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

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

MsC students

14. J. Shirmane

Scientific visits abroad

1. Dr. hab. E. Kotomin, Max Planck Institute for Solid State Research, Stuttgart, Germany (8 months), The Eurasian University, Astana, Kazakhstan (2 weeks).
2. Dr. hab.V. Kuzovkov; Northwestern University, Evanston, USA (3.5 months).
3. Dr. O. Dumbrajs, Max-Planck Institut für Plasmaphysik, Garching, Germany (1 month), University of Maryland, USA (1 month), University of Fukui, Japan (3 months), Karlsruhe Institute of Technology, Germany (1 month).
4. Dr. D. Gryaznov, Max Planck Institute for Solid State Physics, Stuttgart, Germany (7 months), Imperial College London, UK (2 months)
5. Dr. Yu. Mastrikov, University of Maryland, USA (10 months).

6. Dr. S. Piskunov, University of Duisburg-Essen (1 month).
7. Dr. A. Popov, Max Planck Institute for Solid State Research, Stuttgart, Germany (2 months), Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany (10 weeks)
8. Dr. Yu. Zhukovskii, Institute for Materials Research-I, Karlsruhe, Germany (1 month), St. Petersburg State University, Russia (1 week), Technical University of Braunschweig, Germany (3 weeks)
9. D. Bocharov, EC Institute of Transuranum Elements, Karlsruhe, Germany (1 week).
10. A. Gopejenko, Forschungszentrum Karlsruhe, Institut für Materialforschung I, Karlsruhe, Germany (2 months).

International Cooperation

France	1. Laue-Langevin Institute, Grenoble (Dr. G.J. McIntyre, Dr. H. Schober)
Germany	2. Max Planck Institut für Festkörperforschung, Stuttgart (Prof. Dr. J. Maier) 3. Physikalisch-Technische Bundesanstalt, Braunschweig (Dr. Bernd Kästner). 4. Max Planck Institut für Plasmaphysik, Garching (Prof. Dr. H. Zohm) 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)
Greece	10. School of Electrical and Computer Engineering, National Technical University of Athens, Zographou (Dr. K. Avramides)
Israel	11. Ben Gurion University, Beer Sheeva (Prof. A. Aharony, Prof. D. Fuks)
Italy	12. Laboratori Nazionali di Frascati (Dr. S. Bellucci, Dr. M. Cestelli-Guidi)
Japan	13. FIR Center, University of Fukui (Prof. T. Idehara)
Lithuania	14. Institute of Semiconductor Physics (SPI), Vilnius (Dr. E. Tornau)
Poland	15. Warwaw University, Dept of Chemistry (Dr A. Huczko)
Romania	16. University of Craiova (Dr. D. Constantinescu)
Russia	17. St. Petersburg University (Prof. R.A. Evarestov)
UK	18. Imperial College London (Prof. M.Finnis) 19. University College London (Prof. A.L. Shluger)
Ukraine	20. National University of Lviv (Prof. I. Bolesta and Prof. V. Savchyn)
USA	21. Idaho National Laboratory (Dr. S.N. Rashkeev) 22. Northwestern University, Evanston, Illinois (Prof. M.Olvera de la Cruz, Prof. D.E. Ellis) 23. University of Maryland, College Park (Dr. G.S. Nusinovich, Dr. M.M. Kukla)

Main Results

THE MICROSCOPIC APPROACH TO KINETICS OF PATTERN FORMATION OF CHARGED MOLECULES ON SURFACES/INTERFACES

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

Patterning of surfaces is of paramount importance in biophysics, chemistry, technology. In particular, charged patterns generated by the adsorption of cationic and anionic molecules on surfaces and on membranes is of great importance in electrochemistry and biosciences.

