers have been accepted for publication in these proceedings.

A large portion of Session 1 is related to laser and optical techniques and measurements. Papers on computer simulation supplement these contributions, which permit an increase in the efficiency of experimental methods. Other some papers consider the action of laser beams on materials.

Session 2 deals mainly with theoretical aspects of interactions between external fields, photons, fast electrons and condensed matter. Photoionization, polarization, absorption, and scattering are discussed.

Applications of computer simulations have continued to grow in the last few years and Session 3 has acted as a focus for major advances. Considerable advances have also been made in the solution of complex structural dynamics problems and in the use of high performance computing.

Session 4 concerns 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 and

cognitives. Practising engineers, on the other hand, envisage the implementation of the computer techniques as an analysis and design tool.

Many devices are made and/or operating in severe conditions or extreme environment. The fabrication process and service are tightly connected with surface phenomena, defects, and phase transitions. These questions are considered in Session 5, as well as in Sessions 6 and 7.

Session 6 pertains to smart materials, mainly shape memory alloys, and common alloys in nanocrystal state. In spite of their different origins, these materials have much in common, operating as functional devices at a nanoscale level. The focus of the papers presented is the development of models predicting materials behavior.

In reality, all the materials have various defects which influence on their properties. Much important research presented in Session 7 concerns to structure - properties relations, especially mechanical properties. In addition, new experimental and theoretical methods, characterizing structure of real materials at a microscopic and a mesoscopic level, are considered.

Session 8 has a direct relationship to engineering applications. The properties of materials are modelled at a macroscopic level. The focus is on predictions of service performance.

In conclusion, it may be said

That Session One is morning light
One can see subjects sharp and bright
And Session Two gains man's insight
Into the problems which're in mind.

Fifth Session is a clever guy
Who knows life and near by.
And Session Six keeps it in mind,
The world's imperfect and not lined

Next Session Three is like a child
Who opens eyes full of delight
And Session Four resembles a dzinn
Who lead a person to world of dreams

The imperfections, defects, faults
Give Session Seven food for thought.
In Session Eight which's rather old,
There is experience of all the world.

The next Workshop, NDTCS-99 (White Nights in St. Petersburg), is planned for 7-11 June.

Alexander Melker



KIRSANOV Vladislav Vladimirovich
(1937 – 1998)

Vladislav Kirsanov was born on October 11, 1937 in Tver. He graduated from Ural Polytechnic Institute, Energy Faculty, in 1960 and from Ural State University, Physical Faculty, in 1965. After that he does his work as a Senior Research Scientist in the Scientific Research Institute of Nuclear Reactors/Melekes (1965-74) and as the Head of a Department in the Institute of Nuclear Physics/Alma-Ata (1974-86). Returning to his native town Tver, he becomes the Head of High Mathematics (since 1986) and the Vice-Rector for Research (1987-93) of Tver State Technical University. In 1991 he was elected to the membership of the Russian Academy of Natural Sciences, in 1994 and 1997 he was awarded the Soros Professorship and in 1997 he became the Honoured Scientist of the Russian Federation.

Vladislav Kirsanov was among the few physicists who were engaged in computer simulations of radiation processes in solids at the time when this area did not attract such attention as it does now. V.V. Kirsanov first met the problem of radiation damage in 1965 when he entered the Institute of Nuclear Reactors. Already his first studies in radiation solid state physics gave the impressive results. He understood that many practical problems of radiation damage of materials could be successfully solved with the help of computer simulations. He elaborated the computer simulation technique for studying almost all the questions connected with radiation damage of metallic materials. What was typical of him is the ability to attract attention to key problems that are crucial at that time for progress in this area of science and technology. He was among the founders of the All-Union Symposia on Computer Simulation of Radiation Damage in Solids which operated with success from March 1976, when the first Symposium began, and later on he become its Chairman.

Vladislav Kirsanov was a man of great charm. His extraordinary personality attracted to him many people. His collaborates, friends and pupils maintain the bright memory of this person of figure.

