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 six 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, ceramic 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	**PhD students**	**MSc and BSc students**
1. Dr. hab. E. Kotomin	13. D. Bocharov	15. O. Lisovskii
2. Dr. hab. V. Kuzovkov	14. A. Gopejenko	16. P. Merzlakovs
3. Dr hab. Yu.Shunin		17. A. Shirmane
4. Dr. O. Dumbrajs		18. A. Sorokin
5. Dr. R. Eglitis		
6. Dr. D. Gryaznov		
7. Dr. V. Kashcheyevs		
8. Dr. Yu. Mastrikov		
9. Dr. S. Piskunov		
10. Dr. A. Popov		
11. Dr. Yu. Zhukovskii		
12. Dr. G. Zvejnieks		

Scientific visits abroad

1. Dr. hab. E. Kotomin, Max-Planck Institut für Festkörperforschung, Stuttgart, Germany (9 months), University of Beijing, China (1 week)
2. Dr. O. Dumbrajs, Max-Planck Institut für Plasmaphysik, Garching, Germany (2 month), Karlsruhe Institute of Technology, Germany (1.5 months).
3. Dr hab. V. Kuzovkov, Northwesten University, USA (3.5 months)
4. Dr. D. Gryaznov, Max-Planck Institut für Festkörperforschung, Stuttgart, Germany (10 months)

5. Dr. Yu. Mastrikov, University of Maryland, USA (4 months), Institute for Materials Research-I, Karlsruhe, Germany (6 weeks).
6. Dr. S. Piskunov, University of Duisburg-Essen, Germany (2 weeks).
7. Dr. A. Popov, Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany (6 weeks), University of Beijing, China (1 week), National University of Lviv, Ukraine (1 week), Institute of Physics, Tartu, Estonia (2 weeks)
8. Dr. Yu. Zhukovskii, St. Petersburg State University, Russia (6 weeks), Institute for Materials Research-I, Karlsruhe, Germany (1 month), Institute of Nuclear Problems, Belarusian State University, Minsk (2 weeks), Institute of General and Inorganic Chemistry, Russian Academy of Science, Moscow (1 week).

International Cooperation

Belarus	1. Belarusian State University (Prof. S.A. Maksimenko)
Finland	2. Helsinki University of Technology (Dr. T. Kurki-Suonio)
France	3. Laue-Langevin Institute, Grenoble (Dr. G.J. McIntyre, Dr. H. Schober)
Germany	4. Max Planck Institut für Festkörperforschung, Stuttgart (Prof. Dr. J. Maier) 5. Deutsches Elektronen-Synchrotron DESY, Hamburg (Dr. A. Kotlov) 6. EC Institute of Transuranium Elements, Karlsruhe (Dr. P. Van Uffelen). 7. Max Planck Institut für Plasmaphysik, Garching (Dr. V. Igochine, Prof. Dr. K. Lackner, Dr. R. Mayer-Spasche, Prof. Dr. H. Zohm) 8. Institut für Hochleistungsimpuls & Mikrowellentechnik (KIT), Karlsruhe (Dr. S. Kern, Dr. B. Piosczyk) 9. Institut für Materialforschung I (KIT), Karlsruhe (Dr. A. Möslang) 10. Department of Theoretical Chemistry, University of Duisburg-Essen, (Prof. E. Spohr)
Greece	11. School of Electrical and Computer Engineering, National Technical University of Athens, Zographou (Dr. K. Avramides)
Israel	12. Ben Gurion University, Beer Sheeva (Prof. A. Aharony, Prof. D. Fuks)
Italy	13. Laboratori Nazionali di Frascati (Dr. S. Bellucci, Dr. M. Cestelli-Guidi)
Kazakhstan	14. Gumilyov National University, Astana (Prof. A. Akilbekov)
Japan	15. FIR Center, University of Fukui (Prof. T. Idehara)
Lithuania	16. Institute of Semiconductor Physics (SPI), Vilnius (Dr. E. Tornau)
Poland	17. Warsaw University, Dept of Chemistry (Dr A. Huczko)
Romania	18. University of Craiova (Dr. D. Constantinescu)
Russia	19. St. Petersburg State University (Prof. R.A. Evarestov) 20. Institute of General and Inorganic Chemistry, Russian Academy of Sciences, Moscow (Prof. P.N. Dyachkov)
UK	21. Imperial College London (Prof. M.Finnis) 22. University College London (Prof. A.L. Shluger)
Ukraine	23. National University of Lviv (Prof. I. Bolesta and Prof. V. Savchyn)
USA	24. Northwestern University, Evanston, Illinois (Prof. M.Olvera de la Cruz) 25. University of Maryland, College Park (Dr. G.S. Nusinovich, Dr. M.M. Kukla)

Main Results

A. Electronic structure calculations for advanced materials

FIRST-PRINCIPLES NANO-SCALE SIMULATIONS OF CARBON NANOTUBES GROWTH UPON NI AND ALUMINA CATALYSTS

Yu.F. Zhukovskii, S. Piskunov, G. Zvejnieks, E.A. Kotomin,
S. Bellucci (*Laboratori Nazionali di Frascati, Italy*)

Within the EC FP7 CATHERINE project, in collaboration with Dr. S. Bellucci (Laboratori Nazionali di Frascati, Italy) and *Faculty of Computing (University of Latvia)* we have performed large-scale *ab initio* simulations on 2D periodic models of C/Ni(111) (The 5×5 SC model of nickel substrate, Fig. 1) and C/θ-Al_2O_3(010) nanostructures, which can describe peculiarities of the initial stage of growth for the SW CNT bundle upon the catalyst particle.

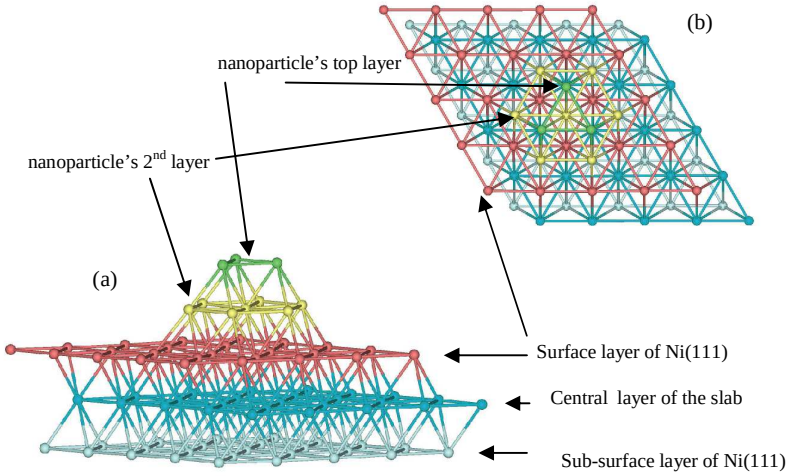

Fig. 1. Schematic illustration of nanostructured Ni(111) catalyst: (a) side view and (b) top view. Each surface plane is shown with different color to guide eyes. The lower light-blue plane is a mirror plane of symmetrically terminated 5-layer slab.

The network of adsorbed carbon atoms, which transforms to the nanotube structures, arise after the dissociation of hydrocarbon molecules *e.g.*, CH_4, flowing towards the substrate when using the CVD method. We estimate the dissociation energies for CH_4 molecules atop both substrates (see Fig. 2 for details) according to the total energy balance of the two-step dissociation mechanism:

$$(CH_4)_{ads} \rightarrow (CH)_{ads} + 3H_{ads}, \quad (1a)$$

$$(CH)_{ads} \rightarrow C_{ads} + H_{ads} \quad (1b)$$

The calculated energies of a complete dissociation (E_{diss}) have been found to be 2.33, 2.17, and 6.40 eV for perfect Ni(111), nanostructured Ni(111), and θ-Al_2O_3(010) substrates, respectively.

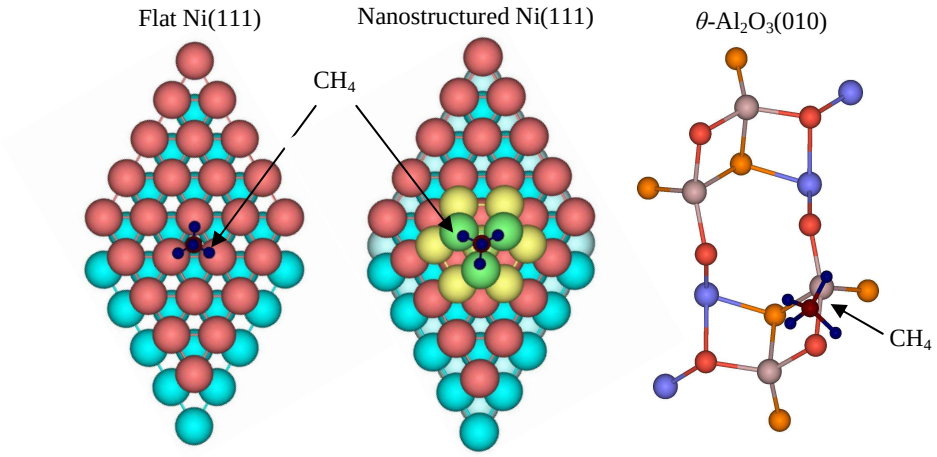

Fig. 2. Schematic illustration of CH_4 dissociation on both Ni(111) and θ-Al_2O_3(010).

As the result of our simulations, we predict an increase of catalytic activity of nanostructured Ni(111) surface, due to nanofacet formation that potentially can play a role in a predictable growth of CNT (Fig. 3). The key stage of carbon nanotube growth from catalyst is an initial swelling of an island consisting of carbon hexagons and pentagons formed from C_{ads} atoms atop the substrate up to creation of semi-fullerene.

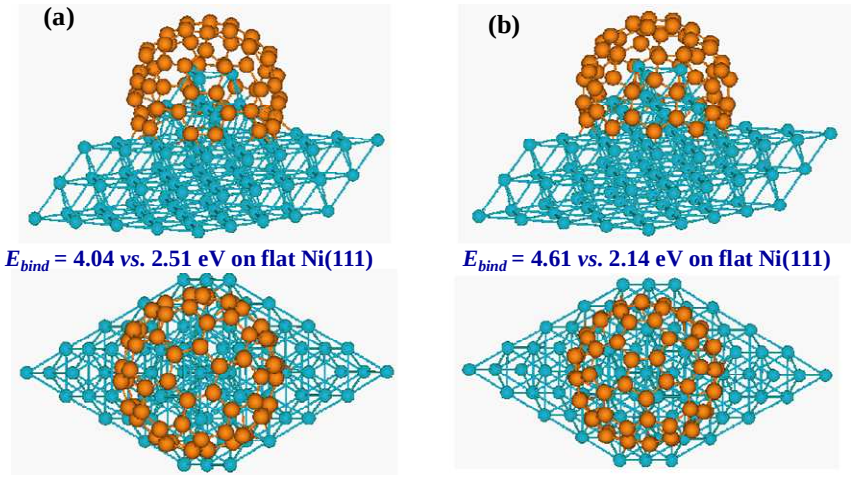

Fig. 3. Aside (upper) and atop (lower) views of 2D supercells containing CNT of either *ac* (a) or *zz* (b) type chirality upon the nanostructured Ni(111) surface.

