NONLINEAR PROCESSES IN SOLIDS

Head of Laboratory *Dr. hab. phys*. Eugene A. Kotomin

Research Area and Main Problems

Our theoretical research interests are focused on four classes of problems related to:

(i) kinetics of diffusion-controlled processes, with emphasis on pattern formation and catalytic surface reactions;
(ii) stochastization of magnetic field lines in magnetized fusion plasma;
(iii) gyrotron development;
(iv) the atomic and electronic structure of numerous advanced materials, with emphasis on calculations of properties of defects, surfaces, metal/insulator interfaces and nanostructures.

We combine several different techniques, including analytical formalisms and large-scale computer simulations (quantum chemical methods, stochastic simulations as well as Monte Carlo/cellular automata modeling).

Scientific staff:

1. Dr. hab. E. Kotomin
2. Dr. hab. V. Kuzovkov
3. Dr. hab. J.R. Kalnin
4. Dr. O. Dumbrajs
5. Dr. Yu. Zhukovskii
6. Dr. A. Popov
7. Dr. R. Eglitis
8. Dr. S. Piskunov
9. Dr. G. Zvejnieks

PhD students:

10. D. Gryaznov
11. V. Kashcheyevs
12. Yu. Mastrikov

Graduate students:

13. D. Bocharov

Visitors from abroad

1. Prof. D.E. Ellis, Northwestern University, Evanston, Illinois, USA (1 week).

Our scientific visits abroad

1. Dr. hab. E. Kotomin, Max Planck Institute for Solid State Physics, Stuttgart, Germany (5.5 months), EU Institute of Transuranium Elements, Karlsruhe, Germany (4.5 months), Northwestern University, Evanston, USA (1 month)
2. Dr. hab. V. Kuzovkov, Braunschweig University of Technology, Germany (3 months)
3. Dr. O. Dumbrajs, Max Planck Institute for Plasma Physics, Garching, Germany (3 months)
4. Dr. Yu. Zhukovskii, Northwestern University, Evanston, USA (4 months), Max Planck Institute for Solid State Physics, Stuttgart, Germany (1 month), National Laboratory of Frascati, Italy (3 weeks), St. Petersburg University, Russia (3 weeks)
5. Dr. A. Popov, Institute Laue-Langevin, Grenoble, France (10 months), National Laboratory of Frascati, Italy (3 weeks)
6. Dr. R. Eglitis, University of Osnabrück, Germany (11 months)

7. Dr. G. Zvejnieks, Institute of Semiconductor Physics, Vilnius, Lithuania (2.5 months), Max Planck Institute for Plasma Physics, Garching, Germany (1 month)
8. Dr. S. Piskunov, Northwestern University, Evanston, USA (5 months)
9. D. Gryaznov, Max Planck Institute for Solid State Physics, Stuttgart, Germany (11 months)
10. V. Kashcheyevs, Tel Aviv University, Israel (11 months)
11. Yu. Mastrikov, Max Planck Institute for Solid State Physics, Stuttgart, Germany (11 months)

International Cooperation

Czech Republic	Institute of Physics, Charles University, Prague (Prof. V. Trepakov)
Estonia	Institute of Physics, Tartu University (Prof. A. Lushchik)
Finland	Helsinki University of Technology (Dr. T.M.J. Ikonen)
France	Laue-Langevin Institute, Grenoble (Dr. G.J. McIntyre)
Germany	EU Institute of Transuranium Elements, Karlsruhe (Dr. R. Konings), Institut für Hochleistungsimpuls&Mikrowellentechnik, Karlsruhe (Dr. B. Piosczyk) Max Planck Institut (MPI) für Festkörperforschung, Stuttgart (Prof. Dr. J. Maier) Max Planck Institut (MPI) für Plasmaphysik, Garching (Prof. Dr. H. Zohm) Technische Universität Braunschweig (Prof. Dr. W. von Niessen) Universität Osnabrück (Prof. Dr. G. Borstel)
Greece	School of Electrical and Computer Engineering, National Technical University of Athens, Zographou (Dr. Y. Kominis)
Israel	School of Physics and Astronomy, Tel Aviv University (Prof. A. Aharony) Ben Gurion University of the Negev, Ber Sheeva (Prof. D. Fuks)
Italy	Laboratori Nazionali di Frascati (Prof. S. Bellucci)
Lithuania	Institute of Semiconductor Physics (SPI), Vilnius (Dr. E. Tornau)
Romania	University of Craiova (Dr. D. Constantinescu)
Russia	St. Petersburg University (SpbU) (Prof. R.A. Evarestov)
Spain	University of Barcelona (Prof. F. Illas)
Sweden	Uppsala University (Prof. K. Hermansson)
UK	King's College London (Prof. L. Kantorovich) University College London (Profs. A.M. Stoneham and A. Shluger)
USA	Northwestern University, Evanston, Illinois (Prof. D.E. Ellis) University of Maryland, College Park (Dr. G.S. Nusinovich) California Institute of Technology, Pasadena (Dr. E. Heifets)

