

LABORATORY OF THEORETICAL PHYSICS AND COMPUTER MODELLING

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

Research Area and Main Problems

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

- kinetics of diffusion-controlled processes, with emphasis on pattern formation and catalytic surface reactions;
- the atomic and electronic structure of numerous advanced materials, with emphasis on calculations of properties of defects, surfaces, metal/insulator interfaces.
- theoretical simulations and experimental studies of nanostructures and nanomaterials;
- modeling of advanced functional materials for energy applications (fuel cells, membranes, Li batteries, fusion and fission reactors);
- stochastization of magnetic field lines in magnetized fusion plasma;
- gyrotron development for thermonuclear reactors .

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. O. Dumbrajs
4. Dr. R. Eglitis
5. Dr. D. Gryaznov
6. Dr. V. Kashcheyevs
7. Dr. Yu. Mastrikov
8. Dr. S. Piskunov
9. Dr. A. Popov
10. Dr. Yu. Zhukovskii
11. Dr. G. Zvejnieks

PhD students

12. D. Bocharov
13. A. Gopejenko

Scientific visits abroad

1. Dr. hab. E. Kotomin, Max Planck Institute for Solid State Research, Stuttgart, Germany (9 months), University of Maryland and Michigan Technological University, USA (2 weeks), The Eurasian University, Astana, Kazakhstan (2 weeks).
2. Dr. hab. V. Kuzovkov, Ludwig-Maximilians-Universität (LMU), München, Germany (1 week); University of Hamburg, Germany (1 month).
3. Dr. O. Dumbrajs, Max-Planck Institut für Plasmaphysik, Garching, Germany (3 months).
4. Dr. D. Gryaznov, EC Institute of Transuranium Elements, Karlsruhe, Germany (9 months), Max Planck Institute for Solid State Physics, Stuttgart, Germany (2 months),
5. Dr. V. Kashcheyevs, Berkeley National Laboratory, USA (2 months), Hebrew University of Jerusalem, Israel (2 weeks), Ben-Gurion University of the Negev, Beer-

- Sheva, Israel (2 weeks), Physikalisch-Technische Bundesanstalt, Braunschweig, Germany (1 week).
6. Dr. Yu. Mastrikov, University of Maryland, USA (11 months).
 7. Dr. S. Piskunov, University of Duisburg-Essen (8 months), Northwestern University, Evanston, USA (1 month), LNF Frascati, Italy (1 month).
 8. Dr. A. Popov, Institute Laue-Langevin, Grenoble, France (3 months), National Laboratory of Frascati, Italy (10 days), Deutsches Elektronen-Synchrotron DESY Hamburg, Germany (10 days) ??
 9. Dr. Yu. Zhukovskii, Northwestern University, Evanston, USA (1 month), Institute for Materials Research I, Karlsruhe, Germany (1 month), St. Petersburg State University, Russia (3 weeks), Max Planck Institute for Solid State Research, Stuttgart, Germany (2 weeks), Technical University of Braunschweig, Germany (2 weeks), EC Institute of Transuranium Elements, Karlsruhe, Germany (1 week).
 10. Dr. G. Zvejniaks, Michigan Technological University, USA (1 week).
 11. D. Bocharov, Max Planck Institute for Solid State Research, Stuttgart, Germany (2 weeks), Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany (1 week), EC Institute of Transuranium Elements, Karlsruhe, Germany (1 week).
 12. A. Gopejenko, Forschungszentrum Karlsruhe, Institut für Materialforschung I, Karlsruhe, Germany (4 months).

International Cooperation

Finland	1. Helsinki University of Technology (Dr. T. Kurki-Suonio)
France	2. Laue-Langevin Institute, Grenoble (Dr. G.J. McIntyre, Dr. H. Schober) 3. ESRF, Grenoble (Dr. A. Rogalev)
Germany	4. Physikalisch-Technische Bundesanstalt, Braunschweig (Dr. Bernd Kästner). 5. Max Planck Institut für Plasmaphysik, Garching (Prof. Dr. H. Zohm) 6. Deutsches Elektronen-Synchrotron DESY, Hamburg (Dr. A. Kotlov) 7. EC Institute of Transuranium Elements, Karlsruhe (Dr. P. Van Uffelen). 8. Max Planck Institut für Plasmaphysik, Garching (Dr. V. Igochine, Prof. Dr. K. Lackner, Dr. R. Mayer-Spasche, Prof. Dr. H. Zohm) 9. Institut für Hochleistungsimpuls & Mikrowellentechnik (KIT), Karlsruhe (Dr. S. Kern, Dr. B. Piosczyk) 10. Institut für Materialforschung I (KIT), Karlsruhe (Dr. A. Möslang) 11. Max Planck Institut für Festkörperforschung, Stuttgart (Prof. Dr. J. Maier)
Greece	12. School of Electrical and Computer Engineering, National Technical University of Athens, Zographou (Dr. K. Avramides)
Israel	13. Ben Gurion University, Beer Sheeva (Prof. A. Aharony, Prof. D. Fuks)
Italy	14. Laboratori Nazionali di Frascati (Dr. S. Bellucci, Dr. M. Cestelli-Guidi)
Japan	15. FIR Center, University of Fukui (Prof. T. Idehara)
Lithuania	16. Institute of Semiconductor Physics (SPI), Vilnius (Dr. E. Tornau)
Romania	17. University of Craiova (Dr. D. Constantinescu)
Russia	18. St. Petersburg University (Prof. R.A. Evarestov)
UK	19. Cavendish Laboratory, University of Cambridge (Dr. M.R. Buitelaar) 20. University College London (Prof. A.L. Shluger)