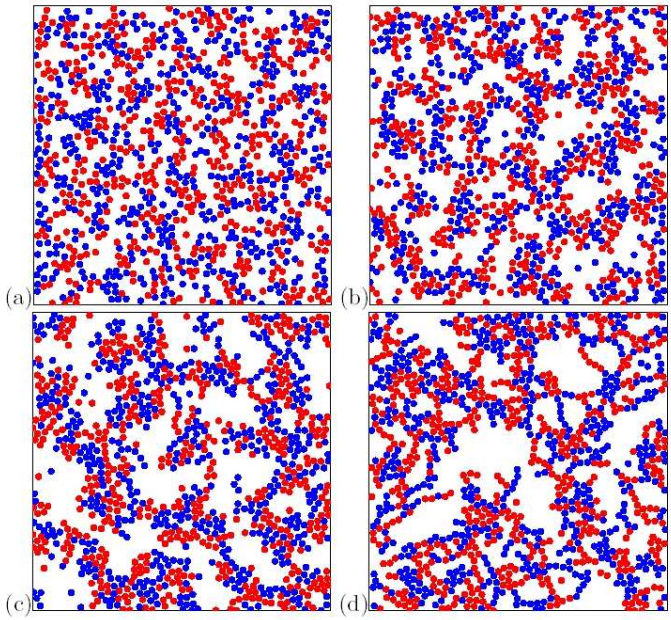

Fig.1. Fragments of the characteristic snapshots obtained using the reverse Monte Carlo for the correlation functions

In collaboration with Northwestern University, Evanston, USA, a microscopic formalism based on computing many-particle densities was applied to the analysis of the diffusion-controlled kinetics of pattern formation of oppositely-charged molecules on surfaces or adsorbed at interfaces with competing long-range Coulomb and short-range Lennard-Jones interactions. Particular attention was paid to the proper molecular treatment of energetic interactions driving pattern formation in inhomogeneous systems. The reverse Monte Carlo method is used to visualize the spatial molecular distribution based on the calculated radial distribution functions (joint correlation functions). We have shown the formation of charge domains for certain combinations of temperature and dynamical interaction parameters. The charge segregation evolves into quasi-crystalline clusters of charges, due to the competing long- and short-range interactions.

FIRST-PRINCIPLES CALCULATIONS ON SINGLE-WALLED BN AND TiO_2 NANOTUBES AND THEIR SYMMETRY ANALYSIS

Yu. Zhukovskii, S. Piskunov,
R.A. Evarestov, A.V. Bandura (*Department of Quantum Chemistry, St. Petersburg University, Russia*)

Use of the line group formalism allows us the construction of nanotubes of different crystalline morphology. The exploitation of the rotohelical symmetry for NTs permits drastic reductions of the computation time. A new approach to the generation of the line group irreducible representations developed *in collaboration with Prof. R.A. Evarestov and Dr. A.V. Bandura (St. Petersburg University, Russia)* is based on the isomorphism between line and plane groups. The application of the approach has been used for thorough theoretical description of BN and TiO_2 single-wall (SW) nanotubes (NTs) of both hexagonal and centered rectangular morphologies.

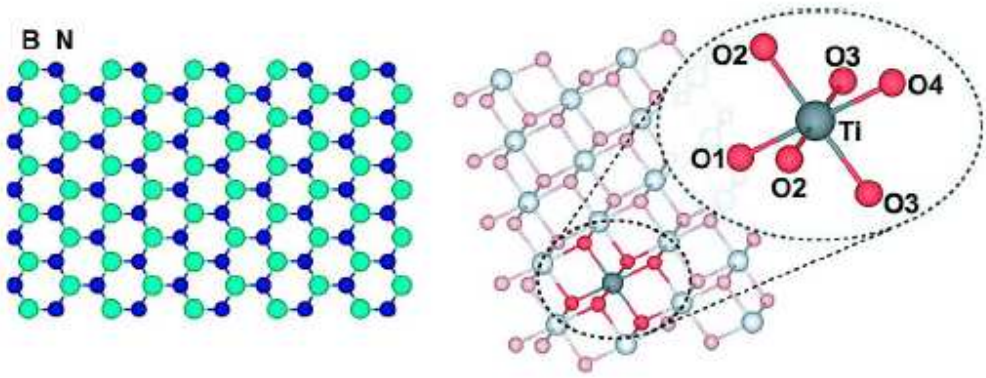

Fig. 2. Stoichiometric hexagonal sheets of BN(0001) and TiO_2(111) scrolling to SW NTs

Large scale *ab initio* LCAO calculations have been performed for the analysis of the atomic and electronic structure of BN and TiO_2 2D sheets and 1D nanotubes produced from the former by rolling up. For this aim, there was applied the hybrid Hartree-Fock/Kohn-Sham exchange-correlation functional *PBE0* with the total geometry relaxation as implemented in the *CRYSTAL* code. To optimize the atomic basis sets, necessary for the proper calculations there was applied the original program package *OPTBAS* interfaced with *CRYSTAL* code. The strain energies of SW BN and TiO_2 nanotubes of different chiralities have been found to be reduced with increasing NT diameter approaching to minimum energy limit beginning with nanotube diameter > 2 nm while their energy band gaps approach to those for the corresponding 2D slabs. To gain a deeper theoretical insight into the technologically important BN and TiO_2 nanomaterials, the next step is outlined to be simulations on the double-wall boron nitride and titania nanotubes.