Main Results

MONTE-CARLO MODELING OF ADSORPTION AND REACTION KINETICS OF OXYGEN AND CARBON MONOXIDE ON Pd(111) SURFACE

V. Kuzovkov and G. Zvejnieks,
V. Petrauskas and E. Tornau (*Semiconductor Physics Institute, Vilnius, Lithuania*)

In collaboration with the *Semiconductor Physics Institute, Vilnius,* we have proposed the model for numerical simulation of the reaction $O + CO \rightarrow CO_2$ and occurring phase

transitions on the Pd(111) surface. We have calculated the phase diagram for this system using kinetic Monte Carlo method. It shows appearance of two phase transitions: $p(2\times2)_O \rightarrow \sqrt{3}\times\sqrt{3}R30^o_O$ and $\sqrt{3}\times\sqrt{3}R30^o_O \rightarrow p(2\times1)_O$ with increase of CO coverage for room and intermediate temperatures, respectively. For the low temperature limit, the direct phase transition $p(2\times2)_O \rightarrow p(2\times1)_O$ is observed. We demonstrate that the reaction rate is the crucial factor determining the occurrence of the $p(2\times1)_O$ phase and vanishing of the $\sqrt{3}\times\sqrt{3}R30^o_O$ with decrease of temperature. The results of correlation function analysis indicate that the reaction proceeds either inside both the $p(2\times2)_O$ and $\sqrt{3}\times\sqrt{3}R30^o_O$ phases, or on the perimeter of the domains of $p(2\times1)_O$ structure.

CALCULATIONS OF THE EFFECTIVE DIFFUSION COEFFICIENT AND CONDUCTIVITY IN HETEROGENEOUS SOLIDS

J.R. Kalnin and E. Kotomin,
J. Maier (*MPI for Solid State Research, Stuttgart, Germany*)

Diffusion in heterogeneous solids is a very relevant topic in many fields of science and technology, ranging from ceramics to biology. This is also relevant for polycrystalline nanomaterials and composites in which the grain boundary exhibits transport coefficients different from the bulk. In order to suggest interpretation to numerous experimental studies of the diffusion and conductivity in nanomaterials performed in collaboration with *Max Planck Institute, Stuttgart,* we have performed the joint theoretical study of this problem. Briefly, we have analyzed results suggested in numerous papers on this subject in the framework of the effective medium approach, analyzed their limitations and suggested new equations. Correctness of our theoretical approach has been confirmed by Monte Carlo (MC) computer calculations.

STOCHASTIC PROCESSES IN GYROTRONS

O. Dumbrajs,
H. Kalis, and A. Reinfelds (*Institute of Mathematics, University of Latvia, Riga*)
G.S. Nusinovich (*University of Maryland, College Park, USA*)

In collaboration with *Institute of Mathematics of University of Latvia*, limits on the power generated by coaxial gyrotrons are investigated. It is shown that among all the operating modes suggested recently for coaxial super power gyrotrons only modes with azimuthal index m lower than about 44 pass the spatial stochasticity test. Modes with higher azimuthal indices cannot be used as operating modes because gyrotron oscillations become chaotic in the azimuthal direction and efficiency is very low. It is argued that there exists a natural upper limit on power generated by gyrotrons, which is about 4 MW

Stability of efficient operation at one of the high-order modes is of great importance for the development of megawatt-level gyrotrons intended for plasma experiments in controlled fusion reactors. Typically such gyrotrons operate at modes with large azimuthal indices, which form a rather dense spectrum of eigenfrequencies. Therefore, instead of considering interaction of electrons with a large number of such modes it is more convenient to analyze the spatial-temporal evolution of an envelope formed by a superposition of these modes with the electrons. In all previous studies of stability of such envelopes it was assumed that

some kind of azimuthal non-uniformity is present in the initial condition for the wave envelope. However, the physical reason for this non-uniformity, which is apparently the non-uniformity of the electron emission, was not analyzed. In collaboration *with University of Maryland, College Park,* the relation between the emission non-uniformity and resulting non-uniformity of the wave envelope is established. Then, results of numerical simulations are given, which demonstrate various changes in the gyrotron dynamics caused by the azimuthal instability of the wave envelope. These results allow one to determine the maximum azimuthal index of the operating mode and show that this maximum index can depend on the degree of azimuthal non-uniformity of the electron emission.