Ukraine	21. National University of Lviv (Prof. I. Bolesta and Prof. V. Savchyn)
	22. Idaho National Laboratory (Dr. S.N. Rashkeev)
USA	23. Northwestern University, Evanston, Illinois (Prof. D.E. Ellis)
	24. University of Maryland, College Park (Dr. G.S. Nusinovich, Dr. M. Kukla)

Main Results

KINETIC MONTE-CARLO SIMULATION OF OXIDIZED SILICON STRIPE FORMATION ON PD(111)

G. Zvejnieks

Recently several papers were published on room temperature decomposition of silane (SiH_4) on oxidized Pd and Pt(111) surfaces. Room temperature fits into a narrow temperature where silane already decomposes, but the temperature is insufficient for formation of various silicides. The most striking result of these experiments was the discovery of Si-O stripe structure. This result was confirmed by vibrational spectra measurements and supported by density functional theory (DFT) calculations.

We propose the model with two interaction constants (nearest neighbor pair repulsion of SiO complexes, v , and their trio attraction in a line, v_t) which demonstrates stripe formation during silane decomposition on oxidized Pd(111) surface. The simplest (2×1) stripe phase is obtained by kinetic Monte Carlo simulation in absence of longer-range attractive interactions which are usually necessary for stripe structure formation. Despite higher energy, this phase is shown to be very stable. Phase diagram for this model is obtained, Figure 1, and (2×1) phase stability is analyzed varying coverage and reaction rate parameters.

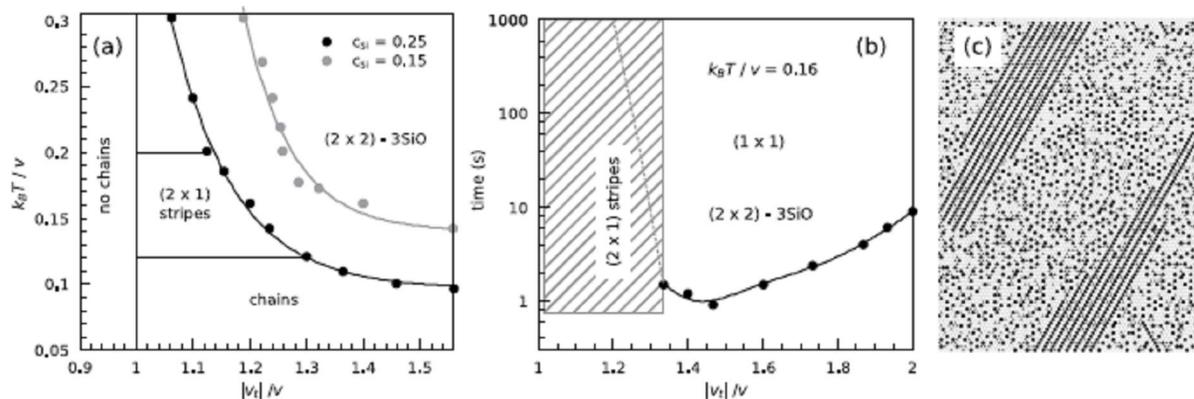


Figure 1 (a) Phase diagram obtained after 10s. (b) Time of (2×1) stripe structure stability (dashed region) and time of (2×2) structure formation from chains at $k_B T / v = 0.16$. (c) Snapshot of (2×1) structure at $|v_t| / v = 1.13$ and $k_B T / v = 0.16$ after 1000 s. Black dots correspond to SiO complexes.

THE ANDERSON LOCALIZATION PROBLEM, THE FERMI-PASTA-ULAM PARADOX AND THE GENERALIZED DIFFUSION APPROACH

V. Kuzovkov

First, based on the interpretation of a quantum tight-binding model in terms of a classical Hamiltonian map, we consider the Anderson localization (AL) problem as the Fermi-Pasta-Ulam (FPU) effect in a modified dynamical system containing both stable and unstable (inverted) modes. Delocalized states in the AL are analogous to the stable quasi-periodic motion in FPU; whereas localized states are analogous to thermalization, respectively. The second aim is to use the classical Hamilton map for a simplified derivation of *exact* equations for the localization operator $H(z)$. The letter was presented earlier [J.Phys.: Condens. Matter **14** (2002) 13777] treating the AL as a generalized diffusion in a dynamical system. We demonstrate that counter-intuitive results of our studies of the AL are similar to the FPU counter-intuitionism.