Our results predict quite effective and reproducible mechanism of growth for carbon nanotubes upon the nickel nanostructured substrate. In absence of catalyst nanoparticles upon the bottom of the nanopores inside alumina membrane the carbon structures could grow from the walls towards the centers of nanopores: either carbon nanoscrolls or rather thick amorphous (soot-like) microtubes. At the bottom level of the multi-scale modeling, *ab initio* methods can be used for determining the electronic structure of the assumed carbon-metal nanocomposites.

FIRST-PRINCIPLES CALCULATIONS ON SINGLE- AND DOUBLE-WALL INORGANIC NANOTUBES AND THEIR STRUCTURAL ANALYSIS

Yu.F. Zhukovskii, S. Piskunov,
R.A. Evarestov, A.V. Bandura (*Department of Quantum Chemistry, St. Petersburg University, Russia*),
E. Spohr (*Department of Theoretical Chemistry, University of Duisburg-Essen, Germany*)

Within the line group irreducible representations developed *in collaboration with Prof. R.A. Evarestov and Dr. A.V. Bandura (St. Petersburg University, Russia)* the one-periodic (1D) nanostructures with rotohelical symmetry have been considered for symmetry analysis of single- and double-wall (SW and DW) boron nitride and titania nanotubes (BN and TiO_2 NTs) formed by rolling up the stoichiometric two-periodic (2D) slabs of hexagonal structure with the same or opposite orientation of translation and chiral vectors. We have simulated the two sets of commensurate double-wall BN NTs and TiO_2 NTs (Fig. 4) with armchair- or zigzag-type chiralities: (n_1,n_1)@(n_2,n_2) or (n_1,0)@(n_2,0), respectively.

a) optimized model of double-wall (6,6)@(12,12) *ac*-TiO_2 NT;

b) optimized model of double-wall (10,0)@(20,0) *zz*- TiO_2 NT.

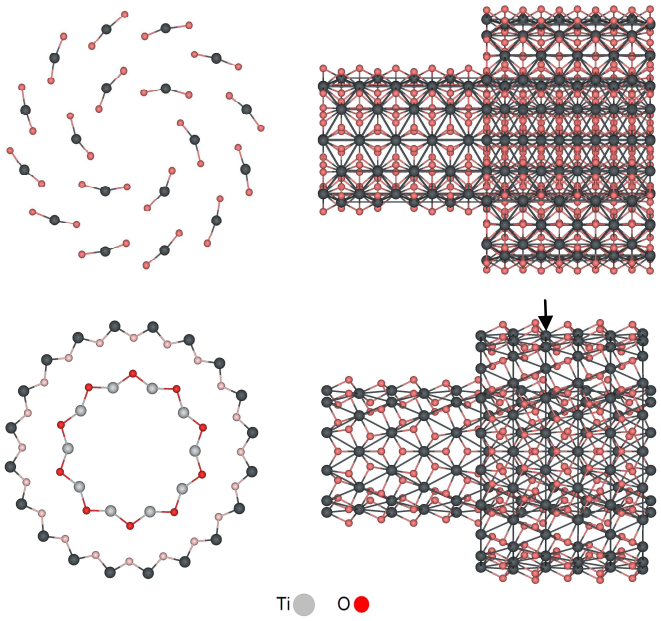

Fig. 4. Cross-sections and aside images of hexagonal DW TiO_2 NTs corresponding to optimized diameters (*i.e.*, left and right parts of models a) and b), respectively) for armchair and zigzag chiralities. For *zz*-DW NT (b), there are also shown atoms of the nearest ring behind the cross-section (as considerably more light circles).

Due to a noticeably larger ionic contribution to inter-wall interaction between three-layer O-Ti-O shells within DW TiO_2 NTs their polarization effects are certainly larger than those in double-wall boron nitride nanotubes which results in the higher electron density localization as compared to DW BN NTs. Considerable interaction between the walls in optimal DW NT configurations results in a decrease of band gaps in double-wall nanotubes as compared to those for SW NTs (this decrease is a more pronounced for DW TiO_2 NTs).

One-dimensional nanostructures synthesized from complex ternary oxides with a perovskite structure have attracted considerable recent interest due to their unique physical properties and promising novel functionalities as compared to bulk materials. At room temperature $SrTiO_3$ possesses a high symmetry cubic structure and, thus, serves as an excellent model material for a wide class of ABO_3 perovskites. Consequently, understanding the behavior of $SrTiO_3$ on the nanoscale is significant for fundamental studies, as well as for shape-controlled synthesis of perovskite nanostructures with predictable properties. Based on *ab initio* calculations performed *in collaboration with Prof. E. Spohr (University of Duisburg-Essen, Germany) and Faculty of Computing (University of Latvia)* we predict that the most energetically stable NTs can be rolled up from (110) nanosheet of rectangular morphology:

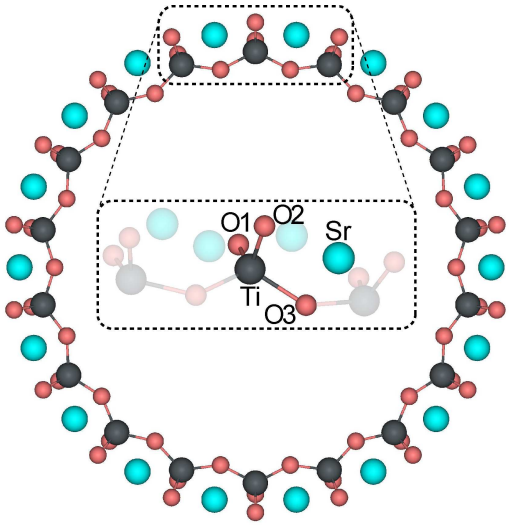

Fig. 5. Atomic structure of the most energetically stable $SrTiO_3$ nanotube.

The increase of the Ti–O bond covalency in the outer shell of strontium titanate NT may lead to an enhancement of adsorption properties which means that they can be used in gas-sensing devices. Quantum confinement effects lead to the widening of the NT band gaps, thus, making them attractive for band gap engineering, *e.g.*, in photocatalytic applications.

THEORETICAL SIMULATIONS ON ELECTRIC PROPERTIES FOR JUNCTIONS OF METALLIC ELECTRODES WITH CARBON NANOTUBES AND GRAPHENE NANORIBBONS

Yu.N. Shunin, Yu.F. Zhukovskii,
S. Bellucci (*Laboratori Nazionali di Frascati, Italy*)

In collaboration with Dr. S. Bellucci (Laboratori Nazionali di Frascati, Italy) within the EC FP7 CATHERINE project, we have developed the model of *'effective bonds'* in the framework of both cluster approach based on the multiple scattering theory formalism and Landauer theory, which can allow us to predict the resistivity properties for C-Me junctions taking into account chirality effects in the interconnects of single-wall (SW) and

multi-wall (MW) CNTs (Fig. 6) as well as single-layer (SL) and poly-layer (PL) GNRs (Fig. 7) with the fitting metals (Me= Ni, Cu, Ag, Pd, Pt, Au) on predefined geometry of carbon nanostructure. We have also developed the model of inter-shell interaction for the MW CNTs, which allows us to estimate the transparency coefficient as an indicator of possible 'radial current' losses.

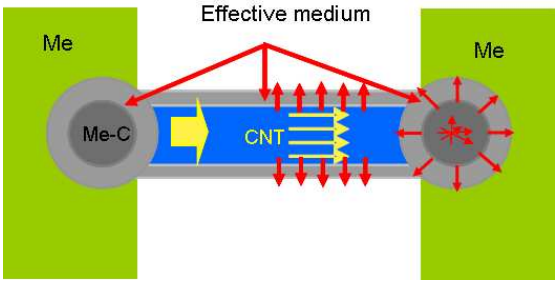

Fig. 6. Model of CNT - Me interconnect.

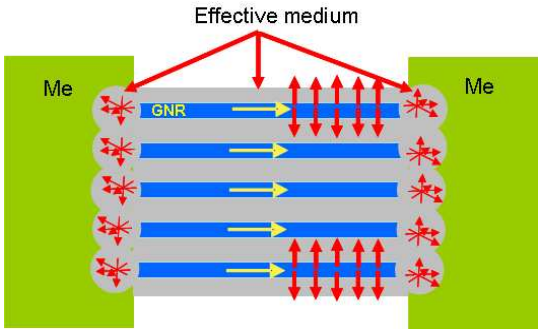

Fig. 7. GNR (polylayered) - Me interconnect.

Figs. 8 and 9 show the generalized results of simulations on resistance of junctions between various metallic substrates with SW CNT and SL GNR, respectively. It is clear that Ag and Au substrates are more effective electrically while Ni is rather a 'worse' substrate for interconnect, although it yields the most effective catalyst for CNT growth.

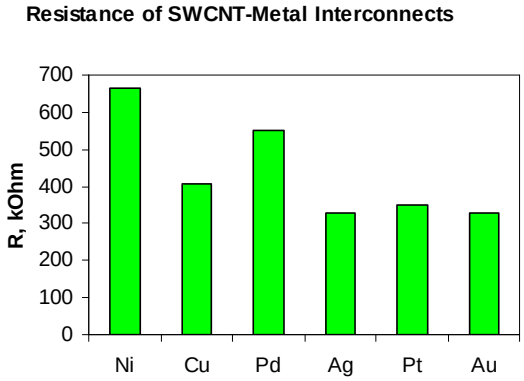

Fig. 8. Resistances of Me interconnects with zigzag-type SW CNT (diameter ~1 nm)

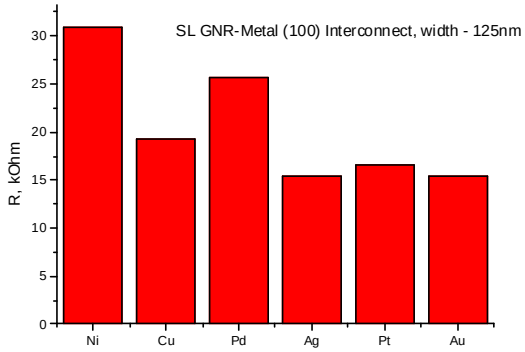

Fig. 9. Resistances of Me interconnects with the SL GNR (width ~125 nm)

Conductance and other current-voltaic parameters depend on the morphology of the nearest shells in MW CNTs and PL GNRs, which results in complications for technological synthesis. Nevertheless, the corresponding nanodevices possess the stable electric characteristics. We are able now to create a database of combinations for different CNT-Me and GNR-Me junctions taking into account a set of parameters, namely: angle of chirality, CNT diameter, numbers of walls or layers, type of metal substrate (Me), orientation of densely-packed metal substrate, *e.g.*, (100), (111) or (110). Thus, we are able to predict interconnect properties for various configurations of SW and MW CNTs as well as SL and PL GNRs.