COAXIAL GYROTRON FOR ITER TOKAMAK

O. Dumbrajs,
B. Piosczyk, T. Rzesnicki, G. Dammertz, S. Illy, J. Jin, W. Leonhardt, G. Michel,
M. Schmid, M. Thumm, and X. Yang (*Forschungszentrum Karlsruhe, Germany*)

ITER is the experimental step between today's studies of plasma physics and tomorrow's electricity-producing fusion power plants. In collaboration with *Forschungszentrum (Institut für Hochleistungsimpuls&Mikrowellentechnik), Karlsruhe,* the cavity has been designed for a first industrial prototype of a 2 MW, CW, 170 GHz coaxial cavity gyrotron. This gyrotron is now under fabrication, the design of critical components has been verified experimentally with a short pulse (~few ms) coaxial gyrotron. This tube utilizes the same quasi-optical (q.o.) RF-output system as designed for the industrial prototype and a very similar electron gun. The performance of the electron gun and beam has been found to be in agreement with the design. Concerning the microwave generation some discrepancy occurred between theory and experiment. In particular, the excited mode spectrum is more dense than expected. The measured pattern of the RF output beam was found to be in agreement with numerical simulations.

STOCHATIZATION AS A POSSIBLE CAUSE OF FAST RECONNECTION DURING SEVERAL MHD MODES ACTIVITY

O. Dumbrajs and G. Zvejnieks,
D. Constantinescu (*University of Craiova, Romania*),
V. Igochine and H. Zohm (*MPI for Plasma Physics, Garching, Germany*)

It was first observed at ASDEX Tokamak in 1982 that externally heated plasmas can suddenly reach an operating regime of improved confinement .In collaboration with *Max Planck Insitute, Garching* and *University of Craiova,* we have analyzed the role of stochastization of magnetic field lines in fast reconnection phenomena occurring in magnetized fusion plasma. A mapping technique has been applied to trace the field lines of toroidally confined plasma where the perturbation parameter is expressed in terms of experimental perturbation amplitudes determined from the ASDEX Upgrade Tokamak. It has been found that fast reconnection observed during amplitude drops of the neoclassical tearing mode instability in the frequently interrupted regime can be related to stochastization. It has been also shown that stochastization can explain the fast lost of confinement during the minor disruption. This demonstrates that stochastization can be regarded as a possible cause for different MHD events in ASDEX Upgrade Tokamak.

HAMILTONIAN MAP DESCRIPTION OF ELECTRON DYNAMICS

O. Dumbrajs,
Y. Kominis, K.A. Avramides, K. Hizanidis, and J.L. Vomvoridis
(*National Technical University of Athens, Greece*)

In collaboration with *National Technical University of Athens*, electron dynamics in gyrotron resonators are described in terms of a Hamiltonian map. This map incorporates the dependency of electron dynamics on the parameters of the interacting rf field and it can be used for trajectory calculations through successive iteration, resulting in a symplectic integration scheme. The direct relation of the map to the physics of the model, along with its canonical form (phase space volume preserving) and the significant reduction of the number of iteration steps required for acceptable accuracy, are the main advantages of this method in comparison with standard methods such as Runge-Kutta. The general form of the Hamiltonian map allows for wide applications as a part of several numerical algorithms, which incorporate CPU-consuming electron trajectories calculations.