AB INITIO CALCULATIONS OF SRTIO₃, BATIO₃, PBTIO₃, CATIO₃ AND BAZRO₃ (001) AND (011) SURFACES

R. I. Eglitis

I present results of calculations of surface relaxations and rumblings for the (001) and (011) surfaces of BaZrO₃ and ATiO₃ perovskites (A = Sr, Ba, Pb and Ca) using a hybrid B3PW description of exchange and correlation. The (001) surface energies of AO, TiO₂ and ZrO₂ terminations are found to be comparable with each other for all five materials. The surface energies for BaZrO₃, SrTiO₃, BaTiO₃, PbTiO₃ and CaTiO₃ (011) surfaces for all terminations are considerably larger than for (001) surfaces. I predict a considerable increase in the Ti-O (Zr-O) chemical bond covalence near the (011) surface as compared both to the bulk and to the (001) surface.

ELECTRON DYNAMICS IN THE PROCESS OF MODE SWITCHING IN GYROTRONS

O. Dumbrajs

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The present paper is devoted to the analysis of electron interaction process in the course of gyrotron switching from one mode to another. This analysis is based on the use of the

Hamiltonian formalism that allows one to construct Poincare plots for different instants of switching time. The study is carried out for a 170 GHz, MW-class gyrotron for the International Thermonuclear Experimental Reactor (ITER)

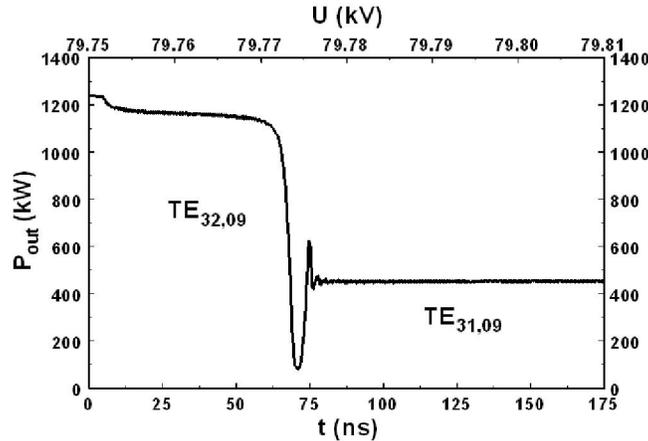


Figure 1. Switching from the operating $TE_{32,09}$ mode at 170.027 GHz to the parasitic $TE_{31,09}$ mode at 166.985 GHz.

FIRST-PRINCIPLES CALCULATIONS OF PURE AND DEFECTIVE PEROVSKITE SURFACES

E. Kotomin, Yu. Zhukovskii, R. Eglitis, S. Piskunov, Yu. Mastrikov,
 J. Maier, R. Merkle, V. Alexandrov, E. Heifets (*Max Planck Institute, Stuttgart, Germany*)
 R.A. Evarestov (*St. Petersburg University, Russia*),
 D.E. Ellis (*Northwestern University, USA*)

ABO₃-type perovskites continue to attract a considerable attention as materials for catalytic and electrochemical applications, *e.g.*, in solid oxide fuel cells (SOFC), ceramic membranes for gas separation, actuators, sensors, *etc.* Mixed oxides with the ABO₃ perovskite structure are flexible systems as their properties can be adjusted or enhanced for specific applications by chemical doping at the A or B cation sites. Alternatively, these oxides can also contain *point defects* in the form of vacancies and trapped electrons/ holes depending on the A, B cation- and dopant nature. In all these applications surfaces play a key role. We performed a series of perovskite studies with a focus on defects and surface properties which are important for high tech applications.

Using Hartree-Fock and DFT hybrid exchange-correlation functionals as incorporated into LCAO computer code *CRYSTAL*, we performed *ab initio* calculations of a surface relaxation and rumpling for (001) and (011) surfaces of BaZrO₃ and ATiO₃ (A=Sr, Ba, Pb,

Ca). The (001) surface energies of AO , TiO_2 and ZrO_2 terminations are close to each other for all five materials. The energies for BaZrO_3 , SrTiO_3 , BaTiO_3 , PbTiO_3 and CaTiO_3 polar (011) surfaces for all terminations are much larger than the (001) surface energies. The considerable increase in the Ti-O (Zr-O) chemical bond covalency is predicted near the (011) surface as compared to the bulk and the (001) surface.

In a close cooperation with Prof. D.E. Ellis (Northwestern University, USA), using the same *CRYSTAL* code, we performed large-scale computer calculations of bulk and surface O vacancies with trapped electrons (known as the F' centers) in three key perovskite crystals: SrTiO_3 , PbTiO_3 and PbZrO_3 . The local lattice relaxation, charge redistribution and positions of defect levels within the band gap have been compared. We have demonstrated that difference in a chemical composition of host materials leads to quite different defect properties: the F' center is a shallow defect in titanates but a deep defect in zirconite. All three perovskites show a considerable trend in O vacancy segregation to the surfaces which is important for the interpretation of the experimental data on mass-charge transport in nanocrystalline materials. The same trend of defect segregation towards surfaces (or internal grain boundaries) was observed in our joint study with V. Alexandrov and Prof. J. Maier (Max Planck Institute, Germany) for the charged F' centers in SrTiO_3 (O vacancy with a single trapped electron).