MECHANISM OF OXYGEN MIGRATION AND INCORPORATION UPON PERFECT AND DEFECTIVE URANIUM NITRIDE (001) SURFACE

D. Bocharov, D. Gryaznov, Yu.F Zhukovskii, E.A. Kotomin,
P. Van Uffelen (*EC Institute for Transuranium Elements, Karlsruhe, Germany*)

For the first time, we have performed detailed first-principles simulations of perfect and defective uranium mononitride (UN) surfaces and their interaction with oxygen, *in collaboration with EC Institute for Transuranium Elements (Karlsruhe, Germany) and Faculty of Computing (University of Latvia).* This is relevant for understanding mechanism of UN nuclear fuel exidation in air. Due to a mixed metallic-covalent nature of the chemical bonding in UN, we predicted a high affinity of adsorbed O towards the UN(001) surface. Indeed, the E_{bind} values of 6.9-7.6 and 5.0-5.7 eV *per* O adatom atop the surface U or N atoms, respectively, are accompanied by 0.5-1.2 *e* charge transfer from the surface towards the O adatom (Fig. 10). The positively charged surface U atom goes outwards, minimizing its distance with the adsorbed O atom while the N atom is strongly displaced from the adsorbed O atom inwards the slab, due to a mutual repulsion between N and O.

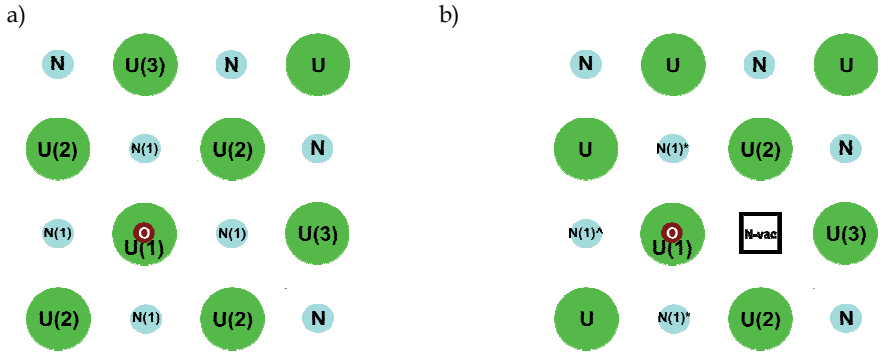

Fig. 10. Schematic top view of O adatoms located atop the surface U atom without (a) and with (b) N vacancy in the proximity of adsorbed O atoms. Numbers in brackets enumerate non-equivalent surface atoms.

Three main migration paths of O upon the UN(001) surface (Fig. 11) are as follows: *1*: between U atom and the nearest N atom, *2*: between the two neighboring U atoms, *3*: between neighboring N atoms. The most favorable migration trajectory has been optimized to be the line joining the sites atop the nearest surface U atoms and the hollow sites between them (path 2). The corresponding energy barriers found (0.36 eV for the 5-layer slab and 0.26 eV for the 7-layer slab) indicate a high mobility of adsorbed O atoms upon UN. The energy barriers along other two migration trajectories are substantially larger.

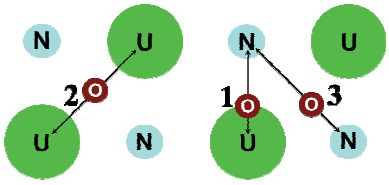

Fig. 11. Different oxygen migration paths upon the UN(001) surface (top view).

Both formation energies of uranium and nitrogen vacancies as well as binding energies of oxygen atoms and molecules adsorbed atop the defective UN(001) surface have been estimated too. Presence of the surface nitrogen vacancy closest to the surface U atom (U_{surf}) results in a low-barrier incorporation of migrating O adatom from position atop U_{surf} towards this vacancy, which can be considered as a trap. Based on the results of calculations discussed above the following stages of oxygen interaction with the UN surfaces were indentified to explain its easy oxidation: (*i*) chemisorption of molecular oxygen, (*ii*) spontaneous breaking of the O_2 chemical bond after molecular adsorption, (*iii*) location of the two newly formed O adatoms atop the adjacent surface U atoms, (*iv*) high mobility of adsorbed O atoms along the surface, (*v*) low-barrier incorporation of O into N-vacancies, *(vi)* stabilization of O atom inside the N-vacancy, (*vii*) further incorporation of O in pre-existed sub-surface N-vacancies as a result of inter-layer diffusion.

AB INITIO SIMULATIONS OF IMPURITY CLUSTERS IN ODS STEELS

A. Gopejenko, Yu.F. Zhukovskii, Yu. Mastrikov, E.A. Kotomin,
P.V. Vladimirov, A. Möslang (*Institut für Materialforschung I, Karlsruhe, Germany*)
V.A. Borodin (*Research Center Kurchatov Institute, Moscow, Russia*)

The understanding of the mechanisms and kinetics of yttria nanoparticle formation in the steel matrix is required of the development of the oxide dispersed strengthened (ODS) steels. The implementation of the ODS steel for fusion- and advanced fission-reactor blanket structures results in increase of the operation temperature by ~100°C which makes this material very promising these reactors. On the other hand, the mechanical properties and radiation resistance of ODS steels are sensitive to the size and spatial distribution of the oxide precipitates. Therefore, it is necessary to perform a large-scale theoretical modeling of the Y_2O_3 formation. Large-scale first principles calculations have been performed *in collaboration with Dr. A. Möslang and Dr. P.V. Vladimirov (Institut für Materialforschung I, Karlsruhe, Germany)* for the γ-Fe lattice containing Y-Y, Y-V_{Fe}, V_{Fe}-V_{Fe}, Y-O (Fig. 12) and O-O pairs as well as different configurations of three-atom clusters Y-O-Y (Fig. 13) and Y-V_{Fe}-Y. These calculations are required to accurately estimate the pair- and triple-wise interaction energies necessary for further lattice kinetic Monte Carlo (LKMC) simulations of ODS growth.

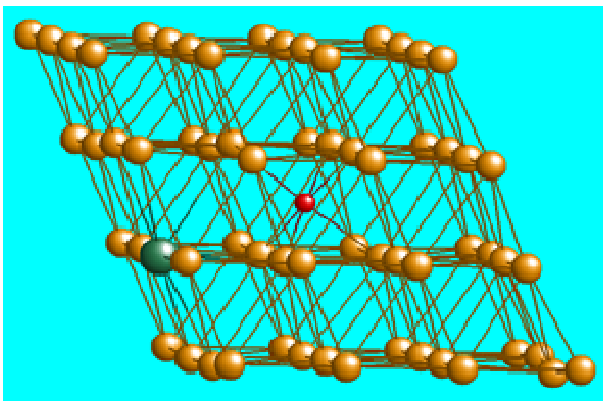

Fig. 12. Relaxed 2nd coordination sphere for configuration of Y-O_{int} pair.

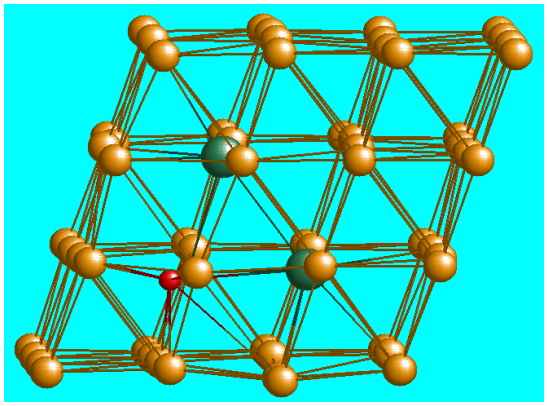

Fig. 13. Relaxed configuration of 2Y-O substitute atoms.

The analysis of the pair-wise interactions calculations show that a certain attraction occurs between the Y substitute atom and Fe vacancy, while no bonding occurs between two Y atoms at any distances. The calculations of the interactions between yttrium and oxygen substitute atoms as well as between two oxygen substitute atoms show similar behavior with the highest binding energies at the distance of 1-NN and the decrease of the binding energy with the increase of the inter-defect distance. No significant bonding has been found between the two Fe vacancies located at different distances.

At the same time, we predict location of Fe vacancies in the proximity of impurity atoms. The calculations on different Y-O-Y cluster configurations clearly show that not only the presence of oxygen atom is required to form certain binding between impurity atoms but also the presence of Fe vacancies favors the growth of the Y_2O_3 precipitates inside the iron crystalline matrix. This has been proven by the calculations of interactions inside the Y-V_{Fe}-Y cluster for which the binding energy has been found to be rather large.

FIRST PRINCIPLES CALCULATIONS OF OXYGEN VACANCY FORMATION AND MIGRATION IN $BA_{1-X}Sr_XCo_{1-Y}Fe_YO_3$ PEROVSKITES

Yu. Mastrikov, E.A. Kotomin,
R. Merkle, J. Maier (Max Planck Institute for Solid State Research, Stuttgart, Germany)
M. M.Kuklja (Materials Science and Eng.Dept., University of Maryland, College Park, USA)

Based on first principles DFT calculations, we analyzed oxygen vacancy formation and migration energies as a function of chemical composition in complex multicomponent (Ba,Sr)(Co,Fe)O_3 perovskites which are candidate materials for SOFC cathodes and permeation membranes. The atomic relaxation, electronic charge redistribution and energies of the transition states of oxygen migration are compared for several perovskites to elucidate the atomistic reason for the exceptionally low migration barrier in $Ba_{0.5}Sr_{0.5}Co_{0.8}Fe_{0.2}O_3$ that was previously determined experimentally. The critical comparison of $Ba_{1-x}Sr_xCo_{1-y}Fe_yO_3$ perovskites with different cation compositions and arrangements shows that in addition to the geometric constraints the electronic structure plays a considerable role for the height of the oxygen migration barrier in these materials. These findings help to understand the fast oxygen permeation and exchange properties of $Ba_{0.5}Sr_{0.5}Co_{0.8}Fe_{0.2}O_3$ as well as some of its limitations

PHONON CALCULATIONS IN CUBIC AND TETRAGONAL PHASES OF $SrTiO_3$: A COMPARATIVE LCAO AND PLANE WAVE STUDY

D. Gryaznov, E.A. Kotomin,
R.A. Evarestov (St. Petersburg State University, Peterhof, Russia)
E. Blokhin, J. Maier (Max-Planck Institute for Solid State Research, Stuttgart, Germany)

The atomic, electronic structure and phonon frequencies have been calculated in a cubic and low-temperature tetragonal $SrTiO_3$ phases at the *ab initio* level. We demonstrated that the use of hybrid exchange-correlation PBE0 functional gives the best agreement with experimental data. The results for the standard Generalized Gradient Approximation (PBE) and hybrid PBE0 functionals are compared for the two types of approaches: a linear combination of atomic orbitals (CRYSTAL09 computer code) and plane waves (VASP 5.2 code). Relation between cubic and tetragonal phases and the relevant antiferrodistortive

phase transition is discussed in terms of group theory and illustrated with analysis of calculated soft mode frequencies at the *Γ*- and *R*-points in the Brillouin zone. Based on phonon calculations, the temperature dependence of the heat capacity is in a good agreement with experiment. This approach is promising for defect modeling in many advanced materials under high operational temperatures.