ANALYTICAL TECHNIQUES FOR CORRELATION EFFECTS IN LOW DIMENSIONAL NANOSTRUCTURES

V. Kashcheyevs,
A. Aharony and O. Entin-Wohlman (*Tel Aviv University, Israel*)

In collaboration with *Tel Aviv University*, we have explored new analytical methods for the description of strong quantum correlations in the electronic nanostructures (quantum dots). When the electrons are confined in a low-dimensional structure, the single particle description becomes inadequate at low temperatures. One of the typical manifestations of the associated many-body effects is the Kondo screening of the spin of a quantum dot with an odd number of electrons. Such systems can be successfully described by model Hamiltonians that derive from a single impurity Anderson model. The latter includes the Coulomb (Hubbard) interaction term only for the impurity site (the quantum dot). Nevertheless, the associated physical quantities (conductance, charge and spin accumulation etc.) are extremely difficult to calculate due to the many-body nature of the problem. Exact solution for some thermodynamic quantities is known in several limiting cases, but obtaining a valid expression for the single-particle Green function in a wide parameter range remains a great challenge. We have applied a method of equations-of-motion to the quantum dot systems, and truncated the well-known hierarchy of exact equations for the electronic Green's functions at high order.

The resulting coupled non-linear integral equations have been solved self-consistently and analytically, using the theory of functions of the complex variable. The resulting expression for the electron Green function has been check against various exact theorems (Fermi liquid relations), and the exact solution (Bethe *ansatz*) in the corresponding limits. We have established that the proposed approximation is very accurate in all regimes except the low-temperature phase dominated by the Kondo screening. For the latter regime, the method gives a correct qualitative picture (e.g. singlet ground state, exponential increase in the spin susceptibility with lowering temperature), but underestimates the Kondo temperature, and more importantly, violates the celebrated Friedel sum rule by up to 30%. A simpler version of the equations-of-motion decoupling which omits the self-consistency and which has been widely used in the recent studies of the Kondo effect in unconventional settings is

shown to be incorrect even on the qualitative level. Thus our method provides a necessary improvement for the studies of strongly correlated nanosystems. We continue investigation of the correlation effects in non-equilibrium settings using the model system of resonant quantum pumping.

DEFECTS, SURFACES, SOLID SOLUTIONS, AND REACTIVITY OF ADVANCED PEROVSKITES

E. Kotomin, Yu Zhukovskii, S. Piskunov, D. Gryaznov, and Yu. Mastrikov
R.A. Evarestov (*St. Petersburg University, Russia*),
F. Illas, N. Lopez, and J. Carrasco (*University of Barcelona, Spain*)
D.E. Ellis (*Northwestern University, Evanston, Illinois, USA*)
E. Heifets (*California Institute of Technology, Pasadena, USA*),
D. Fuks (*Ben Gurion University of the Negev, Ber Sheeva, Israel*),
J. Maier (*MPI for Solid State Research, Stuttgart, Germany*)

In collaboration with *St. Petersburg University, University of Barcelona,* and *Max Planck Institute for Solid State Research, Stuttgart,* we have studied *F* centers (O vacancies) in $SrTiO_3$ perovskite (both bulk and (001) surface of cubic phase stable at room temperature). For first principles calculations on the defective structures of cubic $SrTiO_3$, we have used both *CRYSTAL-03* and *VASP* codes. Due to existence of different kinds of bonds in $SrTiO_3$ one can observe a competition between the tendency to trap the electrons associated with the missing oxygen in vacancy (*F* center) or to localize them on the Ti *3d* orbitals. The creation of a neutral O vacancy results in the new electronic state below the conduction band, which is consistent with experimental estimate indicated small ionization energy for the oxygen vacancy. The formation of oxygen vacancies is accompanied by noticeable relaxation of the first and second nearest neighbors. The lattice relaxation around the *F* center has been found to be sensitive to both shape and size of supercell as well as calculation method. The larger is supercell, the closer *defect energy level* in the band gap lies to the conduction band bottom, approaching the optical ionization energy of 0.49 eV for 270- and 320-atomic supercells, where the distance between neighboring defects is as large as four lattice constants. For these supercells, the defect bandwidth decreases down to 0.02-0.03 eV, *i.e.* the defect-defect interaction becomes negligible.

In collaboration with *Max Planck Institute for Solid State Research, Stuttgart, St. Petersburg University, and California Institute of Technology, Pasadena,* we have performed detailed *ab initio* calculations on technologically important material used as a cathode of the solid oxide fuel cells, *i.e.* $LaMnO_3$ bulk (both high temperature cubic and low temperature orthorhombic phases) and its (100) and (110) surfaces (with emphasis on the surface energies and polarization). We have compared two density functional theory formalisms: DFT-LCAO (as implemented in *CRYSTAL-03* code) and DFT with plane waves (*VASP code*). When comparing results of our calculations with those available in the literature, we have showed that only the hybrid exchange-correlation functional (B3PW) allows us to reproduce the experimental magnetic coupling constants and optical gap. Keeping in mind the fuel cell applications, we have treated the orthorhombic cells with Mn-terminated stoichiometric slabs in the 001 direction. We have found that the surface containing cubic cells is energetically more favorable. Moreover, the (001) surface possesses a lower energy than that of the (110) surface. In these large scale modeling we have increased the slab thickness from 4 to 14 planes. Different spin configurations on Mn

have been used and compared. We also relaxed those surfaces and analyzed the charge density redistribution near the surface indicating the chemical bond covalency.