Alexander Melker, Alexander Suvorov, Yuri Trushin

Contents

xi	<i>Conference Committees</i>
xiii	<i>Introduction</i>
xv	<i>Memorial to Vladislav Kirsanov</i>

SESSION 1 LASER AND OPTICAL TECHNOLOGIES

- 2 **Atlas of molecular iodine absorption lines [3687-01]**
V. E. Privalov, S. K. Savelyev, Baltic State Technical Univ. (Russia)

- 6 **He-Ne laser stabilized by saturated absorption in iodine on vibration protecting system [3687-02]**
P. S. Krylov, V. E. Privalov, Baltic State Technical Univ. (Russia)

- 9 **Compton scattering of laser off electron beams to generate polarized positron beams for future linear colliders [3687-03]**
T. Hirose, K. Dobashi, T. Kumita, Tokyo Metropolitan Univ. (Japan); Y. Kurihara, T. Omori, KEK High Energy Accelerator Research Organization (Japan); T. Okugi, K. Sugiyama, Tokyo Metropolitan Univ. (Japan); A. Tsunemi, Sumitomo Heavy Industry Ltd. (Japan); J. Urakawa, KEK High Energy Accelerator Research Organization (Japan); M. Washio, Waseda Univ. (Japan)

- 23 **Stability and reproducibility of single-frequency He-Ne laser for linear measurements [3687-04]**
A. N. Vlasov, Scientific Production Co. Fulcra (Russia)

- 26 **Nondestructive laser system for the in-situ study of the kinetics of the adsorption processes at solid/liquid interface [3687-05]**
R. Todoran, North Univ. of Baia Mare (Romania); J. P. Sharkany, Uzhgorod State Univ. (Ukraine)

- 29 **Influence of laser noise on sensitivity of fiber optic sensors [3687-06]**
V. M. Nikolaev, O. I. Kotov, L. B. Liokumovich, D. V. Khoptiar, St. Petersburg State Technical Univ. (Russia)

- 31 **Multimode fiber optic interferometer sensor: signals correlation properties [3687-07]**
L. I. Kosareva, O. I. Kotov, E. M. Kotova, A. V. Medvedev, V. M. Nikolaev, V. I. Filimonov, St. Petersburg State Technical Univ. (Russia)

- 34 **Laser technique for anatomical-functional study of the medial prefrontal cortex of the brain [3687-08]**
L. Sanchez-Huerta, A. Hernández, G. Ayala, J. Marroquín, A. B. Silva, K. S. Khotiaintsev, Puebla Autonomous Univ. (Mexico); V. A. Svirid, Mexico National Autonomous Univ.; G. Flores, S. N. Khotiaintsev, Puebla Autonomous Univ. (Mexico)

- 42 **Effect of fanning on the characteristics of double phase-conjugate mirror [3687-09]**
V. Ju. Petrunin, I. A. Vodovatov, I. V. Murashko, St. Petersburg State Technical Univ. (Russia)

- 48 **Application of Wigner's time-frequency distribution for close signals recognition [3687-10]**
A. G. Tkachenko, General Satellite Corp. (Russia)

- 53 **Surface quality laser testing system [3687-11]**
G. V. Laktushkin, V. G. Shemanin, Kuban State Technological Univ. (Russia)
- 56 **Optical instrument for aerosol-dust-air flows diagnosing [3687-12]**
P. V. Charty, V. G. Shemanin, Kuban State Technological Univ. (Russia)
- 59 **Optical pulse probing of coherency gradient in Δ -medium [3687-13]**
I. V. Kazinets, St. Petersburg State Technical Univ. (Russia); I. E. Mazets, A.F. Ioffe Physical-Technical Institute (Russia); B. G. Matisov, St. Petersburg State Technical Univ. (Russia)
- 65 **Time-of-flight characteristics of the conical field: perspectives for application in coincidence spectroscopy [3687-14]**
S. N. Davydov, S. N. Romanov, St. Petersburg State Technical Univ. (Russia)
- 70 **Laser tube for a frequency-stabilized laser [3687-15]**
M. A. Fedotov, E. G. Chulaeva, State Pedagogical Univ. (Russia) and Scientific Research Institute of Gas Discharge Devices (Russia)
- 73 **Advanced holographic nondestructive testing system for residual stress analysis [3687-16]**
A. Kniazkov, Yu. I. Onischenko, G. E. Dovgalenko, G. J. Salamo, Univ. of Arkansas (USA); T. Yu. Latychevskaia, St. Petersburg State Technical Univ. (Russia)
- 82 **Electrostatic spherical mirror analyzer with a position-sensitive detector for electron coincidence spectroscopy [3687-17]**
M. M. Danilov, S. N. Davydov, Yu. K. Golikov, St. Petersburg State Technical Univ. (Russia)