FIRST-PRINCIPLES CALCULATIONS OF THE ATOMIC AND ELECTRONIC STRUCTURE OF PEROVSKITE SURFACES

R.I. Eglitis

The *ab initio* calculations of polar $CaTiO_3$ (111) surface were performed. Surface relaxation, rumpling, energetics, optical band gaps, and charge distribution are obtained using the computer code CRYSTAL and a hybrid exchange-correlation functionals. Using a hybrid B3LYP approach, the surface relaxation for the two possible Ti and CaO_3 (111) surface terminations are calculated. For both Ti and CaO_3-terminated CaTiO3 (111) surfaces upper layer atoms relax inwards, while the second layer atoms, with the sole exception of CaO_3-terminated surface Ca atom, relax outwards. The alculated surface relaxation energy for Ti-terminated surface is more than five times larger than the surface relaxation energy for CaO3-terminated surface. The surface energy for Ti-terminated surface (4.18 eV/cell) is smaller, than the surface energy for CaO_3-termination (5.86 eV/cell).
We calculated also properties of the $SrZrO_3$ (001) surfaceBoth SrO and ZrO_2 terminations were considered. On the (001) surfaces all upper and third layer atoms relax inward, while outward relaxations of all atoms in the second layer are found with the sole exception of SrO-terminated $SrZrO_3$ (001) surface second layer O atom. Calculated surface rumpling for the SrO-terminated SrZrO3 (001) surface (6.77 % of the lattice constant) is by a factor of ten larger than the surface rumpling for the ZrO_2-terminated surface (0.72 % of a_o). A considerable increase in the Zr-O chemical bond covalency near the $SrZrO_3$(001) surface as compared to the bulk is predicted.

FIRST-PRINCIPLES SIMULATIONS ON THE *F* CENTER AGGREGATION IN BAF_2

R.I. Eglitis
H. Shi (School of Science, Beijing Institute of Technology, Beijing, China),
R. Jia (Bergische Universität Wuppertal, Germany)

The *F* center (an electron trapped by a fluorine vacancy) and *R* center (a defect composed of three F centers) in BaF_2 crystal have been studied using density functional theory (DFT) with hybrid exchange-correlation DFT-B3PW functional. Our calculations show that the *F*-center transfer barrier is equal to 1.83 eV. The association energy calculations on R centers indicate energy gain with respect to three isolated *F* centers. During *F*-center aggregation, a considerable covalency arises between two neighbor fluorine vacancies with trapped electrons. Three incompletely paired electrons trapped in the R center have an up-down-up spin arrangements and induce three defect levels in the gaps between valence bands (VB) and conduction bands (CB) for both α- and β-spin polarized band structures, respectively.

More defect bands lead to more complex electron transitions, which were classified into two F- and four M-like transitions. The DOS calculations clearly reveal the components of defect bands.

FIRST-PRINCIPLES CALCULATIONS OF THE ELECTRONIC DENSITY OF STATES FOR SUPERIONIC Ag_2CdI_4 CRYSTALS

A.I. Popov
S. Velgosh, I. Karbovnyk, I. Bolesta, O. Bovgyra
(Ivan Franko National University of Lviv, Ukraine)
W. Ciepluch-Trojane, B. Andriyevsky (Faculty of Electronics and Computer Sciences, Koszalin University of Technology, Poland)
I.V. Kityk (Czestochowa Technical University, Czestochowa, Poland)

Over the past few decades an enhanced interest takes place to the studies of silver-containing fast ionic conductors. These crystals are, first of all, of interest due to phenomena of the reversible transformation of luminescence centers structure as well as mobile silver ions concentration changes within the local irradiated region of the crystals.

This work completes our thorough investigation of Ag_2CdI_4 solid electrolyte. In addition to previous results of electrical, optical and thermal properties of this model compound and following recent report on its microstructure studied by SEM, impedance spectroscopy and fractal dimension analysis as well as infrared spectra and phonon density of states calculation, herewith we focused on the band energy structure calculations of the Ag_2CdI_4 single crystals and determination of partial densities of states in the valence band.
Energy band dispersion calculations have been performed for Ag_2CdI_4 superionic within a framework of local density approximation (Perdew–Zunger parameterization) exploiting the first-principles CASTEP computer code. The *ab-initio* electronic structure simulations were performed for both types of ε-Ag_2CdI_4 crystalline structures. Principal optical functions as well as the density of electronic states in the spectral range of inter-band optical transitions (2.5 eV–20 eV) were determined. Theoretically calculated absorption coefficients derived from the obtained band structure are compared with appropriate experimental data.

B. Kinetics of processes with self-organization

PATTERN FORMATION KINETICS FOR CHARGED MOLECULES ON SURFACES AND INTERFACES: MICROSCOPIC CORRELATION FUNCTION ANALYSIS

V.N. Kuzovkov, E.A. Kotomin, G. Zvejnieks,
M. Olvera de la Cruz (*Northwestern University, Evanston, USA*)

The kinetics of pattern formation and phase separation in a closed system of two types of oppositely charged molecules with competing short- and long-range interactions on surfaces/interfaces was studied combining three methods: a microscopic formalism of the joint correlation functions, Reverse Monte Carlo, and non-equilibrium charge screening factors. The molecular ordering occurs on the background of the Ostwald ripening and thus

is strongly non-equilibrium. It is demonstrated how initial random distribution of molecules is changed for loose similar-molecule aggregates, with further reorganization into dense macroscopic domains of oppositely charged molecules (Fig. 14). Pattern formation process is characterized by the correlation length which monotonically increases in time.

The kinetics of pattern formation was also studied for reversible A+B→0 reaction of mobile oppositely charged molecules at the interface. Using formalism of joint correlation functions, non-equilibrium charge screening and reverse Monte-Carlo methods, it is shown that labyrinth-like percolation structure induced by (even moderate-rate) reaction is principally non-steady-state and is associated with permanently growing segregation of similar reactants and aggregation of similar reactants into domains. A role of short-range and long-range reactant interactions is discussed.

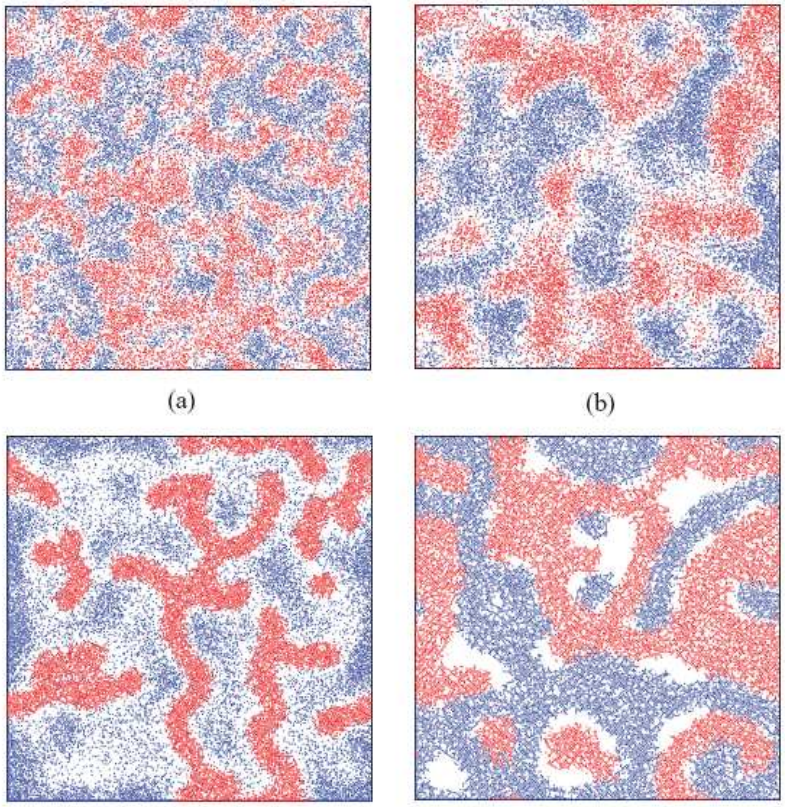

Fig. 14. Fragments of the characteristic snapshots obtained using the reverse Monte Carlo for the correlation functions

In collaboration with Northwestern University, Evanston, USA, the effects of non-equilibrium charge screening in mixtures of oppositely charged interacting molecules on surfaces are analyzed in a closed system. The dynamics of charge screening and the strong deviation from the standard Debye-Hückel theory are demonstrated via a new formalism based on computing radial distribution functions suited for analyzing both short-range and long-range special ordering effects. At long distances, the inhomogeneous molecule distribution is limited by diffusion, whereas at short distances (of the order of several

coordination spheres) by a balance of short-range (Lennard-Jones) and long-range (Coulomb) interactions (Fig. 15). The non-equilibrium charge screening effects in transient pattern formation are further quantified. It is demonstrated that use of screened potentials, in the spirit of the Debye-Hückel theory, leads to qualitatively incorrect results.

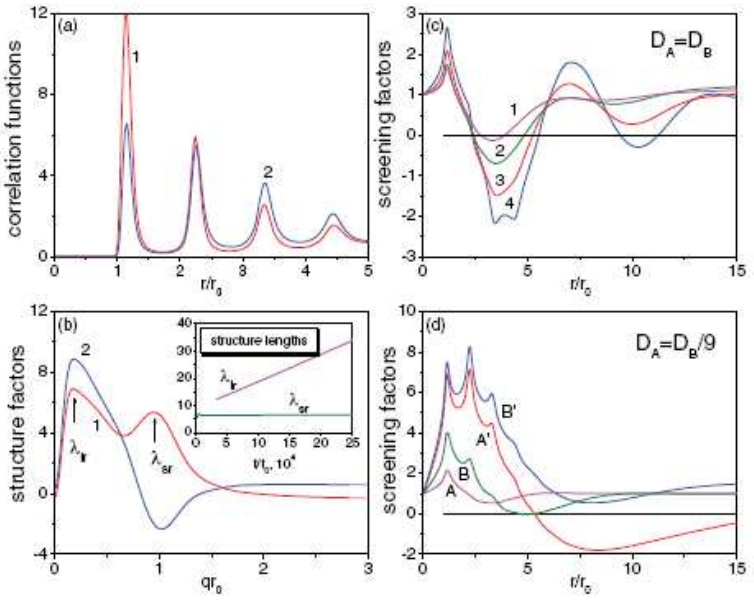

Fig. 15. Ionic binary systems with Lennard-Jones and Coulomb interactions at low temperatures for intermediate density: (a) the joint correlation functions; (b) the partial structure factors; (c) and (d) the non-equilibrium screening factors.