POINT DEFECT MODELLING IN NUCLEAR FUELS

D. Gryaznov, Yu. Mastrikov, Yu. Zhukovskii, E. Kotomin,
P. Van Uffelen (*EC Institute for Transuranium Elements, Karlsruhe, Germany*)
S.N. Rashkeev (*Idaho National Laboratory, USA*)
E. Heifets (*Max Planck Institute, Stuttgart, Germany*)

UO_2 and $(U,Pu)O_2$ solid solutions (the so-called MOX) nowadays are used as commercial nuclear fuels. One of the safety issues during the storage of these fuels is related to their self-irradiation that produces and accumulates point defects and helium therein. *In close collaboration with Dr S. Rashkeev (Idaho National Laboratory) and Dr Van Uffelen (EC Institute for Transuranium Elements, Karlsruhe, Germany)* we have performed DFT calculations on UO_2, PuO_2 and MOX crystalline solids containing He atoms in octahedral interstitial positions.

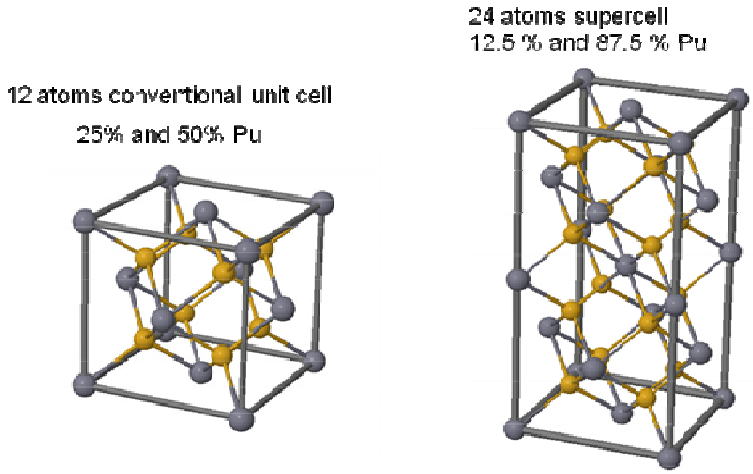

Fig.3. Two models of Pu atom substitutes for U in MOX solid solutions.

In particular, we have calculated the basic MOX properties and He incorporation energies as functions of Pu concentration within the spin-polarized, generalized gradient approximation (GGA) DFT calculations. We have also included the on-site electron correlation corrections using the Hubbard model (in the framework of the so-called DFT + U approach). We have found that PuO_2 remains semiconducting with helium impurity atom in the octahedral position while UO_2 requires a specific lattice distortion. Both materials reveal a positive energy for He atom incorporation, which, therefore, is an exothermic process. He incorporation energy increases with the Pu concentration in the MOX fuel.

COMPUTER MODELLING OF IMPURITY CLUSTERS IN ODS STEELS

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

Development of the oxide dispersion strengthened (ODS) steels for fission and fusion reactors requires a deep understanding of the mechanism and kinetics of Y_2O_3 nanoparticle

precipitation in the steel matrix. Therefore, it is necessary to perform a large-scale theoretical modeling of the Y_2O_3 formation. A series of first principles calculations were performed in *collaboration with Dr. A. Möslang and Dr. P.V. Vladimirov (Institut für Materialforschung I, Karlsruhe, Germany)* on different nanoclusters consisting of pair and triple solute atoms and containing: (*i*) the Y−Fe-vacancy pairs, (*ii*) the two Y atoms substituted for Fe lattice atoms and (*iii*) the O impurity atoms dissolved in *fcc*-Fe matrix. The latter is represented by a face-centered cubic γ-Fe single crystal. This structure is relevant because a phase transition $\alpha \rightarrow \gamma$ occurs in low Cr ferritic-martensitic steels at typically hot isostatic pressing temperatures. The results clearly demonstrate a certain attraction between the Y substitute and Fe vacancy whereas no binding has been found between the two Y substitute atoms. Results of calculations on different Y-O-Y cluster configurations in lattice show that not only a presence of oxygen atom favors a certain binding between the impurity atoms inside the γ-Fe lattice but also the increased concentration of Fe vacancies is required for the growth of the Y_2O_3 precipitates within the iron crystalline matrix