SESSION 2 ELECTRONIC STRUCTURE AND PHYSICAL PROPERTIES OF CONDENSED MATTER

- 90 **Collective effects in resonant negative ion photodetachment [3687-18]**
V. K. Ivanov, G. Yu. Kashenock, St. Petersburg State Technical Univ. (Russia)
- 102 **Quantum fluid dynamics for the simple Coulomb model [3687-19]**
A. L. Sanin, St. Petersburg State Technical Univ. (Russia)
- 105 **Pair charge correlations in silicon nanostructures [3687-20]**
N. T. Bagraev, A.F. Ioffe Physical-Technical Institute (Russia); A. D. Bouravleuv, V. E. Gasumyants, St. Petersburg State Technical Univ. (Russia); W. Gehlhoff, Technische Univ. Berlin (Germany); L. E. Klyachkin, A. M. Malyarenko, A.F. Ioffe Physical-Technical Institute (Russia); A. Naeser, Technische Univ. Berlin (Germany); V. V. Romanov, S. A. Rykov, E. V. Vladimirskaia, St. Petersburg State Technical Univ. (Russia)
- 112 **Quantum interference and conductance in silicon quantum wires [3687-21]**
N. T. Bagraev, A.F. Ioffe Physical-Technical Institute (Russia); W. Gehlhoff, Technische Univ. Berlin (Germany); V. K. Ivanov, St. Petersburg State Technical Univ. (Russia); L. E. Klyachkin, A. M. Malyarenko, A.F. Ioffe Physical-Technical Institute (Russia); A. Naeser, Technische Univ. Berlin (Germany); S. A. Rykov, I. A. Shelykh, St. Petersburg State Technical Univ. (Russia)
- 122 **Electronic spectrum of the three-dimensional quasi crystal [3687-22]**
D. Olenov, E. Isaev, P. Slobodianiuk, Yu. Vekilov, Moscow State Institute of Steel and Alloys (Russia)
- 125 **Evaluation of the carrier effective mass and relaxation time in nonuniformly doped semiconductor structures on the basis of spectrophotometrical experiments [3687-23]**
V. V. Nelayev, B. B. Sevruck, Belorussian State Univ. of Informatics and Radioelectronics

- 127 **Radiative properties of n-ZnSe single crystals doped with Ag** [3687-24]
G. N. Ivanova, V. A. Kasiyan, D. D. Nedeoglo, N. D. Nedeoglo, State Univ. of Moldova
- 129 **Galvanomagnetic properties of heterophase materials at high pressure** [3687-25]
V. V. Shchennikov, S. V. Popova, S. V. Ovsyannikov, Institute of Metals Physics (Russia)