Magnetic perovskites play an important role in spintronics, catalysis and other applications. One of widely used materials, *e.g.*, as a cathode for Solid Oxide Fuel Cells (SOFC), is LaMnO_3 , both pure and Sr-doped. In a close collaboration with Dr E. Heifets and Prof. J. Maier (Max Planck Institute, Germany), we have used plane-wave *VASP* computer code in

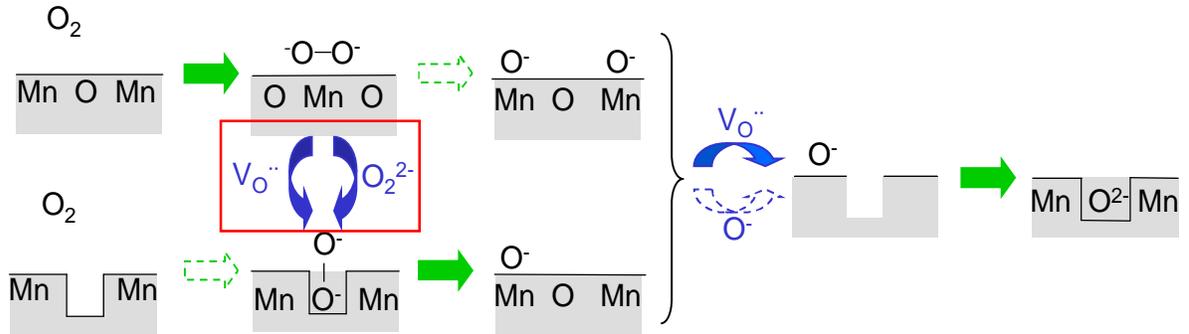


Figure 1: The most probable mechanism of oxygen incorporation on MnO_2 [001]-terminated $\text{La}_{1-x}\text{Sr}_x\text{MnO}_3$ follows the solid arrows. Straight arrows indicate reaction steps (chemisorption, dissociation, O incorporation), bent arrows describe transport (diffusion parallel to the surface). The rate-determining step in the red box is the encounter of an adsorbed molecular oxygen species O_2^- or O_2^{2-} and a surface oxygen vacancy.

a pioneering study of the atomic, electronic and thermodynamic properties of three types of LaMnO_3 surfaces in both cubic and (low-temperature) orthorhombic phases. In particular, thermodynamic analysis demonstrated that the O-terminated (011) surface in both cubic and orthorhombic phases is stable only under very poor O- and Mn-conditions (Fig. 1), whereas under normal SOFC operational conditions O_2 -terminated (011) and MnO_2 -terminated (001) surfaces are the most thermodynamically stable. This study was accompanied with the modeling of oxygen incorporation into LaMnO_3 -based SOFC cathode. Based on the *ab initio* calculations of adsorbates, surface defects, and their

migration, several mechanisms of the O_2 molecule dissociation on the surface and penetration into the cathode were suggested, with a focus on the rate-determining step.

POINT DEFECT MODELLING IN NUCLEAR FUELS

Yu. Zhukovskii, D. Bocharov, E. Kotomin, D. Gryaznov, Yu. Mastrikov,

R.A. Evarestov, A.V. Bandura (*St. Petersburg University, Russia*)

S.N. Rashkeev (*Idaho National Laboratory, USA*)

P. Van Uffelen (*EC Institute for Transuranium Elements, Karlsruhe, Germany*)

Uranium oxide (UO_2) and nitride (UN) are two actinide materials used as the nuclear fuels in fission reactors. Improvement of reactor performance and development of advanced fuels for future (generation IV) reactors needs better understanding the fuel physico-chemical properties, *e.g.*, UN oxidation and UO_2 thermo-mechanical properties under self-irradiation. To this end, we performed *ab initio VASP* modeling of both materials.

In collaboration with Prof. R.A. Evarestov and Dr A.V. Bandura (St. Petersburg University, Russia) we have studied oxygen adsorption on the UN (001) surface using the slab periodic model (Fig. 2). We have studied the binding energies, atomic displacements, and charge redistribution and demonstrated a strong O atom chemisorption typical for metallic surfaces