FIRST-PRINCIPLES CALCULATIONS OF COMPLEX PEROVSKITES FOR FUEL CELLS AND PERMEATION MEMBRANE APPLICATIONS

E. A. Kotomin, D. Gryaznov,
J. Maier, R. Merkle, V. Alexandrov, E. Heifets (*Max Planck Institute, Stuttgart, Germany*)
Yu.Mastrikov, M.M.Kuklja (*Maryland University, USA*)
M.Finnis (*Imperial College London, UK*)

Mixed conducting ABO_3-type perovskites have been used as cathode materials in solid oxide fuel cells (SOFC) since early 1980s, and $La_{1-x}Sr_xMnO_{3\pm\delta}$ (LSM) was the first material which found wide application. Currently, $Ba_{0.5}Sr_{0.5}Co_{0.75}Fe_{0.25}O_{3-\delta}$ (BSCF) shows the best oxygen exchange performance, despite several drawbacks. As it is well understood now, *both* high oxygen vacancy concentration at the SOFC cathode surface and high vacancy mobility are two key factors controlling high BSCF material performance.

While vacancy concentrations and mobilities in the materials bulk are available from experiments, the respective quantites for the surface layer - which are decisive for the surface reaction - are almost impossible to be measured. Thus, *in collaboration with the Max Planck Institute, Stuttgart, Germany, and Maryland University, USA*; we performed an extensive set of large-scale first principles DFT calculations. We have analyzed the atomic and electronic structure of oxygen vacancies, their formation and migration energies in the bulk and in the surface layer and how these properties depend on the chemical composition of the host perovskite. We have shown that optimal BSCF chemical composition is 50-50-80-20 percent.

In collaboration with Prof. M. Finnis (Imperial College London) a detailed study of the electron correlation effects was performed for the pure and defective $LaCoO_3$ and $(La,Sr)(Co,Fe)O_3$. In particular, the results of the electronic and magnetic structure obtained using the GGA+U and hybrid exchange-correlation functionals were compared, the oxygen vacancy formation energy estimated as a function of the temperature.

FIRST-PRINCIPLES CALCULATIONS OF PURE AND DEFECTIVE PEROVSKITE AND FLUORITE SURFACES

R. Eglitis, E.A. Kotomin,
M. Rohlfing (*Universität Osnabrück, Germany*)
H. Shi, X. He (*School of Science, Beijing Institute of Technology, China*)
R. Jia (*Bergische Universität Wuppertal, Germany*)
A. Vassilyeva, A. Dauletbekova (*L. Gumilyov National University, Astana, Kazakhstan*)

In collaboration with University of Osnabruck, Germany, we performed calculations of the surface relaxations, rumplings, energetics, optical band gaps, and charge distribution for the $SrZrO_3$ and $PbZrO_3$ (001) and (011) surfaces using the *ab initio* code CRYSTAL and a hybrid exchange-correlation functionals. Both SrO(PbO) and ZrO_2 terminations of the (001) surface and Sr(Pb), ZrO, and O terminations of the polar $SrZrO_3$and $PbZrO_3$ (011) surfaces were studied. We predict a considerable increase in the Zr-O chemical bond covalency near the $SrZrO_3$ and $PbZrO_3$ (011) polar surfaces as compared to both the bulk and to the (001) surface.

We have calculated also properties of Nb impurities substituting for Ti ions in $SrTiO_3$ perovskite using supercells containing 135 atoms. The local structure optimisation, the electronic charge redistribution, chemical bond covalence and the band-structure changes induced by the defects were analyzed. According to the results of our calculations, Nb is a shallow donor; six nearest O atoms are slightly displaced outwards from the Nb ion. The calculated bond population between nearest Ti and O ions (64 me) is much larger than that between Nb and O ions (8 me), since Nb impurity is more ionic than the host Ti.