SESSION 3 MOLECULAR AND BROWNIAN DYNAMICS OF CONDENSED MATTER

- 132 **Molecular dynamics study of polyethylene extension** [3687-26]
A. I. Melker, D. V. Soloviev, St. Petersburg State Technical Univ. (Russia)
- 142 **Internet-based 3D editor for carbon molecular models** [3687-27]
I. V. Shurtz, I. Krylov, St. Petersburg State Technical Univ. (Russia)
- 148 **Molecular dynamics calculations of the early stages of thin film formation** [3687-28]
G. Betz, W. Husinsky, Technische Univ. Wien (Austria)
- 155 **Embedded-atom interatomic potentials and simulation of planar defects in intermetallic Ti₃Al** [3687-29]
L. I. Yakovenkova, Institute of Metal Physics (Russia); V. V. Kirsanov, Tver State Technical Univ. (Russia); L. E. Karkina, M. Ya. Rabovskaya, Institute of Metal Physics (Russia); A. N. Balashov, Tver State Technical Univ. (Russia)
- 159 **Thermally activated superdislocation transformations in DO₁₉ ordered alloys** [3687-30]
L. I. Yakovenkova, L. E. Karkina, Institute of Metal Physics (Russia)
- 164 **Effective diffusivity of the phosphorus in bcc iron under irradiation** [3687-31]
A. A. Vasiliev, N. N. Khartanovich, St. Petersburg State Technical Univ. (Russia)
- 170 **Radiation-stimulated processes in Si surface layers** [3687-32]
P. W. M. Jacobs, Western Ontario Univ. (Canada); A. E. Kiv, Western Ontario Univ. (Canada) and South Ukrainian Pedagogical Univ.; V. N. Soloviev, T. N. Maximova, Krivoy Rog Pedagogical Univ. (Ukraine); V. V. Chislov, South Ukrainian Pedagogical Univ.
- 175 **Molecular dynamics simulations of unsaturated lipids in monolayers: an investigation of bond ordering** [3687-33]
A. L. Rabinovich, P. O. Ripatti, Institute of Biology (Russia); N. K. Balabaev, Institute of Mathematical Problems in Biology (Russia)
- 182 **Numerical simulation of plastic deformation in polymer crystals** [3687-34]
A. I. Moussienko, Institute of Chemical Physics (Russia); N. K. Balabaev, Institute of Mathematical Problems in Biology (Russia); L. I. Manevitch, Institute of Chemical Physics (Russia)
- 191 **Infrared thermography of damage evaluation in leather products** [3687-35]
M. P. Luong, Lab. de Mechanique des Solides (France)
- 201 **Rotation model of the diffusion mobility of macromolecules in linear polymer crystallites** [3687-36]
U. Gafurov, Institute of Nuclear Physics (Uzbekistan)
- 205 **Molecular dynamics investigation of spall fractures** [3687-37]
A. M. Krivtsov, St. Petersburg State Technical Univ. (Russia); Yu. I. Mescheryakov, Institute for Problems of Mechanical Engineering (Russia)

SESSION 4 COMPUTER TECHNOLOGIES AND VISUALIZATION

- 214 **Overview of VRML applications to architecture [3687-38]**
G. Velez Jahn, Univ. Central de Venezuela
- 220 **Creating large optimized VRML worlds [3687-82]**
V. N. Tolstykh, I. V. Shturtz, St. Petersburg State Technical Univ. (Russia)
- 224 **Case study for natural phenomena visualization: weather effects [3687-39]**
A. B. Grigoriev, St. Petersburg State Technical Univ. (Russia)
- 228 **Classification of scheduling algorithms for real-time systems [3687-40]**
M. V. Khloudova, St. Petersburg State Technical Univ. (Russia)
- 232 **Building an animation system for a virtual reality application [3687-41]**
S. F. Mironov, St. Petersburg State Technical Univ. (Russia)
- 235 **Building an optimal hierarchy of classification features [3687-42]**
V. I. Klovov, St. Petersburg State Technical Univ. (Russia)
- 239 **Data visualization in geoinformation systems [3687-43]**
V. A. Galinsky, St. Petersburg State Technical Univ. (Russia)