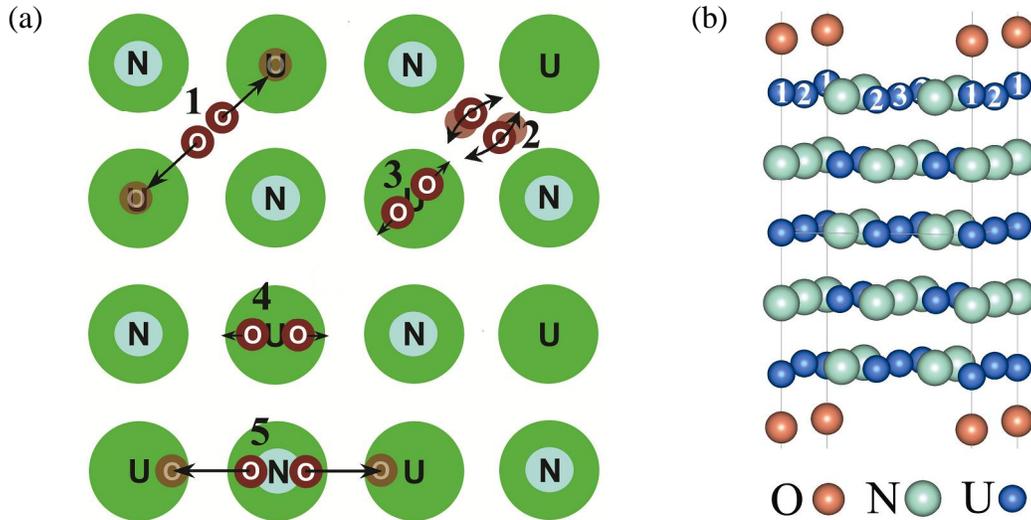


Fig.2. Two periodic slab models: (a) five different horizontal configurations for the O_2 molecule adsorption on the UN(001) surface including those with spontaneous molecular dissociation (*1* and *2*) and (b) two-side periodic adsorption of O atoms (0.25 ML) atop the surface U cations.

which is an important step in the surface oxidation process (O atoms replace for surface N atoms). To check reliability of the plane wave calculations, we employed also the *CRYSTAL LCAO* code and obtained very good agreement with the *VASP* calculations. To shed more light on the initial stage of the adsorbed O_2 molecule dissociation, we have studied this process for different possible molecule configurations on UN surface (Fig. 2a) and demonstrated that the dissociation occurs spontaneously when the molecular centre lies above the surface hollow site or atop N ions, certain activation barrier arises when a molecule sits atop the surface U ion. Besides the UN interaction with oxygen, we studied

also basic defect migration (U, N vacancies and interstitials, as well as O impurities). These *ab initio* energies were used in the fuel performance code *TRANSURANUS* for the analysis of the role of O impurities in the thermal creep in UN. Therefore, a concrete example is provided of how *ab initio* calculations can contribute directly to improve design tools of advanced nuclear fuels.

Lastly, in collaboration with Dr. S.N. Rashkeev (Idaho National Laboratory, USA) and Dr. P. Van Uffelen (EC Institute for Transuranium Elements, Karlsruhe, Germany) a detailed study of the He incorporation into UO₂ fuel has been performed using the DFT+U formalism. We have demonstrated that careful modelling of the fuel structure is necessary for a reliable calculation of the He incorporation energy.

MODELLING OF CLUSTERS CONTAINING Y AND O IMPURITIES AS WELL AS Fe VACANCIES INSIDE THE *fcc* Fe LATTICE

Yu. Zhukovskii, A. Gopejenko, E. Kotomin,
P.V. Vladimirov, A. Möslang (*Institut für Materialforschung I, Karlsruhe, Germany*)

Reduced activation steels strengthened by yttria precipitates are considered as promising construction materials for fusion- and advanced fission-reactors. In particular, use of oxide dispersion strengthened (ODS) steels for fusion reactor blanket structure allows increase of its operation temperature by ~100°C. However, the mechanism of ODS nano-particle formation is still not well understood. Recent experiments indicate that at least part of yttrium oxide particles might be dissolved in the steel matrix during mechanical alloying. If so, yttrium dissolved above its equilibrium solubility limit will precipitate during hot isostatic pressing of mechanically alloyed powder.

Collaborating with Dr. A. Möslang and Dr. P.V. Vladimirov (Institut für Materialforschung I, Karlsruhe, Germany), we have performed the detailed study of the defects in *fcc* Fe lattice stable at high temperatures only (>1100 C). We have analyzed the properties of single and pair defects as well as the Y-O-Y triple-defect complex in the lattice. We also have performed the migration barrier calculations using the Nudge Elastic Band method. The analysis of the results clearly indicates that the presence of iron vacancies is a necessary requirement for the migration of Y atoms. The first calculations on the migration barriers have been performed. They are continued now, with the increased number of the intermediate configurations to precisely estimate the migration barrier. Both defect formation energies and migration barriers will be used for further theoretical simulation of the Y₂O₃ nanocluster growth inside the γ -Fe lattice using kinetic Monte-Carlo method.

CARBON NANOTUBE TECHNOLOGY FOR HIGH-SPEED NEXT-GENERATION NANO-INTERCONNECTS (CATHERINE, EC FP7 PROJECT)

Yu. Zhukovskii, V. Kashheys, S. Piskunov, E. Kotomin,
 Yu. Shunin (*Graduate School of Information Systems Management, Riga, Latvia*)
 M.S. Sarto, A. Tamburrano (*La Sapienza Università, Roma, Italy*),
 S. Bellucci (*Istituto Nazionale di Fisica Nucleare, Laboratori Nazionali di Frascati, Italy*)