In collaboration with *Ben Gurion University, Ber Sheeva*, a special thermodynamic approach has been developed, to predict material properties as the temperature changes, ***i.e.*** to analyze order-disorder transitions. Ground state energies of different Sr-doped $LaMnO_3$ ordered structures have been calculated using first principles method and later used in the thermodynamic approach. This allowed us to conclude that disordering of a technologically important 12.5% Sr-doped $LaMnO_3$ phase with respect to the decomposition into the heterogeneous mixture can occur only at temperatures above the melting point. Along with the thermodynamic analysis, we could also compare two realizations of DFT method for calculation of the properties of Sr-doped $LaMnO_3$, using the packages ***WIEN-2k*** and ***CRYSTAL-03***. Both methods give similar tendencies for predicting the material behavior, however, DFT-LCAO method overestimates temperature of the order-disorder transition as compared to plane wave DFT. Based on ***CRYSTAL-03*** calculations for a number of the $Ba_cSr_{1-c}TiO_3$ (BST) superlattices, we have also developed a thermodynamic approach to these solid solutions. In particular, we have calculated the BST phase diagram and showed that at relatively low temperatures (below 400 K for c=0.5 and 300 K for c=0.1) the spinodal decomposition of the solid solution occurs. As a result, we predict for small Ba concentrations formation of $BaTiO_3$ nanoregions in a predominantly $SrTiO_3$ matrix and vice versa, which is confirmed by the Raman, polarization, ultrasonic, neutron diffraction, and diffusion experiments.

Adsorption of gas-phase oxygen on the ABO_3 perovskite surfaces is important for high temperature oxygen sensors, in photocatalysis, and fuel cell applications. In close cooperation with *Northwestern University, Evanston*, we have performed ***ab initio*** calculations of the energetics, geometry of fully relaxed structure, electronic charge redistribution, and density of states for adsorbed atomic and molecular oxygen on defectless unreconstructed SrO- and TiO_2-terminated $SrTiO_3$(001) surfaces. We have found substantial binding energies for ***atomic O adsorption***: (*i*) atop surface oxygen ion (up to 1.8 eV) and (*ii*) at bridge sites, ***i.e.*** positions between the two adjacent metal and oxygen surface ions on both SrO- and TiO_2-terminated surface (over 2.0 eV). In both cases the strong bonding is rather caused by formation of surface molecular peroxide ion O_2^{2-} which ground state is a singlet. ***For molecular adsorption***, different adsorption sites and orientations of O_2 molecule have been studied, however, adsorption energy never exceeded 0.1 eV. Adsorption of oxygen on strontium titanate has been found to depend significantly on temperature and partial pressures in the gas phase.

FIRST PRINCIPLES MODELING AND THERMODYNAMIC STUDY OF THIN METAL FILMS ON METAL OXIDES AND PEROVSKITES

Yu. Zhukovskii and E. Kotomin,
A.M. Stoneham (*University College London, UK*),
D. Fuks (*Ben Gurion University of the Negev, Ber Sheeva, Israel*),
D.E. Ellis (*Northwestern University, Evanston, Illinois, USA*)
P. Balaya and J. Maier (*MPI for Solid State Research, Stuttgart, Germany*),

In collaboration with *Northwestern University, Evanston, Ben Gurion University Ber Sheeva,* and *University College London,* we have continued ***ab initio*** calculations (using

hybrid B3LYP method) and thermodynamic study of copper and silver adhesion onto both perfect and defective magnesia substrate. For a defectless magnesia surface, we confirm the experimentally observed submonolayer growth of 3D metallic islands (Ag possesses a higher trend than Cu). Their shapes have been found to be pyramid-like. Formation of O vacancies on the substrate markedly enhances metal atom adsorption as compared to physisorption over regular sites on a defect-free substrate. For the first time, we predict that the presence of these surface defects (beginning with concentrations of 5 per cent for Cu and 22 per cent for Ag) can stimulate the growth of uniform 2D metallic sublayers.