SESSION 5 BEAMS AND NANOTECHNOLOGIES

- 244 **Nonconventional transition layer formation during PLD of nanometer-period multilayers [3687-44]**
A. A. Gorbunov, K. Brand, H. Geisler, Technische Univ. Dresden (Germany); J. Noetzel, Forschungszentrum Rossendorf (Germany); B. Wehner, A. Tselev, Technische Univ. Dresden (Germany); V. S. Kharlamov, A.F. Ioffe Physical-Technical Institute (Russia); H. Mai, Fraunhofer-Institut für Werkstoff- und Strahltechnik (Germany); J. Thomas, Institut für Festkörper- und Werkstofforschung (Germany); H. Lichte, W. Pompe, Technische Univ. Dresden (Germany); J. Trushin, A.F. Ioffe Physical-Technical Institute (Russia); E. Wieser, Forschungszentrum Rossendorf (Germany); H. Worch, Technische Univ. Dresden (Germany)
- 254 **Theoretical and experimental studies of $(\text{AlN})_{1-x}(\text{SiC})_x$ layer structures formed by N+ and Al+ coimplantation in 6H-SiC [3687-45]**
D. V. Kulikov, A.F. Ioffe Physical-Technical Institute (Russia); J. Pezoldt, Technische Univ. Ilmenau (Germany); P. V. Rybin, A.F. Ioffe Physical-Technical Institute (Russia); W. Skorupa, Forschungszentrum Rossendorf (Germany); Yu. V. Trushin, A.F. Ioffe Physical-Technical Institute (Russia); R. A. Yankov, Forschungszentrum Rossendorf (Germany)
- 258 **Fabrication of the nanocrystal structures $\text{ZrO}_2(\gamma):\text{Zr}$ and $\text{SiO}_2:\text{Si(p)}$ by ion implantation [3687-46]**
O. N. Gorshkov, D. O. Filatov, A. P. Kasatkin, V. A. Novikov, D. I. Tetelbaum, S. A. Trushin, M. V. Stepihova, Univ. of Nizhnii Novgorod (Russia)
- 264 **Processes responsible for the long-range effects in metals at low-intensity ion and light irradiations [3687-47]**
D. I. Tetelbaum, Yu. A. Semin, V. V. Khabibulov, A. Yu. Azov, A. A. Trofimov, Univ. of Nizhnii Novgorod (Russia)
- 268 **Experimental study and computer simulation of AlN and BN sputtering [3687-48]**
S. S. Elovikov, E. Yu. Zykova, A. A. Promokhov, V. E. Yurasova, Moscow State Univ. (Russia)

- 274 **Displacement threshold energies of impurity atoms in GaAs heterostructures** [3687-49]
B. Ja. Ber, Yu. A. Kudrjavitsev, V. S. Kharlamov, Yu. V. Trushin, A.F. Ioffe Physical-Technical Institute (Russia); E. E. Zhurkin, St. Petersburg State Technical Univ. (Russia)
- 278 **Modeling of light-nuclei interaction** [3687-50]
I. G. Golikov, A. V. Golovin, I. I. Loshchakov, St. Petersburg State Technical Univ. (Russia)
- 283 **Transport equations calculation of energy deposition distribution in atomic collisions cascade** [3687-51]
E. E. Zhurkin, D. P. Ivanov, St. Petersburg State Technical Univ. (Russia)
- 290 **Physical model of copper clusters formation in hydrogenated amorphous carbon grown by ion cosputtering of graphite and copper** [3687-52]
D. V. Kulikov, Yu. V. Trushin, V. S. Kharlamov, A.F. Ioffe Physical-Technical Institute (Russia)
- 292 **Discrete-cluster model of condensation from metal vapor** [3687-53]
S. I. Igolkin, S. K. Savelyev, Baltic State Technical Univ. (Russia)
- 297 **Cluster model of amorphized particles formation by plasma spraying of metallic powder** [3687-54]
B. K. Barakhtin, E. V. Nesterova, CRISM Prometey (Russia)