C. Physics of Plasma

A LOW-DIMENSIONAL MODEL SYSTEM FOR QUASI-PERIODIC PLASMA PERTURBATIONS

D. Constantinescu[1], O. Dumbrajs[2], V. Igochine[3], K. Lackner[3],
R. Meyer-Spasche[3], H. Zohm[3] and ASDEX Upgrade team[3]

[1]Dept.Applied Mathematics, University of Craiova, Association Euratom-MECI, Romania
[2]Institute of Solid State Physics, University of Latvia, Association Euratom-UL, Latvia,
[3]Max-Planck Institut für Plasmaphysik, Association Euratom-IPP, Germany

Larger scale plasma instabilities not leading to an immediate termination of a discharge often result in periodic nonlinear perturbations. A simplest possible model is suggested for description of the system with drive and relaxation processes with different time scales. The model is based on two equations: the first being responsible for the relaxation dynamics and the second one for the drive (Fig. 16). The model can be generalized to describe the pellet injection.

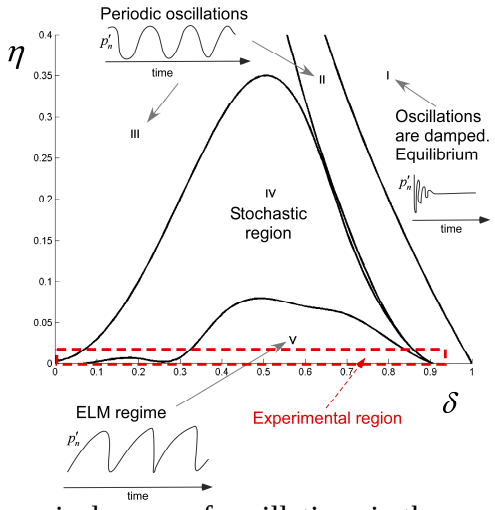

Fig. 16. Dynamical zones of oscillations in the parameter space

UNDERSTANDING COMPLEX MAGNETOHYDRODYNAMIC ACTIVITIES WITH A RELAXATION IN THE HT-7 TOKAMAK

Erzhong Li[1], Liqun Hu[1], V Igochine[2], O Dumbrajs[3] and Kaiyun Chen[1]

[1]Institute of Plasma Physics, Chinese Academy of Science, Hefei, China
[2]MPI f¨ur Plasmaphysik, Euratom-Association, D-85748 Garching, Germany
[3]Institute of Solid State Physics, Association Euratom-University of Latvia, Riga, Latvia

A new relaxation instability with complex magnetohydrodynamics (MHD) activities is found in the HT-7 tokamak operational region, which manifests itself in bursts of hydrogen alpha-ray radiations, electron cyclotron emission and soft x-ray (SX) radiations on outer channels, as well as complex MHD perturbations, but without hard disruptions. It is found that a stochastic annular belt resulted just before the relaxation due to the m/n = 5/3 island overlapping with m/n = 2/1 and m/n = 3/2 islands (Fig. 17).

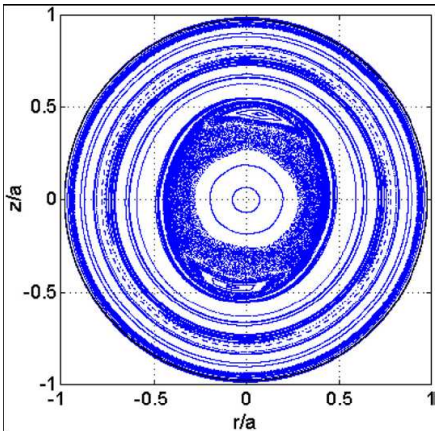

Fig. 17. The Poincare mapping where a stochastic annular belt of magnetic field lines could be observe

EFFECT OF POSSIBLE REFLECTIONS ON THE OPERATIONS OF EUROPEAN ITER GYROTRONS

O Dumbrajs

Theory describing the effect of reflections on operation of gyrotrons with radial output is applied the ITER 170 GHz 2 MW coaxial cavity gyrotron, which is under development, and to the 170 GHz 1 MW cylindrical cavity gyrotron as a fall back solution.

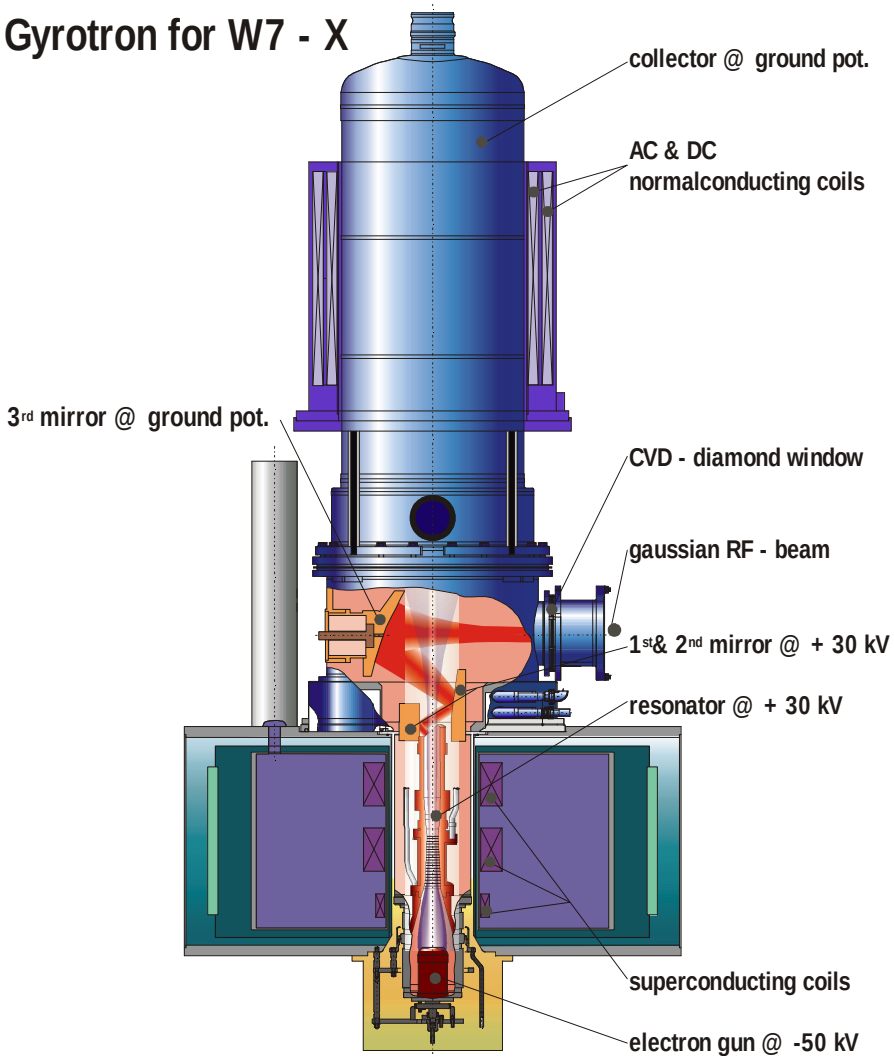

Fig. 18. European 140 GHz, 1 MW, CW Gyrotron

Publications in year 2011

SCI

1. R.A. Evarestov, **Yu.F. Zhukovskii**, A.V. Bandura, **S. Piskunov**, and M.V. Losev, Symmetry and models of double-wall BN and TiO_2 nanotubes with hexagonal morphology. – J. Phys. Chem. C, 2011, **115**, p. 14067–14076.
2. **S. Piskunov**, T. Jacob, and E. Spohr, Oxygen adsorption at $La_{1-x}Sr_xMnO_3$(001) surfaces: Predictions from first principles. - Phys. Rev. B, 2011, **83**, 073402 (p. 1-4).
3. R.A. Evarestov, E. Blokhin, **D. Gryaznov**, **E.A. Kotomin**, and J. Maier, Phonon calculations in cubic and tetragonal phases of $SrTiO_3$: A comparative LCAO and plane-wave study. - Phys. Rev. B, 2011, **83**, 134108 (p. 1-9).
4. **V.N. Kuzovkov**, **E.A. Kotomin,** and **G. Zvejnieks**, Pattern formation kinetics for charged molecules on surfaces: microscopic correlation function analysis. - J. Phys. Chem. B, 2011, **115**, p. 14626–14633.
5. **E.A. Kotomin**, V. Aleksandrov, **D. Gryaznov**, R.A. Evarestov, and J. Maier, Confinement effects for ionic carriers in $SrTiO_3$ ultrathin films: first-principles calculations of oxygen vacancies. - Phys. Chem. Chem. Phys., 2011, **13**, p. 923-926.
6. **V.N. Kuzovkov**, **E.A. Kotomin**, and **G. Zvejnieks**, Atomistic theory of mesoscopic pattern formation induced by bimolecular surface reactions between oppositely charged molecules. - J. Chem. Phys., 2011, **135**, 224503 (p. 1-5).
7. **V.N. Kuzovkov**, **E.A. Kotomin**, and M. Olvera de la Cruz, The non-equilibrium charge screening effects in diffusion-driven systems with pattern formation. - J. Chem. Phys., 2011, **135**, 034702 (p. 1-6).
8. **E.A. Kotomin**, **Yu.A. Mastrikov**, M.M. Kuklja, R. Merkle, A. Roytburd, and J. Maier, First principles calculations of oxygen vacancy formation and migration in mixed conducting $Ba_{0.5}Sr_{0.5}Co_{1-y}Fe_yO_{3-\delta}$ perovskites - Solid State Ionics (2.496), 2011, **188**, p. 1-5.
9. S. Velgosh, B. Andriyevsky, I. Karbovnyk, I. Bolesta, O. Bovgyra, W. Ciepluch-Trojanek, I.V. Kityk, and **A.I. Popov**, First-principles simulations of the electronic density of states for superionic Ag_2CdI_4 crystals. - Solid State Ionics, 2011, **188**, p. 31-35.
10. H. Shi, R. Jia, and **R.I. Eglitis**, First-principles simulations on the aggregation of F centers in BaF_2: R center. - Solid State Ionics, 2011, **187**, p. 1-7.
11. E. Li, L. Hu, V. Igochine, **O. Dumbrajs**, and K. Chen, Understanding complex magnetohydrodynamic activities associated with a relaxation in the HT-7 tokamak. - Plasma Phys. Control. Fusion, 2011, **53**, 085019 (p. 1-13).
12. D. Constantinescu, **O. Dumbrajs**, V. Igochine, K. Lackner, R. Meyer-Spasche, H. Zohm, and ASDEX Upgrade Team, A low-dimensional model system for quasi-periodic plasma perturbations. - Phys. Plasmas (2.320), 2011, **18**, 062307 (p. 1-7).
13. V. Pankratov, **A.I. Popov**, L. Shirmane, A. Kotlov, and C. Feldmann, $LaPO_4$:Ce,Tb and YVO_4:Eu nanophosphors: Luminescence studies in the vacuum ultraviolet spectral range. - J. Appl. Phys., 2011, **110**, 053522 (p. 1-7).
14. **D. Bocharov**, **D. Gryaznov**, **Yu.F. Zhukovskii**, and **E.A. Kotomin**, DFT calculations of point defects on UN(001) surface. - Surf. Sci., 2011, **605**, p. 396-400.