Carbon nanotubes (CNTs) become an important constituent of future nanoelectronics which is still hindered by inability to reproduce a growth of CNT with predetermined chirality indices since existing methods of nanotube synthesis yield a mixture of metallic and semiconducting nanotubes. The chemical vapor deposition (CVD) growth of CNTs above the particles of metallic catalyst is believed to be the promising approach for gaining a control over the properties of nanotubes. In collaboration with Dr S. Bellucci (Istituto Nazionale di Fisica Nucleare, Laboratori Nazionali di Frascati, Italy), we have performed the large-scale DFT-LCAO calculations on 2D-periodic models of the nanostructured C/Ni(111) interface (Fig. 3, values of E_{bind} describe carbon species bonding *per* C atom). Initial appearance of carbon atoms upon the catalyst surface (when using the CVD method) follows from the dissociation of hydrocarbon molecules, *e.g.*, CH₄. As a next step, we have simulated the C/Ni(111) interface, where carbon adatoms initially form periodic 2D islands then transforming to nanotube embryos, looking as semi-fullerenes, and finally to capped CNTs ($d_c \approx 1.42 \text{ \AA}$) of either armchair (*ac*) or zigzag (*zz*) chirality. Periodicity of this system results (Figs. 3,4) in models of infinite bundles of single-walled (SW) CNT (Fig. 4) with diameter 1.0-1.1 \AA and inter-tube distance 3.4-3.8 \AA (depending on chirality).

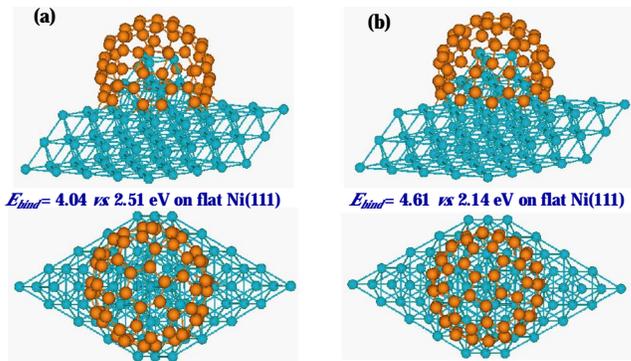
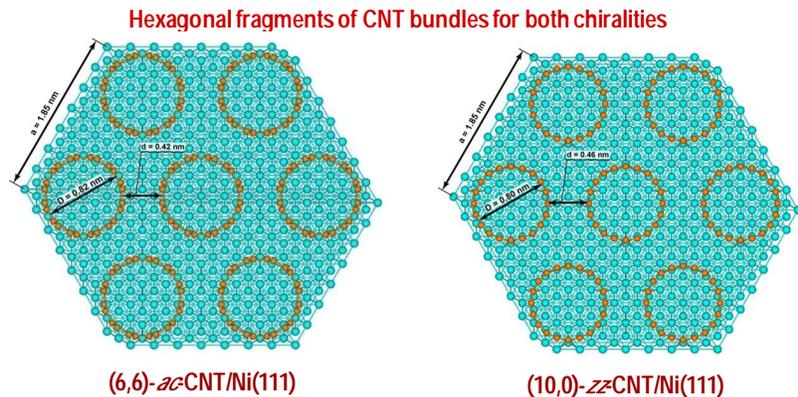


Fig. 3. Aside (upper) and atop (lower) views of 2D supercells containing CNT of either *ac* (a) or *zz* (b) type chirality upon the nanostructured Ni(111) surface.

Fig. 4. Hexagonal fragments of the CNT/Ni(111) interconnect sectioned across the bundle junctions and containing seven supercells shown in Fig. 3 for both *ac*- and *zz*-type chiralities.



Excellent conductivity properties of metallic CNT are the main reason for choosing them as the next-generation material for interconnects. However, the state-of-the-art estimates for the number of conducting channels in existing literature, which so far have been used in electrodynamical simulations, are based upon the limited microscopic modeling (room temperature, low voltage only, limited ensemble of chiralities, no doping). In collaboration with Prof. M.S. Sarto and Dr A. Tamburrano (La Sapienza Università, Roma, Italy), we have performed in-depth simulations (based on the orthogonal tight-binding, OTB, simulations, validated for simple examples by *ab initio* DFT calculations) producing the new quantitative analytic and numerical results which allow us to lift the above limitations. The key quantity, connecting CNT transport properties with the band structure is the number of conducting channels, $N(E)$, at particular energy E . It is defined by the positions of the bottoms for the conduction sub-bands and those on the tops of valence sub-bands. The values of $N(E)$ are not only the functions of energy, but also the nanotube diameter, temperature, bias voltage and chemical potential.

Based on the formalism of scattering theory, we have developed the coherent-potential approach considered as an effective-medium-approximation (CPA EMA). The first step of CPA-EMA modeling is the construction of potentials, both atomic and crystalline which uses the special well-tested analytical procedures. For proper description of CNT-Ni interconnect, including its resistivity, the CPA-EMA model has been developed in the current study, in collaboration with Dr S. Bellucci (Istituto Nazionale di Fisica Nucleare, Laboratori Nazionali di Frascati, Italy). Within the formalism of electronic transport it consists of two regions supporting two different electron transport mechanisms: ballistic (elastic, valid for carbon nanotubes *per se*) and collisional (non-elastic, valid for metal-CNT junctions). Taking into account that not all the electrons participate in a conduction process with the Fermi velocity, we have defined the so-called “thermally activated electrons” responsible for conductivity in the interconnect area. In the framework of this formalism, the interconnect resistance between the various transition metal substrates and either single-walled (SW) or multi-walled (MW) CNTs have been quantitatively estimated.