SESSIONS 6-7 PHASE TRANSITIONS, DEFECTS, AND MECHANICAL PROPERTIES OF SOLIDS

- 302 **Residual stresses induced by martensite transformation in NiTi alloy** [3687-55]
T. Breczko, Olsztyn Univ. of Agriculture and Technology (Poland); V. V. Rubanick, Jr., Institute of Technical Acoustics (Belarus)
- 310 **Behavior of NiTi alloy under action of ultrasound** [3687-56]
T. Breczko, Olsztyn Univ. of Agriculture and Technology (Poland); V. V. Rubanick, Jr., Institute of Technical Acoustics (Belarus)
- 313 **Tensorial generalization of a phenomenological material law for shape memory alloys** [3687-57]
P. Terriault, F. Trochu, V. Brailovski, Ecole Polytechnique de Montréal (Canada)
- 324 **Phase transformation analysis from the point of view of the theory of nonelasticity with cross-links** [3687-58]
B. E. Melnikov, I. Yu. Kadashevich, St. Petersburg State Technical Univ. (Russia)
- 330 **Modeling of strain accumulation and recovery due to fcc-hcp transformation at thermocycles** [3687-59]
M. E. Evard, A. E. Volkov, St. Petersburg State Univ. (Russia)
- 335 **Application of atomic force microscopy for investigation of magnetic structure of steels** [3687-60]
I. S. Kalashnikov, Institute of Aviation Materials (Russia); G. L. Klimchitskaya, North-West Polytechnical Institute (Russia); R. Prioli, S. I. Zanette, A. O. Caride, Ctr. Brasileiro de Pesquisas Físicas (Brazil); O. Acsehrad, E. M. Silva, R. A. Simão, Univ. Federal de Rio de Janeiro (Brazil)

- 342 **Computer simulation of diffusion processes in microelectronics: approach to the solution of statistical problems [3687-61]**
V. V. Nelayev, M. V. Kazitov, Belorussian State Univ. of Informatics and Radioelectronics;
S. I. Vatlin, A. M. Voronkovskaya, A. M. Semenkova, Belorussian Ctr. of Medical Radiation
Technology
- 347 **Effect of structural imperfection on kinetics of alpha-gamma phase transformation in
constructional steel near Ac1 temperature [3687-62]**
T. I. Chashchukhina, M. V. Degtyarev, L. M. Voronova, L. S. Davydova, Institute of Metal
Physics (Russia)
- 350 **Residual stress investigations of a ferritic steel welded plate by a nondestructive neutron
diffraction technique [3687-63]**
Yu. V. Taran, Joint Institute for Nuclear Research (Russia); G. Albertini, G. Bruno, Univ.
of Ancona (Italy); F. Cernushi, ENEL-CRAM (Italy); F. Rustichelli, Univ. of Ancona (Italy)
- 360 **Comparative evaluation of high-cycle fatigue strength and wear resistance for PDI material
processed by heat treatment and gas carburizing furnace and ADI material [3687-64]**
S. Uesaka, S. Doi, Oita Univ. (Japan); K. Mitsunaga, Kagoshima Senior Women's School (Japan)
- 365 **Evaluation of microtexture using x-ray pole figures obtained from single grains [3687-65]**
N. Yu. Ermakova, N. Yu. Zolotarevsky, V. R. Mirsoev, Yu. F. Titovets, St. Petersburg State
Technical Univ. (Russia)
- 371 **Mechanism of creating nanodefects on metal surfaces under load [3687-66]**
V. I. Vettegren, S. Sh. Rakhimov, V. N. Svetlov, A.F. Ioffe Physical-Technical Institute (Russia)
- 373 **Characteristic features of the formation of dislocation structures in poly-, micro-, and
nanocrystalline materials [3687-67]**
G. A. Malygin, A.F. Ioffe Physical-Technical Institute (Russia)
- 375 **Misfit defect configurations associated with stacking faults in thin crystalline film/substrate
systems [3687-68]**
M. Yu. Gutkin, K. N. Mikaelyan, I. A. Ovid'ko, Institute of Machine Science Problems (Russia)
- 377 **Structure and morphology of surfaces of alkali-halide under heating in an electrical field
[3687-69]**
V. A. Feodorov, L. G. Kariev, O. A. Meksichev, Tambov State Univ. (Russia)
- 379 **X-ray residual stress analysis of free-standing ceramics [3687-70]**
I. Kraus, G. Gosmanová, N. Ganev, Czech Technical Univ./Prague; D. Fröhlich, L. Pfeiffer,
H.-D. Tietz, Westsächsische Hochschule Zwickau (Germany)

