

Alexander VOZNYI

Postdoctoral fellow, DFT modeling of self-assembled monolayers on semiconductor surfaces

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WORK EXPERIENCE

Oct 2004 – present **Postdoctoral fellow**, University of Sherbrooke, Sherbrooke, QC, Canada

EDUCATION

2001-2004	Ph. D. in Physics of semiconductors and dielectrics, Chernivtsi National University, Ukraine
2000-2001	M. Sc. in Semiconductor microelectronics, Chernivtsi National University, Ukraine
1996-2000	B. Sc. in Semiconductor microelectronics, Chernivtsi National University, Ukraine

RESEARCH EXPERIENCE

- **Functionalization of semiconductor surfaces for bio-detection**
 - Using *ab initio* modeling as a complementary characterization tool to understand the atomic level processes of thiols SAM formation on GaAs
 - Verification of the interface robustness
 - Improvement of thiol deposition technique
 - Estimation of the applicability limits of current materials and finding more suitable materials (choice of thiols type and endgroup, semiconductor material and surface orientation / reconstruction)
 - Participation in bio-sensor architecture design
 - Choice of signal for sensing (QDs vs surface, label-free vs fluorescence sensing)
 - Development of technique for selective-area deposition of thiol SAMs
 - Concept of quantum-well structure for improved sensitivity of optical signal to virus immobilization
- **Characterization of group-III nitrides**
 - *Ab initio* modeling of disorder and strain effect on stability and optical properties of ternary alloys
 - Characterization of III-nitride surfaces using wetting angle measurements
 - Surface free energy and molecule-surface interactions theory and *ab initio* modeling
- **Laser assisted quantum well intermixing (QWI) for applications in photonics**
 - Finding optimal laser parameters for improved lateral resolution
 - Finite element method (FEM) modeling of light adsorption, heat propagation, thermal diffusion and confined energy levels shift in quantum wells.
 - *First principles* modeling of defects formation and propagation at semiconductor-insulator interface under laser irradiation

EXPERTISE

- **Density Functional Theory**
 - Techniques
 - Electronic band structure calculations using localized and plane-wave basis sets
 - Chemical bond analysis: orbitals, hybridization and energetics
 - Optical properties and analysis of optical transitions
 - Phonon dispersion spectra
 - Surface energy calculations
 - Problems
 - Physisorption and chemisorption of molecules on surface
 - Self-assembly
 - Semiconductor surfaces (reconstructions, electron counting, passivation)
 - Doping and point defects
 - Disordered alloys
 - Packages
 - SIESTA, personally developed Empirical Pseudopotential Method code, Materials Studio, HyperChem

- **Finite Element Method**
 - FEMLAB package: Heat transfer, Diffusion, Shroedinger equation and Structural mechanics modules
- Basic knowledge in **analysis of experimental data**: STM, XPS, FTIR, ellipsometry, PL, wetting angle.
- **Programming languages**: FORTRAN, C++, Delphi, PHP, SQL, HTML
- Fluent in English, French, Russian, Ukrainian

TEACHING EXPERIENCE

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| 2005, 2006 | Practical part of the M. Sc. course "Principles of lasers and laser assisted microfabrication":
<i>Finite Element Method modeling of laser light and heat propagation in semiconductors.</i>
University of Sherbrooke, Sherbooke, QC, Canada |
| 2002, 2003 | Practical part of the M. Sc. course " <i>Theory of electrical and electronic circuits</i> "
Chernivtsi National University, Ukraine |