15. **S. Piskunov**, **G. Zvejnieks**, **Yu.F. Zhukovskii**, and S. Bellucci, Atomic and electronic structure of both perfect and nanostructured Ni(111) surfaces: First-principles calculations. - Thin Solid Films, 2011, **519**, p. 3745–3751.

16. V. Pankratov, **A.I. Popov**, A. Kotlov, and C. Feldmann, Luminescence of nano- and macrosized $LaPO_4$:Ce,Tb excited by synchrotron radiation. - Opt. Mater., 2011, **33**, p. 1102–1105.

17. H. Shi, Y. Wang, R. Jia, and **R.I. Eglitis**, *Ab initio* calculations of the hydroxyl impurities in BaF_2. - Comput. Mater. Sci., 2011, **50**, p. 3101-3104.

18. **A. Gopejenko**, **Yu.F. Zhukovskii**, P.V. Vladimirov, **E.A. Kotomin**, and A. Möslang, Modeling of yttrium, oxygen atoms and vacancies in γ-iron lattice. - J. Nucl. Mater., 2011, **416**, p. 40-44.

19. **D. Bocharov**, **D. Gryaznov**, **Yu.F. Zhukovskii**, and **E.A. Kotomin**, *Ab initio* modeling of oxygen impurity atom incorporation into uranium mononitride surface and sub-surface vacancies. - J. Nucl. Mater., 2011, **416**, p. 200-204.

20. **V.N. Kuzovkov**, The Anderson localization problem, the Fermi–Pasta–Ulam paradox and the generalized diffusion approach. - Phys. Scr., 2011, **84**, 065002 (p. 1-8).

21. R.A. Evarestov, **Yu.F. Zhukovskii**, A.V. Bandura, and **S. Piskunov**, Symmetry and models of single-walled TiO_2 nanotubes with rectangular morphology. - Centr. Eur. J. Phys., 2011, **9**, p. 492-501.

22. A. Kalinko, A. Kotlov, A. Kuzmin, V. Pankratov, **A.I. Popov**, and L. Shirmane, Electronic excitations in $ZnWO_4$ and $Zn_xNi_{1-x}WO_4$ (x = 0.1 − 0.9) using VUV synchrotron radiation. - Centr. Eur. J. Phys., 2011, **9**, p. 432-437.

23. E. Klotins, **A.I. Popov**, V. Pankratov, L. Shirmane, and D. Engers, Polar nanoregions in $Pb(Mg_{1/3}Nb_{2/3})O_3$ (PMN):insights from a supercell approach. - Centr. Eur. J. Phys., 2011, **9**, p. 438-445.

24. **Yu.N. Shunin**, **Yu.F. Zhukovskii**, N. Burlutskaya, and S. Bellucci, Resistance simulations for junctions of SW and MW carbon nanotubes with various metal substrates. - Centr. Eur. J. Phys., 2011, **9**, p. 519-529.

25. A.F. Vassilyeva, **R.I. Eglitis**, **E.A. Kotomin**, and A.K. Dauletbekova, Ab initio calculations of the atomic and electronic structure of MgF_2 (011) and (111) surfaces. - Centr. Eur. J. Phys., 2011, **9**, p. 515-518.

26. **Yu.F. Zhukovskii**, **S. Piskunov**, **E.A. Kotomin**, and S. Bellucci, Simulations on the mechanism of CNT bundle growth upon smooth and nanostructured Ni as well as θ-Al_2O_3 catalysts. - Centr. Eur. J. Phys., 2011, **9**, p. 530-541.

27. **R.I. Eglitis**, First-principles calculations of the atomic and electronic structure of $CaTiO_3$ (111) surfaces, Ferroelectrics, 2011, **424**, p. 1-6.

28. V. Alexandrov, **S. Piskunov**, **Yu.F. Zhukovskii**, **E.A. Kotomin**, and J. Maier, First-principles modeling of oxygen interaction with $SrTiO_3$(001) surface: Comparative density-functional LCAO and plane-wave study. - Integr. Ferroelectr., 2011, **123**, p. 10-17.

29. E. Blokhin, **D. Gryaznov**, **E.A. Kotomin**, R.A. Evarestov, and J. Maier, A comparative hybrid DFT study of phonons in several $SrTiO_3$ phases. - Integr. Ferroelectr., 2011, **123**, p. 18-25.

30. **R.I. Eglitis**, *Ab initio* calculations of $SrZrO_3$ (001) surfaces. - Integr. Ferroelectr., 2011, **123**, p. 26-31.
31. E. Klotins, **A.I. Popov**, V. Pankratov, L. Shirmane, and D. Engers, Numerical evidences of polarization switching in PMN-type relaxor ferroelectrics. - Integr. Ferroelectr., 2011, **123**, p. 32-39.
32. **Yu.N. Shunin**, **Yu.F. Zhukovskii**, V.I. Gopejenko, N. Burlutskaya, and S. Bellucci, *Ab initio* simulations on electric properties for junctions between carbon nanotubes and metal electrodes. - Nanosci. Nanotechnol. Lett., 2011, **3**, Nr 6, p. 1-10.
33. **S. Piskunov** and E. Spohr, $SrTiO_3$ nanotubes with negative strain energy predicted from first principles. - J. Phys. Chem. Lett., 2011, **2**, p. 2566–2570.
34. **Yu.F. Zhukovskii**, R.A. Evarestov, A.V. Bandura, and M.V. Losev, First-principles calculations on double-walled inorganic nanotubes with hexagonal chiralities. - IOP Conf. Ser.: Mater. Sci. Eng., 2011, **23**, 012014 (p. 1-4).
35. M.M. Kuklja, **Yu.A. Mastrikov**, S.N. Rashkeev, and **E.A. Kotomin**, The structural disorder and lattice stability of $(Ba,Sr)(Co,Fe)O_3$ complex perovskites. - Electrochem. Soc. Transactions, 2011, **35**, p. 2077-2084.
36. **E.A. Kotomin**, R. Merkle, **Yu.A. Mastrikov**, M.M. Kuklja, and J. Maier, First principles modeling of oxygen mobility in perovskite SOFC cathode and oxygen permeation membrane materials. - Electrochem. Soc. Transactions, 2011, **35**, p. 823-830.
37. **Yu.N. Shunin**, **Yu.F. Zhukovskii**, N. Burlutskaya, and S. Bellucci, Theoretical simulations on electric properties of CNT-Me and GNR-Me interconnects using effective media approach. – Proc. Comput. Sci., 2011, **7**, p. 343–345.

Chapters in Scientific Books

1. E. Heifets, **E.A. Kotomin**, **Yu.A. Mastrikov**, **S. Piskunov**, and J. Maier, Thermodynamics of ABO3-type perovskite surface. - Chapter in a book: Thermodynamics - Interaction studies - Solids, liquids and gases (InTech Open Access Publishers), 2011, p. 491-518.
2. **V.N. Kuzovkov**, **E.A. Kotomin**, **G. Zvejnieks**, K.D. Li, T.H. Ding, and L.M. Wang, Void Superlattice Formation in Electron Irradiated Materials. - Chapter 11 in e-book Series: "Advances in Materials Science Research" (Ed. Maryann C. Wythers, Nova Science Publishers), 2011, Vol. 2, p. 191-216. pdf

Non-SCI

1. I. Karbovnyk, P. Savchyn, **A.I. Popov**, A. Huczko, M. Cestelli-Guidi, and C. Mirri, Infrared characterization of silicon carbide nanowires. - Nanomaterials: applications & properties. - Proc. Internat. Conf. "Nanomaterials: applications & properties (Alushta, Ukraine)" (Eds. A. Pogrebnjak, T. Lyutyy, and S. Protsenko, Publ. Sumy State University, Ukraine), 2011. Vol. 2, Part 1, p. 134-136.
2. S. Velgosh, I.Karbovnyk, I. Kityk, **A.I. Popov**, and I. Rovetskyy, Luminescence studies of the pure and In, Sb, and Sn doped cadmium iodide crystals. - Electronics and information technologies, 2011, Nr. 1, p. 36–43 (in Ukrainian, with English & Russian abstracts).

3. **Yu.F. Zhukovskii**, **E.A. Kotomin**, and **S. Piskunov**, "First-principles simulations on dissociative adsorption of methane molecules upon nickel substrate resulting in a growth of nanotubes". - Proc. Internat. Conf. „Physics, Chemistry and Application of Nanostructures (Nanomeeting-2011, Minsk, Belarus)" (Eds. V.E. Borisenko, S.V. Gaponenko, V.S. Gurin, and C.H. Kam; World Scientific, New Jersey, London, Singapore), 2011, p. 91-94.

4. **Yu.N. Shunin**, **Yu.F. Zhukovskii**, N. Burlutskaya, and S. Bellucci, "Theoretical simulation on electric properties of CNT-Me and GNR-Me interconnects". - Proc. Internat. Conf. „Physics, Chemistry and Application of Nanostructures (Nanomeeting-2011, Minsk, Belarus)" (Eds. V.E. Borisenko, S.V. Gaponenko, V.S. Gurin, and C.H. Kam; World Scientific, New Jersey, London, Singapore), 2011, p. 283-286.

Science popularization

1. **O. Dumbrajs**, Vai Vācija spēs izdzīvot bez kodolenerģijas? - Enerģija un pasaule, 2011, **5**, p. 66-69 (In Latvian).

2. **E. Kotomin**, European Materials Science Project in the Institute of Solid State Physics, University of Latvia. Diskusiju Forums, N4, Augusts 2011, lp.61.

3. V.I. Florovs, A. Cebers, D. Docenko, **D. Bocharov**, and **V. Kashcheyevs**, The 35th Open Olympiade of Latvia in Physics. - The Starry Sky, 2011, **211**, p. 40-46 (In Latvian)

4. V.I. Florovs, A. Cebers, **D. Bocharov**, J.Timošenko, D. Docenko, and **V. Kashcheyevs**, The 36th Open Olympiade of Latvia in Physics. - The Starry Sky, 2011, **214**, p. 38-44 (In Latvian).