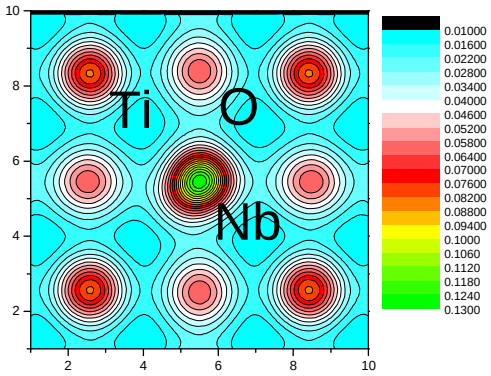

Fig.4. Charge density map of Nb doped SrTiO3 bulk from (001) side view

Similar calculations were also performed *in collaboration with L.Gumilyov University, Kazakhstan* for optical materials-- MgF_2 (001) and (011) surfaces. These neutral and polar surfaces show very small relaxation and negligible increase of covalent contribution to the chemical bonding thus remaining considerably ionic. The calculated bulk optical band gap is in a good agreement with the experimental value, whereas optical band gap for the polar (011) surface is reduced by 0.6 eV compared with the calculated bulk value, in contrast to the (001) surface gap which remains very close to the bulk.

The ground state of interstitial F ions (*H*-centrers) was calculated in SrF_2 for two different arrangements, which are oriented along either [100] or [111] axes. The local atomic relaxation and charge redistribution are discussed. Lastly, we studied also two different configurations of the *H* center at the BaF_2 (111) surface which considerably differ in the electron density, lattice relaxation and spin distributions.

ON THE THEORY OF HIGH-POWER GYROTRONS WITH UPTAPERED RESONATORS

O. Dumbrajs,
G.S. Nusinovich (*Institute for Research in Electronics and Applied Physics, University of Maryland, USA)*

In high-power gyrotrons it is desirable to combine an optimal resonator length with the optimal value of the resonator quality factor. In resonators with the constant radius of the central part, the possibilities of this combination are limited because the quality factor of the resonator sharply increases with its length. Therefore, the attempts to increase the length for maximizing the efficiency leads to such increase of the quality factor which makes the optimal current too small. Resonators with slightly uptapered profiles offer more flexibility in this regard. In such resonators, one can separate optimization of the interaction length from optimization of the quality factor, because the quality factor determined by diffractive losses can be reduced by increasing the angle of uptapering.

These issues were analyzed *in collaboration with Maryland University*, by studying a typical high-power $170GHz$ gyrotron which is currently under development in Europe for ITER (http://en.wikipedia.org/wiki/ITER). The effect of a slight uptapering of the resonator wall on the efficiency enhancement and the purity of the radiation spectrum in the process of the gyrotron start-up and power modulation are studied. Results show that optimal modification of the shape of a slightly uptapered resonator may result in increasing the gyrotron power from $1052kW$ to $1360kW$.

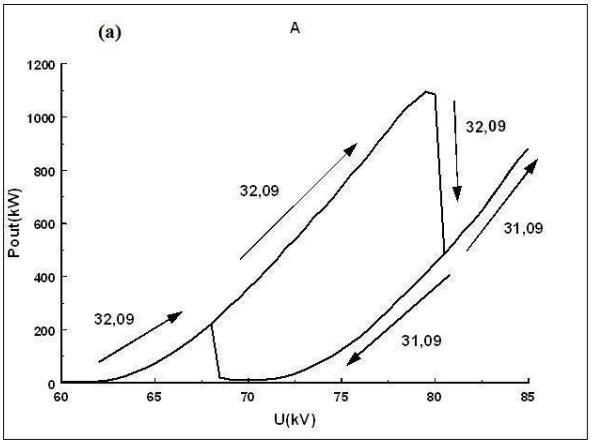

Fig. 5. Output power as a function of voltage in a gyrotron with the cavity ***A***. Calculations were carried out from $60kV$ to $85kV$ and from $85kV$ to $60kV$. The parasitic $TE_{31,09}$

parasitic is excited at $80.5kV$. Due to the hysteresis, this mode survives when the voltage decreases until $64.5kV$ where the operating $TE_{32,09}$ mode reappears. A clear hysteresis loop can be observed.

STRUCTURE AND DYNAMICS OF SAWTEETH CRASHES IN ASDEX UPGRADE

O. Dumbrajs,
V. Igochine, S. Günter, H. Zohm, K. Lackner, G. Pereverzev (*MPI für Plasmaphysik, Garching, Germany*)
J. Boom, I. Classen (*FOM-Instituut voor Plasmafysica Rijnhuizen, Nieuwegein, The Netherlands*)

The crash phase of the sawteeth in ASDEX Upgrade tokamak was investigated in detail by means of soft X-ray (SXR) and electron cyclotron emission (ECE) diagnostics. Analysis of pre-cursor and post-cursor (1,1) modes shows that the crash does not affect the position of the resonant surface q=1. Our experimental results suggest that sawtooth crash models should contain two ingredients to be consistent with experimental observations: (1) the (1,1) mode structure should survive the crash; (2) the flux changes should be small to preserve the position of the q=1 surface close to its original location. Detailed structure of the reconnection point was investigated with ECE imaging diagnostic. It is shown that reconnection starts locally. The expelled core is hot which is consistent with SXR tomography results. The observed results can be explained in the framework of a stochastic model.