SESSION 8 METHODS OF CONTINUUM AND COMPUTATIONAL MECHANICS

- 382 **Global behavior of periodic assemblies of elastic contact bodies [3687-71]**
B. A. Schrefler, Univ. of Padua (Italy); H. Zhang, Dalian Univ. of Technology (China);
U. Galvanetto, Univ. of Padua (Italy)
- 391 **Corotational variables in nonlinear mechanics of solids [3687-72]**
V. Palmov, St. Petersburg State Technical Univ. (Russia)
- 395 **Analytical methods in mechanics of granular-elastic media [3687-73]**
O. I. Zayats, A. N. Nezlobin, V. G. Cheremensky, N. M. Dobrova, St. Petersburg State
Technical Univ. (Russia)

- 401 **Method of approximation of the weak solution of elasticity problems [3687-74]**
I. E. Anoufrieve, L. V. Petukhov, St. Petersburg State Technical Univ. (Russia)
- 405 **Algorithm for solving the viscoelastic rolling contact problem with a periodic speed pattern [3687-75]**
D. L. Chertoc, Simon Fraser Univ. (Canada); J. M. Golden, Dublin Institute of Technology (Ireland); G. A. C. Graham, Simon Fraser Univ. (Canada)
- 419 **Adequacy of the multisurface theory and structural model with the complexity of plastic deformation processes [3687-76]**
I. N. Izotov, N. P. Kuznetsov, B. E. Melnikov, A. G. Mityukov, A. Yu. Musienko, St. Petersburg State Technical Univ. (Russia)
- 427 **Computer simulation of kinked fatigue crack propagation at sharp notches [3687-77]**
A. S. Semenov, S. Sahn, Dresden Technical Univ. (Germany); B. E. Melnikov, St. Petersburg State Technical Univ. (Russia)
- 437 **New approach to mathematical and finite element modeling of delaminations in multidirectional multilayered laminated composite structures: I. Fracture criteria and finite element algorithm [3687-78]**
A. I. Borovkov, Yu. Y. Misnik, St. Petersburg State Technical Univ. (Russia)
- 445 **New approach to mathematical and finite element modeling of delaminations in multidirectional multilayered composite structures: II. Numerical examples [3687-79]**
A. I. Borovkov, Yu. Y. Misnik, St. Petersburg State Technical Univ. (Russia)
- 455 **Finite element stress, vibration, and buckling analysis of laminated beams with the use of refined elements [3687-80]**
A. I. Borovkov, I. Avdeev, A. Artemyev, St. Petersburg State Technical Univ. (Russia)
- 465 **Computer synthesis of human motion as a part of an adequate motion analysis experiment [3687-81]**
A. A. Ivanov, V. A. Sholukha, A. V. Zinkovsky, St. Petersburg State Technical Univ. (Russia)
- 470 *Author Index*

SESSION 1

Laser and Optical Technologies

Atlas of molecular iodine absorption lines.

Vadim E. Privalov

Sergey K. Savelyev

*Baltic State Technical University, 1-st Krasnoarmeyskaya, 1, St. Petersburg, Russia
root@ssav.spb.su*

ABSTRACT

A computerised atlas of molecular iodine - 127 is presented. Reference data for some practically interesting lines are presented.

1. ATLAS OVERVIEW

The four of the five reference wavelengths accepted as length measurement standard are determined on the base of lasers stabilised by saturated absorption in iodine. The actual problem in this field is to enlarge the range of the investigated iodine lines. That is why during last period we have been investigating some separate ranges of the visible part of iodine absorption spectra.

This paper presents the computerised atlas with about 800000 of lines of iodine - 127 B-X absorption band in the range 0.499 - 0.829 μm . Atlas is developed for Windows environment and enables to view the list of lines in the form of a chart and a diagram. A system of filters provides an efficient search for a wanted line by its notation or a wavelength¹⁻³. The form of the screen is presented in Fig. 1.