FIRST-PRINCIPLES CALCULATIONS ON SINGLE-WALLED AND DOUBLE-WALLED TiO₂ NANOTUBES AND THEIR SYMMETRY ANALYSIS

Yu. Zhukovskii, S. Piskunov,

R.A. Evarestov, A.V. Bandura, M.V. Losev (*St. Petersburg University, Russia*)

The formalism of line groups for 1D nanostructures with rotohelical symmetry has been applied for construction of TiO₂ nanotubes (NTs), both single- and double-walled (SW and DW, respectively). They can be formed by rolling up the stoichiometric 2D sheets cut from the stable (101) anatase surface containing either 6 (O-Ti-O_O-Ti-O) or 3 (O-Ti-O) atomic layers. After optimization of geometry the former keeps the centered rectangular symmetry of initial slab while the latter is spontaneously reconstructed to the hexagonal fluorite-type (111) sheet. For SW NTs, we consider 4 sets of titania nanotubes with optimized 6- and 3-layer structures: the two pairs of either anatase $(-m, m)$ and (m, m) or fluorite (n, n) and (n, \emptyset) chiralities, respectively. For DW NTs, we consider only 2 sets of nanotubes consisting of the two optimized three-layer walls with identical fluorite chiralities: $(m', m') @ (m'', m'')$ and $(n', 0) @ (n'', 0)$ where inter-wall distances are about 3-4 Å, to keep them quasi-isolated.

In a close cooperation with Prof. R.A. Evarestov, Dr A.V. Bandura and MS M.V. Losev (St. Petersburg University, Russia), we have performed large-scale *CRYSTAL* calculations on both titania slabs and nanotubes, using the hybrid Hartree-Fock/Kohn-Sham exchange-correlation functional PBE0, in order to analyze the properties of SW and DW TiO₂ NTs. We have also compared the key properties of SW and DW nanotubes, for example, the strain energies of DW NTs has been found to be ~5% smaller than those separately calculated for 3-layer SW NTs (that indicates a larger stability of DW NTs), while the band gaps of DW NTs have been found to be smaller by ~25% than those for 3-layer SW NTs.

CSPbCl₃ NANOCRYSTALS DISPERSED IN THE Rb_{0.8}Cs_{0.2}Cl MATRIX STUDIED BY FAR-INFRARED SPECTROSCOPY

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^fInstitute Laue Langevin, 6 rue Jule Horowitz, 38042, Grenoble, France

The comparative far-infrared spectroscopy studies of Rb_{0.8}Cs_{0.2}Cl and Rb_{0.8}Cs_{0.2}Cl containing CsPbCl₃ nanocrystals between 170 and 320 K are performed. Far infrared reflectivity of Rb_{0.8}Cs_{0.2}Cl crystals was measured at the Daphne Light IR station, Laboratori Nazionali di Frascati in Italy. Obtained reflectivity spectra have been analyzed using FOCUS software. Detailed analysis of FIR spectra allows to determined and analyzed, in particular, the temperature dependences of phonon frequencies (in cm⁻¹), damping constants and optical dielectric constants of Rb_{0.8}Cs_{0.2}Cl and Rb_{0.8}Cs_{0.2}Cl:Pb. The effect of cesium lead chloride nanocrystals on the phonon modes of the host matrix, particularly manifested in different temperature behavior of LO–TO splitting and the temperature dependence of high frequency dielectric constant, was demonstrated [a].

[a] A. Voloshynovskii, P. Savchyn, I. Karbovnik, S. Myagkota, M. Gestelli Guidi, M. Piccinini, and **A.I. Popov**, Solid State Commun., 2009, **149**, p. 593-597.

<http://dx.doi.org/10.1016/j.ssc.2009.01.032>

SURFACTANT-ASSISTED SYNTHESIS OF $Cd_{1-x}Co_xS$ NANOCUSTER ALLOYS AND THEIR STRUCTURAL, OPTICAL AND MAGNETIC PROPERTIES

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We report the synthesis of Co-doped CdS nanoclusters ($Cd_{1-x}Co_xS$) for different doping concentrations ($x= 0.10, 0.20$ and 0.30) and characterization of their structural, optical, and magnetic properties. Co^{2+} ions were doped with CdS nanoclusters by surfactant-assisted synthesis technique. The structural properties studied by X-ray diffraction revealed hexagonal-greenockite structure and a decrease of the lattice parameters (a and c) with doping, showing incorporation of Co in the lattice. The morphology of the nanoclusters was studied by scanning electron microscopy. Grain size of the CdS nanoclusters increases with increase in Co doping concentration. The optical absorption studies, using diffused reflectance spectroscopy, revealed that Co doping modifies the absorption band edge. Ferromagnetic phase was observed in the magnetization measurements at room-temperature due to high carrier concentration. X-ray absorption near edge fine structure measurements at the sulfur (S) K-edge of the Co-doped samples revealed that the valence remains divalent and that there are some changes with Co doping in the spectral intensity. The structural, optical, and magnetic properties of $Cd_{1-x}Co_xS$ nanoclusters demonstrate diluted magnetic semiconductors behavior [b].