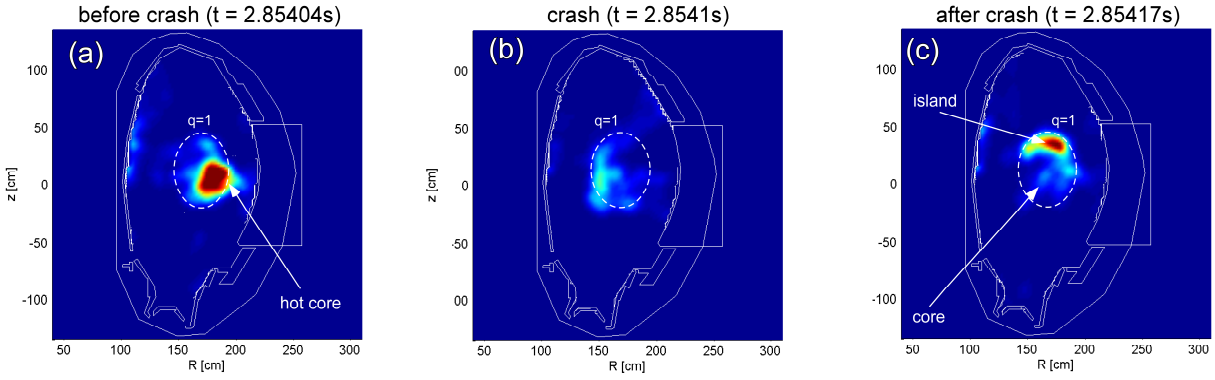

Fig.6. Soft X-ray tomography of the sawtooth crash (#25854, t=2.85s). Three different time frames are shown: (a) hot core rotates in clockwise direction before the crash; (b) crash phase; (c) hot island rotates in clockwise direction after the crash. q=1 position is marked by the dashed line. (Each figure has its own color scheme to increase the contrast.)

It should be noted that electrons with different azimuthal coordinates of guiding centers exhibit different dynamics in the process of mode switching. This can be considered as a specific feature of the electron interaction with the fields of more than one mode. In the

case of single-mode operation, electrons with different azimuthal coordinates of guiding centers exhibit the same behavior in the phase space. However, in the process of mode switching, where two modes are present, electron dynamics depends on the azimuthal coordinate of the guiding center. This can be explained by the fact that the phase difference of these modes is azimuthally dependent. This conclusion can be illustrated by the right figure in the second row in Fig. 2 showing electron distribution at the exit for *t=72*

DESIGN OF AN OPTIMIZED RESONANT CAVITY FOR A COMPACT SUB-TERAHERTZ GYROTRON)

O. Dumbrajs,
T. Idehara, S. Sabchevski (*Research Center for Development of Far-Infrared Region, University of Fukui, Japan*)

Coherent sources of radiation in the sub-terahertz and the terahertz frequency range are in great demand for various spectroscopic studies (e.g. electron spin resonance spectroscopy, DNP/NMR spectroscopy *etc*.). The required levels of the output power as well as the needed specific spectral characteristics make the gyrotrons the most promising and high-performance devices for such applications. Recently, an initial design of a versatile second harmonic gyrotron utilizing a compact cryo-free 8T superconducting magnet has been accomplished. *In collaboration with the University of Fukui, Japan,* we presented an optimized resonator for this gyrotron. Instead of a regular (cylindrical) part as in the conventional cavities it contains an uptapered section. Such configuration offers a significant increase of the efficiency and improves the overall performance of the tube.