Presentations at scientific conferences, congresses, meetings, schools and workshops

I. 27th ISSP Conference (Riga, Latvia, February, 2011).

1. A. Gopejenko, Yu.F. Zhukovskii, P.V. Vladimirov, E.A. Kotomin, and A. Möslang, „Ab initio calculations of binding energies between defects in fcc Fe lattice". Abstracts: p. 6.

2. O. Dumbrajs, „Nuclear power: history, status, prospects". Abstracts: p. 21.

3. D. Bocharov, Yu.F. Zhukovskii, G. Gryaznov, and E.A. Kotomin, "Oxygen diffusion processes on UN (001) surface". Abstracts: p. 23.

4. P. Merzlyakov, G. Zvejnieks, V.N. Kuzovkov, E.A. Kotomin, K.D. Li, and L.M. Wang, „Self-organization of vacancy clusters in CaF_2: experimental data analysis and theoretical modeling". Abstracts: p. 24.

5. V. Pankratov, A.I. Popov, S.A. Chernov, and C. Feldmann, "Mechanism for energy transfer processes between Ce^{3+} and Tb^{3+} in $LaPO_4$:Ce, Tb nanocrystals by time-resolved luminiscence spectroscopy". Abstracts: p. 44.

6. V. Pankratov, L. Shirmane, A.I. Popov, A. Kotlov, and C. Feldmann, „Luminescence of nano- and macrosized $LaPO_4$:Ce,Tb excited by synchrotron radiation". Abstracts: p. 45.

7. L. Shirmane, V. Pankratov, A.I. Popov, A. Kotlov, and C. Feldmann, „Luminescence properties of YVO_4:Eu^{3+} nanoctystals under synchrotron radiation". Abstracts: p. 47.

8. R.A. Evarestov, Yu.F. Zhukovskii, S. Piskunov, and A.V. Bandura, „Symmetry and models of single-wall inorganic nanotubes". Abstracts: p. 49.

9. E. Klotins, A.I. Popov, V. Pankratov, L. Shirmane, and D. Engers, „Polar nanoregions in $Pb(Mg_{1/3}Nb_{2/3})O_3$ (PMN)". Abstracts: p. 50.

10. A. Sorokin, D. Bocharov, S. Piskunov, and V. Kashcheyevs, „Quantum chemistry simulations of $LaAlO_3/SrTiO_3$ interface electronic structure". Abstracts: p. 133a.

II. 45th Russian School on Condensed State Physics (St. Petersburg, Russia, March, 2011).

11. D. Bocharov, D. Gryaznov, Yu.F. Zhukovskii, and E.A. Kotomin, „Quantum-chemical modeling of oxidation processes on surface of nitride nuclear fuel". Abstracts: p. 27.

12. D. Bocharov, A. Kuzmin, J. Purans, and Yu.F. Zhukovskii, „Interpretation of X-Ray absorption spectra using quantum chemistry methods". Abstracts: p. 28

***III. TMS-2011 Annual Meeting, Symposium on Computational Thermodynamics and Kinetics (San Diego, California, USA, February-March, 2011)**.*

13. R. Glass, D. Fuks, E.A. Kotomin, and J. Maier, "Thermodynamic analysis of phase transformations in $La_c\ Sr_{1-c}\ MnO_3$ perovskite solid solutions". Abstracts: p. 249.

IV. International conference "Functional materials and nanotechnologies" FM&NT-2011 (Riga, Latvia, April, 2011).

12. R. Merkle, L. Wang, Yu.A. Mastrikov, E.A. Kotomin, and J. Maier, "Mechanistic insight into oxygen exchange on mixed conducting oxides from experiments and theory". Abstracts: p. 13.

13. E.A. Kotomin, R. Merkle, Yu.A. Mastrikov, M.M. Kuklja, D. Fuks, and J. Maier, "First principles modeling of oxygen incorporation into oxygen permeation membranes and SOFC cathodes". Abstracts: p. 18.

16. Yu.F. Zhukovskii, D. Bocharov, D. Gryaznov, and E.A. Kotomin, "First-principles simulations on initial stage of uranium nitride surface oxidation". Abstracts: p. 20.

17. O. Dumbrajs, "European gyrotrons for ITER". Abstracts: p. 21

18. D. Gryaznov, M. Finnis, R.A. Evarestov, and J. Maier, "Thermodynamic calculations on defects in perovskites: DFT and frozen phonon method". Abstracts: p. 39.

19. E. Blokhin, D. Gryaznov, E.A. Kotomin, R.A. Evarestov, and J. Maier, "Phonon calculations in perfect and defective SrTiO3 perovskites". Abstracts: p. 65.

20. R.I. Eglitis, "Ab initio calculations of $SrTiO_3$, $BaTiO_3$, $PbTiO_3$, $CaTiO_3$, $BaZrO_3$, $SrZrO_3$ and $PbZrO_3$ (001) and (011) surfaces as well as Nb impurity segregation towards the SrTiO3 surface". Abstracts: p. 67.

21. Yu.N. Shunin, Yu.F. Zhukovskii, N. Burlutskaya, V.I. Gopeyenko, and S. Bellucci, "Theoretical simulations of fundamental properties of CNT-Me and GNR-Me interconnects for novel electronic nanodevices". Abstracts: p. 69.

22. I.D. Karbovnyk, V.M. Lesivtsiv, I.M. Bolesta, S.R. Velgosh, I.M. Rovetsky, V. Pankratov, and A.I. Popov, "The luminescence of BiI_3 nanoclusters embedded in CdI_2 layered crystals". Abstracts: p. 116.

23. A.I. Popov, V. Pankratov, D. Jakimovicha, E. Klotins, L. Shirmane, and A. Kotlov, "Luminiscence properties of $BaZrO_3$ perovskites under synchrotron radiation". Abstracts: p. 117.

24. A.I. Popov, V. Pankratov, V. Bratus, and A. Kotlov, "Electronic excitation and luminiscence of 3C-SiC pure and neutron-irradiated silicon carbide". Abstracts: p. 118.

25. A.I. Popov, V. Pankratov, A. Lushchik, E. Klotins, L. Shirmane, V.E. Serga, L.D. Kulikova, and A. Kotlov, "Comparative study of the luminiscence properties of macro and nanocrystalline MgO using synchrotron radiation". Abstracts: p. 119.

26. P.V. Savchyn, V.V. Vistovskyy, A.S. Voloshinovskii, V. Pankratov, A. Kotlov, and A.I. Popov, "Luminescence of Eu^{2+} doped $LaCl_3$ microcrystals embedded into NaCl host". Abstracts: p. 122.

27. A.F. Fix, R.I. Eglitis, E.A. Kotomin, A.K. Dauletbekova, and F.U. Abuova, "Ab initio calculations of bulk and surface F centers in MgF_2". Abstracts: p. 158.

28. F.U. Abuova, E.A. Kotomin, and A.K. Dauletbekova, "The electronic structure calculations of hole centers in MgF_2". Abstracts: p. 159.

29. R.I. Eglitis, H. Shi, and R. Jia, "Ab initio calculations of surface H centers in BaF_2". Abstracts: p. 160.

30. R.I. Eglitis, L. Yue, R. Jia, X. He, and H. Shi, "First-principles calculations for the H center in SrF_2 crystals". Abstracts: p. 161.

31. R.I. Eglitis, "Semi-empirical Hartree-Fock calculations for pure and Li-doped $KTaO_3$". Abstracts: p. 162.

32. A. Sorokin, Yu.F. Zhukovskii, J. Purans, and E.A. Kotomin, "Influence of Al and Ga dopants on electronic properties of ZnO: ab initio simulations". Abstracts: p. 164.

33. A. Gopejenko, Yu.F. Zhukovskii, P.V. Vladimirov, E.A. Kotomin, and A. Möslang, "Ab initio calculations of pair-wise interactions between defects for ODS steels". Abstracts: p. 165.

34. D. Bocharov, Yu.F. Zhukovskii, D. Gryaznov, and E.A. Kotomin, "UN (110) surface properties: ab initio calculations". Abstracts: p. 166.

35. D. Gryaznov, E. Heifets, and E.A. Kotomin," Density functional theory calculations on magnetic properties of actinide compounds". Abstracts: p. 167.

36. E. Klotins, A.I. Popov, and V. Pankratov, "Density functional theory beyond translational invariance: Discrete variable representation". Abstracts: p. 168.

37. R.A. Evarestov, Yu.F. Zhukovskii, S. Piskunov, A.V. Bandura, and M.V. Losev, "First-principles simulations on double-wall BN and TiO_2 nanotubes with hexagonal morphology". Abstracts: p. 170.

38. N.A. Zaporina, J. Grabis, A. Krumina, M. Maiorov, G. Heidemane, and D. Bocharov, "Methods of obtaining nanodisperse Ni ferrite, their structure and magnetic properties". Abstracts: p. 183.

V. 9th International Conference "Information Technologies and Management", IT&M'2011 (Riga, Latvia, April, 2010).

39. Yu.F. Zhukovskii, "Simulation on multi-wall inorganic nanostructures with spherical (0D) and cylindrical (1D) morphology". Abstracts: p. 18-20.

40. A. Gopejenko, Yu.F. Zhukovskii, P.V. Vladimirov, E.A. Kotomin, and A. Möslang, "Interactions between Y and O impurity atoms as well as Fe vacancies in iron lattice: Ab initio modeling". Abstracts: p. 46.

41. Yu.N. Shunin, Yu.F. Zhukovskii, N. Burlutskaya, V.I. Gopeyenko, and S. Bellucci, "Theoretical simulations on fundamental properties of CNT-Me and GNR-Me interconnects". Abstracts: p. 131-132.

VI. Spring European Materials Research Society (E-MRS) Meeting (Nice, France, May, 2011).

42. R.I. Eglitis, "Ab initio calculations of $SrTiO_3$, $BaTiO_3$, $PbTiO_3$, $CaTiO_3$, $BaZrO_3$, $SrZrO_3$ and $PbZrO_3$ (001) and (011) surfaces as well as Nb impurity segregation towards the surfaces/interfaces". Abstracts: AA-6.

43. R.I. Eglitis, H. Shi, and R. Jia, "Ab initio calculations of surface H centers in BaF_2". Abstracts: BP2-25.

44. E.A. Kotomin, D. Gryaznov, R.A. Evarestov, V.E. Alexandrov, and J. Maier, "Confinement effects for ionic carriers in perovskite ultrathin films". Abstracts: CL-4

45. Yu.N. Shunin, Yu.F. Zhukovskii, N. Burlutskaya, and S. Bellucci, "Electric properties of junctions between 1D carbon nanostructures and metal substrate: theoretical simulations". Abstracts: EP-8.

