NONLINEAR PROCESSES IN SOLIDS

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

Research Area and Main Problems

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

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

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

Scientific staff:

1. Dr. hab. E. Kotomin
2. Dr. hab. V. Kuzovkov
3. Dr. hab. J.R. Kalnin (left in September)
4. Dr. O. Dumbrajs
5. Dr. Yu. Zhukovskii
6. Dr. A. Popov
7. Dr. R. Eglitis
8. Dr. G. Zvejnieks
9. Dr. S. Piskunov
10. Dr. D. Gryaznov

PhD students:

11. V. Kashcheyevs
12. Yu. Mastrikov
13. D. Bocharov

Scientific visits abroad

1. Dr. hab. E. Kotomin, EC Institute of Transuranium Elements, Karlsruhe, Germany (10 months), Max Planck Institute for Solid State Research, Stuttgart, Germany (3 weeks), Imperial College, London, UK (1 week).
2. Dr. O. Dumbrajs, Max Planck Institute for Plasma Physics, Garching, Germany (3 months).
3. Dr. Yu. Zhukovskii, Northwestern University, Evanston, USA (10 weeks), Max Planck Institute for Solid State Research, Stuttgart, Germany (7 weeks), National Laboratory of Frascati, Italy (5 weeks), St. Petersburg State University, Russia (1 month), EC Institute of Transuranium Elements, Karlsruhe, Germany (1 week), Uppsala University, Sweden (1 week).
4. Dr. A. Popov, Institute Laue-Langevin, Grenoble, France (10 months), National Laboratory of Frascati, Italy (1 month).

5. Dr. R. Eglitis, University of Osnabrück, Germany (8 months), Sung Kyun Kwan University, Suwon, Korea (3 months).
6. Dr. G. Zvejnieks, Institute of Semiconductor Physics, Vilnius, Lithuania (1.5 months).
7. Dr. S. Piskunov, Forschungszentrum Jülich, Germany (6 months), Northwestern University, Evanston, USA (4 months).
8. Dr. D. Gryaznov, Max Planck Institute for Solid State Physics, Stuttgart, Germany (9 months), EC Institute of Transuranium Elements, Karlsruhe, Germany (2 months).
9. V. Kashcheyevs, Tel Aviv University, Israel (8 months), Ben-Gurion University of the Negev, Beer-Sheva, Israel (3 months).
10. Yu. Mastrikov, Max Planck Institute for Solid State Rcsearch, Stuttgart, Germany (11 months).

International Cooperation

Austria	1. Institute of Chemical Technologies and Analytics, Vienna University of Technology, Vienna (Prof. Dr. J. Fleig)
Estonia	2. Institute of Physics, Tartu University (Prof. A. Lushchik)
Finland	3. Helsinki University of Technology (Dr. T.M.J. Ikonen)
France	4. Laue-Langevin Institute, Grenoble (Dr. G.J. McIntyre)
Germany	5. EC Institute of Transuranium Elements, Karlsruhe (Dr. P. van Uffelen), 6. Institut für Hochleistungsimpuls & Mikrowellentechnik, Karlsruhe (Dr. B. Piosczyk) 7. Institut für Werkstoffe und Verfahren der Energietechnik, Forschungszentrum Jülich (Prof. Dr. E. Spohr) 8. Max Planck Institut (MPI) für Festkörperforschung, Stuttgart (Prof. Dr. J. Maier) 9. Max Planck Institut für Plasmaphysik, Garching (Prof. Dr. H. Zohm) 10. Technische Universität Braunschweig (Prof. Dr. W. von Niessen) 11. Universität Osnabrück (Prof. Dr. G. Borstel)
Greece	12. School of Electrical and Computer Engineering, National Technical University of Athens, Zographou (Dr. Y. Kominis)
Israel	13. School of Physics and Astronomy, Tel Aviv University (Prof. A. Aharony) 14. Ben Gurion University of the Negev, Ber Sheeva (Prof. D. Fuks)
Italy	15. Laboratori Nazionali di Frascati (Dr. S. Bellucci)
Japan	16. FIR Center, University of Fukui (Prof. T. Idehara)
Korea	17. Sung Kyun Kwan University, Suwon (Dr. J.C. Lee)
Lithuania	18. Institute of Semiconductor Physics (SPI), Vilnius (Dr. E. Tornau)
Romania	19. University of Craiova (Dr. D. Constantinescu)
Russia	20. St. Petersburg University (SpbU) (Prof. R.A. Evarestov)
Spain	21. University of Barcelona (Prof. F. Illas)
Sweden	22. Uppsala University (Prof. K. Hermansson)
UK	23. Imperial College London (Prof. R.W. Grimes) 24. King's College London (Prof. L. Kantorovich) 25. University College London (Profs. A.M. Stoneham and A. Shluger)