In collaboration with *Northwestern University, Evanston,* we have continued *CRYSTAL-03* calculations for copper adsorption on a regular, defect-free TiO_2- and BaO- terminated (001) surfaces of a cubic $BaTiO_3$, using the hybrid B3PW method (instead of ***a posteriori*** HF-CC used earlier). To clarify the nature of the interfacial bonding, we use slab models of the Cu/$BaTiO_3$(001) interfaces with different one-side substrate coverages, varied from 1/8 monolayer (ML) up to 1/2 ML, over both TiO_2- and BaO-terminated surfaces. TiO_2 termination has been found to be energetically more favorable for the adsorption of copper atoms. In agreement with previous experimental and theoretical data, our calculations indicate essential contribution of atomic polarization into the interaction between Cu atoms and surface O^{2-} ions. An increase of substrate coverage by copper simultaneously reduces the binding energy (***per*** adatom) and enhances the interatomic interactions inside growing metallic film. For mostly ionic BaO-terminated substrate we compare our results with earlier obtained data for the perfect Cu/MgO(001) interface.

In collaboration with *Max Planck Institute for Solid State Research, Stuttgart,* we present theoretical support for experimentally observed storage anomaly for nanocomposites in the context of lithium batteries. According to experimental investigations on Ru/Li_2O nanocomposite (2-5 nm), an extra Li storage is possible resulting in a capacitive voltage-charge behavior, which is neither due to homogeneous (insertion) nor heterogeneous (conversion) reactions. The low potential (1.2-0.02 V ***vs.*** Li^+/Li) extra capacity, obtained in metal/Li_2O nanocomposite can be explained by an "interfacial storage mechanism". ***Ab initio*** calculations on the atomic and electronic structure of Ti(0001)/Li_2O(111) model interface performed using hybrid B3PW method, both indicate the validity of the phenomenological model of the interfacial Li storage mechanism and predicts conditions of its realization. Compared to a pure Li_2O, a Ti/Li_2O(111) interface can store at least a monolayer of additional Li per interface with electrons being transferred largely to the titanium adatoms. In addition it highlights the occurrence of a varied stoichiometry of nanosized solids compared to massive phases.

FIRST PRINCIPLES SIMULATION OF ELECTRONIC STRUCTURE OF PERFECT AND DEFECTIVE CaF_2

R. Eglitis
H. Shi and G. Borstel (*University of Osnabrück, Germany*),

In collaboration with *Osnabrück University,* we have performed ***ab initio*** calculations on technologically important calcium fluoride (perfect and defective bulk and densely-packed surfaces), using hybrid B3PW method as implemented in *CRYSTAL'03* code, which provides the best agreement with experiment for the band gap width (11.0 ***vs.*** 12.1 eV, respectively). When comparing results of calculations on CaF_2 (111), (110), and (100)

surfaces, we confirm that the CaF_2(111) surface is the most stable one, in agreement with the experiment. The characterization of *F* centers in CaF_2 is still a question of debate. We found, that the vacancy formation energy in CaF_2 is 7.87 eV. The charge-density map of the *F* center in CaF_2 shows that the charge is well localized inside the vacancy. The spin density in *F* center has been found to be 0.716 *e*. The relaxation of atoms around the *F* center is rather small. *F* center level within band gap suggests a possible mechanism for explanation of the optical absorption observed experimentally in CaF_2 at 3.3 eV.

EXPERIMENTAL AND THEORETICAL STUDIES OF NANOSTRUCTURED ALUMINIUM NITRIDE

A. Popov and Yu. Zhukovskii
C. Balasubramanian and S. Bellucci (*National Laboratory of Frascati, Italy*),
A. Ivanov and H. Schober (*Institut Laue Langevin, Grenoble, France)*
V. Savchyn, N. Krutyak, and I. Karbovnyk (*National University of Lviv, Ukraine*)

AlN nanotubes (NTs) and nanoparticles (NPs) have been synthesized by using a highly nonequilibrium direct-current (DC) arc plasma method. The nanotubes sample contained around 80% NTs (~25-30 nm in diameter, ~700 nm length) and the rest NPs. The nanoparticles sample contained more than 95% NPs, with diameter varying between 40–60 nm, and the rest were NTs. In collaboration with *National Laboratory of Frascati* we have studied cathodoluminescence (CL) spectra of powder samples containing mostly AlN NTs, and of powder samples consisting mostly of AlN NPs, in comparison to that of the commercially available aluminum nitride powder. A clear difference between emission spectra of commercial AlN, AlN NPs and AlN NTs has been found. Commercial AlN emits light at 3.5 eV. For the sample, containing AlN NPs, this peak is slightly shifted to higher energies. It is well known that the position of this emission band depends on oxygen content in the sample. We suggest that the slight difference in the band positions might be due to the different concentration of oxygen impurities in the investigated samples. The CL spectrum of aluminum nitride NTs shows an additional emission peak near 2.25 eV.