46. V. Pankratov, A.I. Popov, and E.A. Kotomin, "Polarons in complex oxides". Abstracts: LP-15.

47. A.I. Popov, E.A. Kotomin, V. Pankratov, and J. Maier, "Generalization of Rabin-Klick diagram for a whole family of alkali halides". Abstracts: LP-16.

48. L. Petit, A. Svane, E.A. Kotomin, and D. Gryaznov, "First-principles calculations of the electronic and atomic structures of radiation defects in PuO_2". Abstracts: L6-2.

49. A. Gopejenko, Yu.F. Zhukovskii, P.V. Vladimirov, V.A. Borodin, E. A. Kotomin, and A. Möslang, "Modelling of interactions between Y, O and vacancy clusters in fcc Fe lattice". Abstracts: VP-7.

50. D. Bocharov, Yu.F. Zhukovskii, D. Gryaznov, and E.A. Kotomin, "First-principles simulations on initial stages of UN(001) surface oxidation". Abstracts: V4-17.

51. D. Gryaznov, M.W. Finnis, and J. Maier, "First principles DFT calculations on $La_{0.875}Sr_{0.125}Co_xFe_{1-x}O_3$ and point defects therein". Abstracts: X13-3.

52. E.A. Kotomin, R. Merkle, Yu.A. Mastrikov, M.M. Kuklja, D. Fuks, S.N. Rashkeev, and J. Maier, "First-principles modeling of oxygen incorporation into SOFC cathode and permeation membranes". Abstracts: X13-5.

VII. 219th Meeting of Electrochemical Society (Montreal, Canada, May, 2011).

53. E.A. Kotomin, R. Merkle, Yu.A. Mastrikov, M.M. Kuklja, and J. Maier, "First principles modeling of oxygen mobility in perovskite SOFC cathode and oxygen permeation membrane materials". Abstracts B7-976.

54. M.M. Kuklja, Yu.A. Mastrikov, N. Rashkeev, and E.A. Kotomin, "The structural disorder and lattice stability of $(Ba,Sr)(Co,Fe)O_3$ complex perovskites". Abstracts: B7-839.

VIII. Science for Our Nation's Energy Future: Summit and Forum (Washington, D. C., USA, May, 2011).

55. P.K. Jha, V. Kuzovkov, B.A. Grzybowski, and M. Olvera de la Cruz, "Light induced self assembly of switchable colloids". Abstracts: P1-H24.

IX. International Conference NANOMEETING-2011 (Minsk, Belarus, May, 2011).

56. Yu.F. Zhukovskii, E.A. Kotomin, and S. Piskunov, "First-principles simulations on dissociative adsorption of methane molecules upon nickel substrate resulting in a growth of nanotubes".

57. Yu.N. Shunin, Yu.F. Zhukovskii, N. Burlutskaya, and S. Bellucci, "Theoretical simulation on electric properties of CNT-Me and GNR-Me interconnects".

X. The Future European Technologies Conference, FET'2011 (Budupest, Hungary, May, 2011).

58. Yu.N. Shunin, Yu.F. Zhukovskii, N. Burlutskaya, and S. Bellucci, "Theoretical simulations on electric properties of CNT-Me and GNR-Me interconnects using Effective Media Approach".

XI. Regional Conference "Nuclear energy - global trends and perspectives in south-east Europe" (Podgorica, Montenegro, May, 2011).

59. O. Dumbrajs, "Nuclear fission and fusion: rivals or companions?".

XII. NATO Advanced Research Workshop "Nanomaterials and Nanodevices for Ecological Security" (Jurmala, Latvia, June, 2011).

60. Yu.N. Shunin, Yu.F. Zhukovskii, N. Burlutskaya, and S. Bellucci, "Simulation of fundamental properties of CNT-metal interconnects for development of new sensor systems". Abstracts: OA5.

61. Yu.F. Zhukovskii, "Nanoelectronic devices containing isolated arrays of CNTs contacting to metallic substrate and their ecological advantage as compared to nowadays microelectronic deviced". Abstracts: OA6.

62. R.I. Eglitis, "Ab initio calculations of $SrTiO_3$, $BaTiO_3$, $PbTiO_3$, $CaTiO_3$, $BaZrO_3$, $SrZrO_3$, $PbZrO_3$ (001) and (011) nano-surfaces as well as Nb impurity segregation towards the perovskite nano-surfaces". Abstracts: OB-7.

63. V. Pankratov, A.I. Popov, and L. Shirmane, "Luminescence properties of nanosized phosphors under synchrotron radiation". Abstracts: PB04.

64. A.I. Popov, V. Pankratov, L. Shirmane, E. Klotins, and A. Kotlov, "Synchrotron radiation studies on luminescence properties of macro- and nano-sized $MgAl_2O_4$". Abstracts: PB05.

65. A. Gopejenko, Yu.F. Zhukovskii, P.V. Vladimirov, E.A. Kotomin, and A. Möslang, "Interaction of O and Y impurity atoms as well as Fe lattice: Ab initio modeling". Abstracts: PB06.

XIII. CECAM workshop on Understanding Structure and Functions of Reducible Oxide Systems (Zaragoza, Spain, June, 2011).

66. E.A. Kotomin, R. Merkle, J. Maier, Yu. Mastrikov, and M.M. Kuklja, "First-principles simulations of oxygen defects in reducible perovskites". Abstracts: p. 38.

XIV. Annual Monitory Meeting of European Fusion Development Agreement, EFDA - 2011 (Frascati, Italy, June, 2011).

67. Yu.A. Mastrikov, Yu.F. Zhukovskii, E.A. Kotomin, P.V. Vladimirov, and A. Möslang, "Models of point defects in bcc-Fe lattice for simulation of ODS nanocluster".

XV. International Symposium on Reactivity of Solids (Bordeaux, France, June-July, 2011).

68. R. Merkle, L. Wang, Yu. Mastrikov, E.A. Kotomin, and J. Maier, "Mechanistic insight into oxygen exchange on mixed conducting oxides from experiments and theory". Abstracts: O2

XVI. 18th International Conference on Solid State Ionics (Warsaw, Poland, July, 2011).

69. E.A. Kotomin, R. Merkle, Yu.A. Matrikov, M.M. Kuklja, and J. Maier, "First princliples modeling of oxygen vacancy formation and mobility in (Ba,Sr)(Co,Fe)O_{3-d} perovskites".

XVII. 8th International Workshop "Strong Microwaves and Teraherz Waves: Sources and Applications" (Nizhny Novgorod, Russia, July, 2011).

70. D. Constantinescu, O. Dumbrajs, V. Igochine, K. Lackner, R. Meyer-Spasche, H. Zohm, and ASDEX Upgrade team, "A low-dimensional model system for quasi-periodic plasma perturbations".

XVIII. 16th International conference on Radiation Effects in Insulators, REI-16 (Beijing, China, August, 2011).

71. E.A. Kotomin, D. Gryaznov, R.A. Evarestov, V.E. Alexandrov, and J. Maier, "Confinement effects for oxygen vacancies in nanosized perovskites". Abstracts:.O-7, p. 49.

72. A.I. Popov, E.A. Kotomin, J. Maier, A.Ch. Lushchik, and Ch.B. Lushchik, "Analysis of excitonic mechanism of radiation-induced defect formation in insulating materials". Abstracts: O-1, p. 43.

73. D. Gryaznov, E.A. Kotomin, and S.N. Rashkeev, "GGA+U modeling of basic radiation defects in MOX nuclear fuels". Abstracts: PA-28, p. 124.

XIX. International Symposium on Nano and Giga Challenges in Electronics, Photonics and Renewable Energy, NGC2011 (Moscow, Russia, September, 2011).

74. Yu.N. Shunin, Yu.F. Zhukovskii, N. Burlutskaya, V.I. Gopeyenko, and S. Bellucci, "Theoretical simulations on electronic transport properties of CNT-Me and GNR-Me interconnects". Abstracts: OCMS-4.

XX. International Workshop on Nanoscience and Nanotechnology, n&n-2011 (Frascati, Italy, September, 2011).

75. Yu.N. Shunin, Yu.F. Zhukovskii, V.I. Gopeyenko, N. Burlutskaya, and S. Bellucci, "Simulations on electromagnetic properties for CNT- and GNR-metal interconnect". Abstracts: p. 56-59.

76. Yu.F. Zhukovskii, S. Piskunov, and S. Bellucci, "Theoretical simulations on inter-shell interactions in double-wall carbon nanotubes of different morphology". Abstracts: p. 74-77.

XXI. E-MRS 2011 Fall Meeting (Warsaw, Poland, September, 2011).

77. R. I. Eglitis, "First-principles calculations of $SrTiO_3$, $BaTiO_3$, $PbTiO_3$, $CaTiO_3$, $BaZrO_3$, $SrZrO_3$ and $PbZrO_3$ (001) and (011) surfaces as well as Nb impurity segregation towards the perovskite surfaces". Abstracts: K IX-4.

78. R. I. Eglitis, H. Shi, R. Jia, L. Yue, and X. He, "Ab initio calculations of H center in SrF_2, surface H centers and aggregation of F centers in BaF2". Abstracts: G III-4.

79. R. I. Eglitis, "Ab initio calculations of $PbZrO_3$ (001) and (011) surfaces as well as oxygen vacancy at ZrO_2-terminated (001) surfaces". Abstracts: H H-33.

XXII. School „Synergy between modelling and experiments for the investigation of nuclear fuels" (Cambridge, UK, September, 2011).

80. D. Bocharov, Yu.F. Zhukovskii, D. Gryaznov, and E.A. Kotomin, "A comparative study of the UN (100) and (110) surfaces: first principles DFT calculations".

XXIII. European Congress on Advanced Materials and Processes, EUROMAT-2011 (Montpellier, France, September, 2011).

81. A. Weizman, D. Fuks, E.A. Kotomin, and J. Maier, "Ab-initio thermodynamic analysis of the (La,Sr)CoO_3 solid solutions".

XXIV. 1st International conference "Nanomaterials: applications & properties" (Alushta, Ukraine, September, 2011).

82. I. Karbovnyk, P. Savchyn, A.I. Popov, A. Huczko, M. Cestelli-Guidi, and C. Mirri, "Infrared characterization of silicon carbide nanowires".

XXV. Materials Science and Technology, MS&T-2011 (Columbus, Ohio, USA, October, 2011).

83. E.A. Kotomin, D. Gryaznov, L. Petit, and A. Svane, "First principles calculations of the electronic and atomic structure of radiation defects in PuO_2". Abstracts: p. 97.

84. E.A. Kotomin, D. Gryaznov, E. Blokhin, R.A. Evarestov, V. Alexandrov, and J. Maier, "Confinement effects for ionic carriers in $SrTiO_3$ ultrathin films". Abstracts: p. 61.

85. E.A. Kotomin, R. Merkle, Yu.A. Mastrikov, M.M. Kuklja, and J. Maier, "First principles calculations of oxygen incorporation into SOFC cathode materials". Abstracts: p. 89.