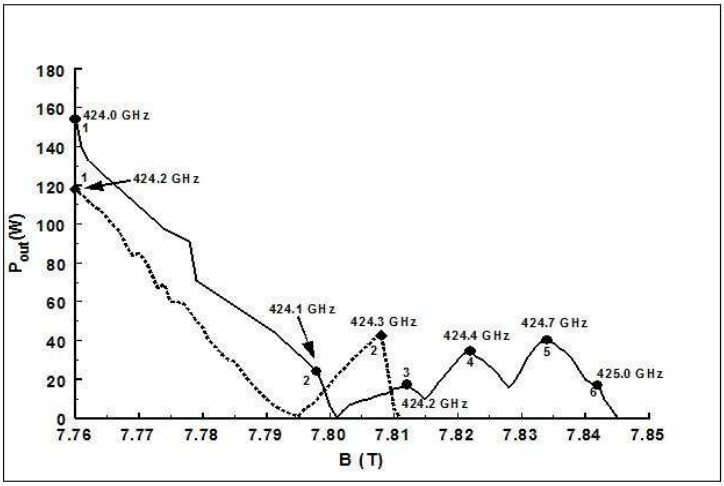

Fig. 7. Output power and frequency as a function of the magnetic field in the cylindrical cavity (dashed) and in the uptapered cavity (solid). Positions of the axial wave numbers q are marked by diamonds and dots respectively. The output power forms a fingerlike shape. In the mode transition region, the output power is small but nonzero and the oscillation frequency can be smoothly tuned.

BASIC PROPERTIES OF THE F-TYPE CENTERS IN HALIDES, OXIDES AND PEROVSKITES

A.I. Popov , E.A. Kotomin,
J. Maier (*Max Planck Institute for Solid State Research, Stuttgart, Germany*)

Recently, *in collaboration with Prof. J.Maier from Max Planck Institute for Solid State Research, Germany* we presented (Nucl. Instr. Meth. B, 2010, **268**, p. 3084-3089) a short survey of the optical properties of primary radiation-induced point defects in alkali halides, simple oxides and some ABO_3 perovskites. We have discussed in details the optical properties of the single-electron *F* and F^+ centers in rock-salt (f.c.c.) alkali halides and oxides and show that the Mollwo-Ivey law well-known for the *F*-type centers in alkali halides may be extended for other rock-salt structure insulators (Fig.8).

We discussed in details the major differences in point defect production mechanisms in halides and oxides. It was known for a long time that in alkali halides with NaCl (f.c.c.) structure absorbed energy to produce the *F-H* pair varied inversely with the space available to accept an interstitial ion. It can be characterised by *S/D*, the ratio of the separation between halogen ions in the [110] direction and the diameter of the halogen ion *D*.

We have shown how the Rabin-Klick diagram may be generalized for a whole family of alkali halides (NaCl (f.c.c.) CsCl (b.c.c.) structures. The *F*-type center migration and aggregation into metal colloids in alkali halides and oxides was also discussed.

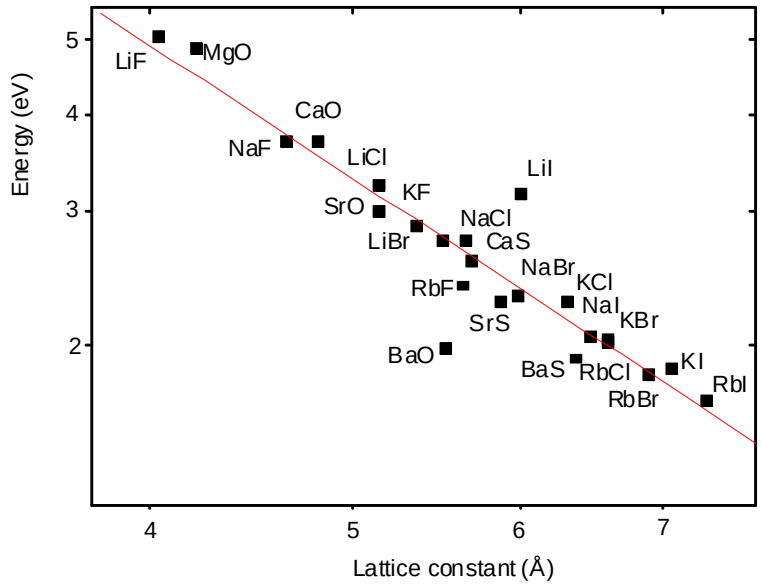

Fig.8. The generalized plot of Mollwo-Ivey relation for the *F* band in alkali halides and F^+ oxides and sulfides with f.c.c. structure.