In collaboration with *Institut Laue Langevin, Grenoble,* we have performed the neutron scattering study of synthesized AlN NTs. We discuss the generalized density of phonon states G(ω) for the NTs in comparison with bulk AlN. *G*(ω) for the bulk features two main bands at low (~30 meV) and high (~80 meV) frequencies. Both bands are completely smeared out in the nanomaterial indicating a broad distribution of force constants induced by structural disorder. Apart from the smearing out of the vibrational bands we observe enhanced intensities at low frequencies (< 10 meV) as usually found in disordered systems. The observed changes in the microscopic dynamics must lead to appreciable differences in the thermal and transport properties of the NTs with respect to the bulk material.

Theoretical simulations serve as the effective tool for a study of both the atomic and electronic structure of AlN nanotubes and can complement the corresponding experiments for the comprehensive development of nanotube engineering. In collaboration with *National Laboratory of Frascati,* we have constructed single-walled models of AlN nanotubes with two different chiralities: armchair- and zigzag-type. To analyze dependence of their electronic structure on the thickness of AlN NT, we have considered two different diameters for both NT types: 1 nm and 6 nm. It allows us to analyze how a curvature of NT changes their properties as compared to both AlN bulk and n-type densely packed surfaces

(with either wurtzite or zincblende structures). We have found, the smaller diameter of AlN NT, the closer its total density of one-electron states to that for bulk material, and *vice versa*, the properties of thick nanotubes approach to surface. Our periodic 1D calculations performed using *CRYSTAL-03* code show that various configurations of AlN NTs are energetically stable with a smooth tubular single wall and a uniform diameter. The larger NT diameter, the closer its properties to AlN(0001) surface and smaller dependence of NTs on their chirality, *i.e.* their armchair- and zigzag-structures become energetically closer.

Scientific papers published in 2005

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2. H. Shi, R.I. Eglitis, and G. Borstel, *Ab initio* calculations of the CaF_2 electronic structure and *F* centers. - *Physical Review B*, 2005, **72**, 045109, (p. 1-9).
3. R.A. Evarestov, E.A. Kotomin, Yu.A. Mastrikov, D. Gryaznov, E. Heifets, and J. Maier, Comparative density-functional LCAO and plane-wave calculations of $LaMnO_3$ surfaces. - *Physical Review B*, 2005, **72**, 214411, (p. 1-12).
4. S. Piskunov, E. Heifets, E.A. Kotomin, J. Maier, R.I. Eglitis, and G. Borstel, Hybrid DFT calculations of the atomic and electronic structure for ABO_3 perovskite (001) surfaces. - *Surface Science*, 2005, **575**, p. 75-88.
5. V.N. Kuzovkov and W. von Niessen, The phase diagram of the multi-dimensional Anderson localization *via* analytic determination of Lyapunov exponents. - *European Physics Journal B*, 2004, **42**, p. 529-542.
6. R.I. Eglitis and G. Borstel, Towards a practical rechargeable 5 V Li ion battery. - *Physica Status Solidi (a)*, 2005, **202**, p. R13-R15.
7. R.A. Evarestov, A.V. Bandura, V.E. Alexandrov, and E.A. Kotomin, DFT LCAO and plane wave calculations of $SrZrO_3$. - *Physica Status Solidi (b)*, 2005, **242**, p. R11-R13.
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9. H. Shi, R.I. Eglitis, and G. Borstel, First-principles calculations of the CaF_2 bulk and surface electronic structure. - *Physica Status Solidi (b)*, 2005, **242**, p. 2041-2050.
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11. O. Dumbrajs and G.S. Nusinovich, Azimuthal instability of radiation in gyrotrons with overmoded resonators. – *Physics of Plasmas*, 2005, **12**, 053106 (p. 1-9).
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