PUBLICATIONS

- **O. Voznyy**, J. J. Dubowski,
Kinetics of thiols adsorption on GaAs (001) surfaces: evidences of SAM formation on As-overlayer,
In preparation for *Phys. Rev. Lett.*
- **O. Voznyy**, J. J. Dubowski,
Recombinative adsorption energetics of hydrogen sulfide and alkanethiols on different GaAs (001) surface
reconstructions,
In preparation for *Phys. Rev. B*
- **O. Voznyy**, J. J. Dubowski,
Structure, bonding nature, and binding energy of alkanethiolate on As-rich GaAs (001) surface: a density functional
theory study,
J. Phys. Chem. B, **110** (47), 2006, p. 23619.
- **O. Voznyy**, R. Stanowski, J. J. Dubowski,
Multibandgap quantum well wafers by IR laser quantum well intermixing: simulation of the lateral resolution of the
process,
Journal of Laser Micro / Nanoengineering, **1**, 2006, p. 48.
- R. Stanowski, **O. Voznyy**, J. J. Dubowski,
Finite element model calculations of temperature profiles in Nd:YAG laser annealed GaAs/AlGaAs quantum well
microstructures,
Journal of Laser Micro / Nanoengineering, **1**, 2006, p. 17.
- V. Deibuk, **O. Voznyy**,
Thermodynamic stability and charge redistribution in ternary AlGa_N, InGa_N, and InAl_N alloys,
Semiconductors, **39** (6), 2005, p. 623.
- **O. Voznyy**, V. Deibuk,
The role of alloying effects in the formation of electronic structure of unordered group III nitride solid solutions,
Semiconductors, **38** (3), 2004, p. 304.
- V. Deibuk, **O. Voznyy**, M. M. Sletov,
Features of optical properties of aluminum gallium nitride solid solutions,
Semiconductors, **36** (4), 2002, p. 398.
- V. Deibuk, **O. Voznyy**, M. M. Sletov,
Band structure and spatial charge distribution in AlGa_N,
Semiconductors, **34** (1), 2000, p. 35.

CONFERENCES

- **O. Voznyy**, J. J. Dubowski,
Kinetics of thiols adsorption on different GaAs (001) reconstructions and evidences of binding to As-overlayer,
E-MRS 2007 Spring Meeting, Symposium O, Strasbourg, France.
- **O. Voznyy**, J.J. Dubowski,
First-principles study of adsorption energetics of alkanethiols on GaAs(001) (poster),
MRS 2006 Fall Meeting, Symposium D, Boston, MA, USA.
- **O. Voznyy**, J.J. Dubowski,
Adsorption and self-assembly of alkanethiols on GaAs (001) surface (oral),
IEEE Lasers & Electro-Optics Society Annual Meeting, Montreal, October 29, 2006.
- **O. Voznyy**, J.J. Dubowski,
Ab-initio study of self-assembled monolayers of thiols on (001) GaAs (oral),
Photonics North, Nanophotonics and Photon-based Atomic Level Manipulation, Quebec City, Quebec, Canada, June 7, 2006.
- **O. Voznyy**, J.J. Dubowski,
Ab-initio modeling of GaAs-thiol interface (poster),
RQMP annual meeting, Montreal, May 26, 2006.
- J. Genest, R. Stanowski, **O. Voznyy**, J.J. Dubowski,
Laser-based quantum well and quantum dot intermixing (poster),
RQMP annual meeting, Montreal, May 16, 2005.
- **O. Voznyy**, R. Stanowski, J. J. Dubowski,
Multibandgap quantum well wafers by IR laser quantum well intermixing: simulation of the lateral resolution of the process (oral),
The 6th International Symposium on *Laser Precision Microfabrication 2005*, April 4, 2005, Williamsburg, VA, USA.
- R. Stanowski, **O. Voznyy**, J. J. Dubowski,
Modelling of temperature profiles in Nd:YAG laser annealed GaAs/AlGaAs quantum well microstructures (oral),
Laser Applications in Microelectronic and Optoelectronic Manufacturing LAMOM 2005 - Photonics West, San Jose, January 22-27, 2005.
- L. Ostrovskaya, A. Vasin, **O. Voznyy**, V. Deibuk, M. Sletov.
Study of the wettability of III-N thin films with different bond ionicity and surface layers polarity (poster),
E-MRS 2005 Fall meeting, Warsaw, Poland.
- **O. Voznyy**, V. Deibuk,
Optical properties of ordered group-III nitride alloys (poster),
E-MRS 2003 Fall Meeting, Symposium N, Warsaw, Poland.
- **O. Voznyy**, V. Deibuk,
Thermodynamic stability of bulk and film group-III nitride alloys (oral),
XV International workshop "*Physics and technology of thin films*", Ivano-Frankivsk, Ukraine, 2003.
- V. Deibuk, **O. Voznyy**, M. Sletov,
Effect of antisites on electronic band structure and charge densities of Ga_{1-x}Al_xN (poster),
XXVIII International School on *Physics of Semiconducting Compounds*, Jaszowiec, Poland, 1999.

REFERENCES

Prof. Jan J. Dubowski

Canada research chair in Quantum Semiconductors
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