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SILICON CARBIDE NANOWIRES: SYNTHESIS AND CATHODOLUMINESCENCE

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One of the most interesting SiC features is a possibility to use it in light emitting devices for the entire visible range. Current intensive research of the novel SiC nanostructures allow us for obtaining of enhanced and tunable emission by varying the size of nanoparticles or the length/diameter of nanowires as well. The present study deals with the fabrication of stable 1D SiC nanostructures by means of combustion synthesis and its further optical characterization that originates from the deep defect levels in the band gap. Comparative cathodoluminescence (CL) measurements allow us for understanding the factors influencing the change of the luminescence yield and the emission lines shifts when one moves from bulk material to confined structures. The results of CL studies on SiC 1D nanostructures are compared with the CL data collected for the commercial SiC micropowder, in which the band at 2.38 eV and a less intensive one at 1.97 eV are prevailing. 2.38 eV line corresponding to band-to-band transition in 3C-SiC was found to be much less intensive in nanopowders than in commercial sample. Further experiments indicated that isolated and purified 3C-SiC nanowires exhibit stronger emission line at 1.97 eV. The intensity of this line depends on the purification degree. CL yield at 1.97 eV is enhanced significantly when one compares a bulk SiC to double-purified silicon carbide SiC nanowires. The origin of this band can be ascribed to \mathcal{D} irradiative centers. The obtained experimental results lead to the conclusion that deep vacancy states density (that determines the 1.97 eV line intensity) is higher in nano-SiC than compared to the bulk material. Another additional reason of the enhancement of 1.97 eV CL in double-purified SiC nanowires is that the energy transfer from band-to-band electronic states (2.38 eV) to \mathcal{D} irradiative center is more efficient. In this case the purification process leads to the strong decrease of the concentration of the imperfection/defect states responsible for non-radiative relaxation of electronic excitations. As a result, CL yield at 1.97 eV is significantly higher than that observed from the commercial bulk SiC or less purified nanowires. Summarizing, a morphological characterization of the fabricated 3C-SiC 1D nanostructures has been performed by combining electron microscopy with CL measurements. Using those techniques as complementary tools can be helpful in the analysis of various nanomaterials having pronounced defect structure [c,d]

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FAR IR SPECTRA OF Ag_2CdI_4 AT TEMPERATURE RANGE 10–420 K: COMPLEMENTARY EXPERIMENTAL AND FIRST-PRINCIPLE THEORETICAL STUDY

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Ag_2MX_4 compounds, where $M = \text{Cd}, \text{Hg}, \text{Zn}, \text{etc.}$, belong to a class of *superionic solids* which are promising materials for use in *solid state batteries and fuel cells* due to extraordinarily high ionic conductivity at supercritical temperatures.. We have performed a complete IR characterization of the ternary superionic compound Ag_2CdI_4 . Far IR spectroscopy was performed at the Daphne Light synchrotron IR facility. The influence of temperature on the far-infrared (FIR) spectrum of polycrystalline Ag_2CdI_4 has been investigated in details. We complement FTIR spectroscopy with Kramers-Kronig analysis and complex dielectric response modeling with a number of quantum-chemical DFT calculations of the central-zone vibrational spectrum of Ag_2CdI_4 . This combination of different techniques allowed us to validate the IR-active optical modes, describe mode splitting in polycrystalline Ag_2CdI_4 , obtain dielectric parameters in the IR-range and thus bridge the gap in studying of Ag_2MX_4 superionic compounds. The present approach can be further applied to study the lattice dynamics in other complex polycrystalline solids [e].

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FUNDAMENTAL AND APPLIED NANOELECTRONIC ELEMENTS

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We study coherent electron transport in time-dependent nanoelectronic elements – nanotubes and quantum dots. In collaboration with Dr. Mark Buitelaar (Cavendish Laboratory, University of Cambridge, UK), we have investigated charge pumping in carbon nanotube quantum dots driven by the electric field of a surface acoustic wave. It was found that, at small driving amplitudes, the pumped current reverses polarity as the conductance is tuned through a Coulomb blockade peak using a gate electrode. This

behavior was systematically investigated as a function of wave amplitude, frequency, and direction and a model was developed in which our results can be understood as resulting from adiabatic charge redistribution between the leads and quantum dots on the nanotube. In collaboration with Dr. Bernd Kästner (Physikalisch-Technische Bundesanstalt, Braunschweig, Germany) we have described a new mechanism for charge quantization in dynamic quantum dots. These elements can be formed by time-dependent electrostatic potentials in nanoelectronic devices, such as gate- or surface-acoustic-wave-driven electron pumps. Ability to control the number of captured electrons with high precision is required for applications in fundamental metrology and quantum information processing, but the available models are limited. We have described stochastic decrease in the electron number of a shrinking dynamic quantum dot by a nuclear decay cascade model with "isotopes" being different charge states of the dot. Unlike the natural nuclei, the artificial confinement is time-dependent and tunable, so the probability distribution for the final "stable isotopes" depends on the external gate voltage. An explicit fitting formula was derived to extract the sequence of decay rate ratios from the measurements of averaged current in a periodically driven device. This provides a microscopic fingerprint of the initialization process, allows to compare different devices and architectures, and predict the upper limits of initialization accuracy.

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