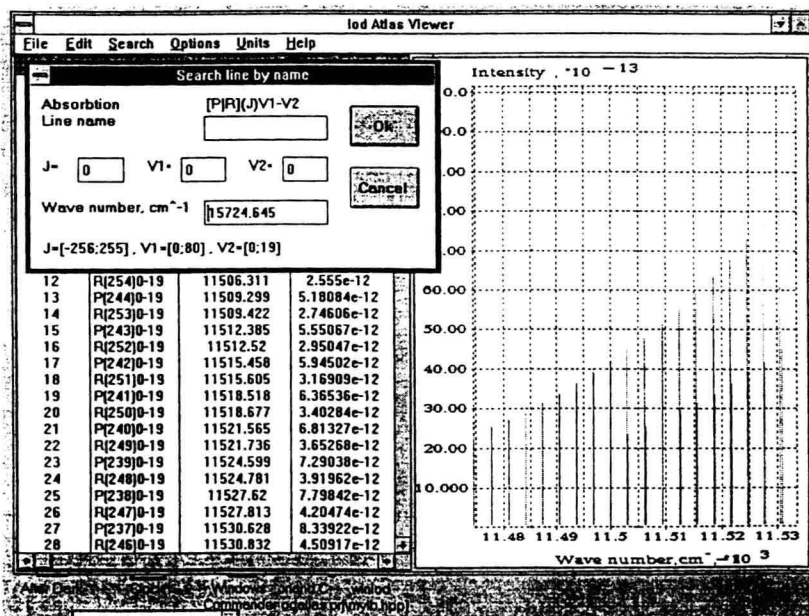


Fig. 1. A window of iodine atlas during a search operation.

2. RESULTS

As the example let us present the table of the lines in the nearby area of a line 0.510554 μm of laser on Cu vapour ⁴.

Table 1. Absorption lines of iodine-127 near the line 0.510554 μm .

Line	Wave number, cm^{-1}	Detuning, MHz	Absorption coefficient, arb. units
R(10)70-2	19586.660	+2813	0.16E-01
P(14)47-0	19586.725	+4746	0.22E+00
R(16)47-0	19586.553	-410	0.25E+00
P(16)71-2	19586.393	-5215	0.24E-01
R(20)72-2	19586.592	+762	0.29E-01
R(26)75-2	19586.518	-1465	0.36E-01
R(27)76-2	19586.598	+938	0.37E-01
R(43)56-1	19586.457	-3281	0.14E+00
R(70)50-0	19586.592	+762	0.43E+00
P(70)61-1	19586.492	-2227	0.15E+00
R(76)63-1	19586.672	+3164	0.14E+00
P(82)68-1	19586.391	-5273	0.13E+00
P(84)52-0	19586.549	-527	0.37E+00
R(91)53-0	19586.518	-1465	0.34E+00
R(106)57-0	19586.549	-527	0.25E+00

As it is seen from the table 1 the most suitable lines for the operation in this range are R(70)50-0, P(84)52-0 and R(91)53-0. The use of these lines for the distant testing of iodine presence in the atmosphere may enable to solve the problem with determination of the presence of this element.

Table 2. Absorption lines of iodine-127 near the line 0.576295 μm .

Line	Wave number, cm^{-1}	Detuning, MHz	Absorption coefficient, arb. units
R(6)73-13	17352.377	+4570	0.80E-07
P(6)73-13	17352.219	-176	0.80E-07
R(12)74-13	17352.158	-1992	0.15E-06
P(15)43-10	17352.156	-2051	0.52E-06
R(15)75-13	17352.193	-938	0.18E-06
R(17)43-10	17352.244	+586	0.58E-06
R(17)76-13	17352.232	+234	0.21E-06
R(20)79-13	17352.389	+4922	0.24E-06
P(20)79-13	17352.145	-2402	0.24E-06
P(24)56-12	17352.396	+5156	0.80E-06
P(29)29-6	17352.107	-3516	0.45E-07
P(30)32-7	17352.311	+2578	0.13E-03
P(31)39-9	17352.414	+5684	0.19E-05
R(33)32-7	17352.424	+5977	0.14E+00
R(39)57-12	17352.207	-527	0.11E-05