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

A.I. Popov,

R. Sathyamoorthy, P. Sudhagar (*R & D Department of Physics, Kongunadu Arts & Science College, Coimbatore, Tamilnadu, India);*

A. Balerna, S. Bellucci (*INFN-Laboratori Nazionali di Frascati, Frascati, Italy*);

C. Balasubramanian (*Facilitation Centre for Industrial Plasma Technologies, Institute for Plasma Research, Bhat, Gandhinagar 382428, India*);

K. Asokan (*Inter University Accelerator Centre, New Delhi, India*);

The synthesis of Co-doped CdS nanoclusters ($Cd_{1-x}Co_xS$) was performed for different doping concentrations (x = 0.10, 0.20 and 0.30) and characterization of their structural, optical, and magnetic properties. 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. 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

Publications

SCI

1. **Yu.A. Mastrikov**, M.M. Kuklja, **E.A. Kotomin**, and J. Maier, First-principles modelling of complex perovskite $(Ba_{1-x}Sr_x)(Co_{1-y}Fe_y)O_{3-d}$ for solid oxide fuel cell and gas separation membrane applications. - Energy Environ. Sci., 2010, **3**, p. 1544–1550.
2. **V. Kashcheyevs** and B. Kaestner, Universal decay cascade model for dynamical quantum dot initialization. - Phys. Rev. Lett., 2010, **104**, 186805 (p. 1-4).
3. R.A. Evarestov, **Yu.F. Zhukovskii**, A.V. Bandura, and **S. Piskunov**, Symmetry and models of single-wall BN and TiO_2 nanotubes with hexagonal morphology. - J. Phys. Chem. C, 2010, **114**, p. 21061-21069.
4. **Yu.A. Mastrikov**, R. Merkle, E. Heifets, **E.A. Kotomin**, and J. Maier, Pathways for oxygen incorporation in mixed conducting perovskites: a DFT-based mechanistic analysis for (La, Sr)$MnO_{3-\delta}$. - J. Phys. Chem. C, 2010, **114**, p. 3017-3027.

5. **D. Gryaznov**, E. Heifets, and D. Sedmidubsky, Density functional theory calculations on magnetic properties of actinide compounds. - Phys. Chem. & Chem. Phys., 2010, **12**, p. 12273–12278.

6. **D. Gryaznov**, R.A. Evarestov, and J. Maier, Hybrid density-functional calculations of phonons in $LaCoO_3$. - Phys. Rev. B, 2010, **82**, 224301 (p. 1-5).

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I. 26th ISSP Conference (Riga, Latvia, February, 2010).

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2. *D. Bocharov, D. Gryaznov, Yu.F. Zhukovskii and E.A. Kotomin, "Surface and subsurface vacancies in uranium nitride: first principles calculations". Abstracts: p. 31.*
3. *P. Merzlakovs and G. Zvejnieks, "Modeling of cluster scaling behavior with kinetic Monte-Carlo and cellular automata methods". Abstracts: p. 32.*
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5. *Yu.F. Zhukovskii, S. Piskunov, E.A. Kotomin and S. Bellucci, "Growth mechanism for CNT bundle upon both flat and nanostructured Ni catalyst: ab initio simulations". Abstracts: p. 16.*
6. *R.A. Evarestov and Yu.F. Zhukovskii, "Symmetry and models of BN and TiO_2 nanotubes". Abstracts: p. 21.*
7. *E.A. Kotomin, Yu.A. Mastrikov, R. Merkle and J. Maier, "Oxygen incorporation reaction into mixed conducting ABO_3 - type perovskites for fuel cell applications". Abstracts: p. 22.*
8. *Yu.N. Shunin, Yu.F. Zhukovskii, S. Bellucci and N. Burlutskaya, "Resistance simulations for junctions of SW and MW carbon nanotubes with various metal substrates". Abstracts: p. 33.*
9. *G. Zvejnieks and E.E. Tornau, "Modeling of Au-Ni surface alloy instability". Abstracts: p. 35.*
10. *D. Bocharov, D. Gryaznov, Yu.F. Zhukovskii and E.A. Kotomin, "First principles calculations on oxygen impurities incorporated in the vacancies of UN(001) substrate". Abstracts: p. 37.*
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12. *D. Gryaznov, R.A. Evarestov, E.A. Kotomin and J. Maier, "Electronic, phonon and magnetic structure of pure and Sr-doped $LaCoO_3$". Abstracts:p. 39.*
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51. *S. Kern, K.A. Avramidis, O. Dumbrajs, G. Gantenbein, S. Illy, A. Samartsev, A. Schlaich, M. Thumm, and A.R. Choudhury "Simulation and experimental investigations on dynamic after cavity interaction (ACI)".*

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61. E. Heifets, and D. Gryaznov, "Density Functional Theory Calculations on Magnetic Properties of Actinide Compounds". Abstracts: Q 14.6.

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