Ukraine 26. National University of Lviv (Prof. I. Bolesta and Prof. V. Savchyn)

USA 27. Northwestern University, Evanston, Illinois (Prof. D.E. Ellis)
28. University of Maryland, College Park (Dr. G.S. Nusinovich)
29. California Institute of Technology, Pasadena (Dr. E. Heifets)

Main Results

RANDOM WALK APPROACH TO THE ANALYTICAL SOLUTION OF DISORDERD SYSTEMS WITH MULTIPLICATIVE NOISE – THE ANDERSON LOCALIZATION PROBLEM

V. Kuzovkov,
W. von Niessen (*Braunschweig Technical University, Germany*)

Understanding fundamental properties of low-dimension disorded systems continue to attract great attention. *In collaboration with Technische Universität Braunschweig, Germany*, we developed a new analytical random walk approach for calculating the phase-diagram of spatially extended systems with multiplicative noise. We study the *Anderson localization* problem as an example. The transition from delocalized to localized states was treated as a generalized diffusion with a noise-induced first-order phase transition. The generalized diffusion manifests itself in the divergence of averages of wave functions (correlators) controlled by the Lyapunov exponent, which is the inverse of the localization length. The appearance of the generalized diffusion arises due to the instability of a fundamental mode corresponding to correlators. The generalized diffusion could be described in terms of a signal theory, which operates with the concepts of input and output signals and the filter function. Delocalized states correspond to the bounded output signals whereas localized states to unbounded output signals, respectively. The transition from bounded to unbounded signals is defined uniquely by the filter function.

CO OXIDATION AT Pd(111) SURFACE

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

Catalytic surface reactions still remain an actual research topic, which is supported by both search of effective catalysts in automotive industry and challenges for applicability of theoretical methods. *In collaboration with the Semiconductor Physics Institute (Vilnius),* the model has been proposed to simulate numerically the reaction $O + CO \rightarrow CO_2$ and occurring phase transitions on Pd(111) surface. We calculated the phase diagram for this system by means of the kinetic Monte Carlo method. We have shown existence of the phase transitions $p(2\times2)_O \rightarrow \sqrt{3}\times\sqrt{3}R30^o{}_O$ and $p(2\times2)_O \rightarrow \sqrt{3}\times\sqrt{3}R30^o{}_O \rightarrow p(2\times1)_O$ with increase of CO coverage for room and intermediate temperatures, respectively, while in the low temperature limit the direct $p(2\times2)_O \rightarrow p(2\times1)_O$ phase transition is observed. We demonstrated that the reaction rate is the crucial factor determining the occurrence of the $p(2\times1)_O$ phase and vanishing of the $\sqrt{3}\times\sqrt{3}R30^o{}_O$ with temperature decrease. The results of correlation function analysis indicated that the reaction proceeds inside both the $p(2\times2)_O$ and $\sqrt{3}\times\sqrt{3}R30^o{}_O$ phases, but on the perimeter of the domains of $p(2\times1)_O$ structure.

STOCHASTIC PROCESSES IN ASDEX UPGRADE TOKAMAK

O. Dumbrajs and G. Zvejnieks,
V. Igochine, H. Zohm and A. Flaws (*MPI für Plasmaphysik, Garching, Germany*),
D. Constantinescu (*University of Craiova, Romania*)

One of major problems in fusion tokamak is plasma stability. *In collaboration with Max Planck Institute, Garching*, the diffusion coefficient was determined (by means of the mapping technique) for stochastic field lines arising in fast reconnection phenomena in magnetized fusion plasma during the frequently interrupted regime of neoclassical tearing mode (FIR-NTM), as well as in non-complete Sawtooth reconnection in ASDEX Upgrade tokamak in ASDEX Upgrade tokamak. Solution of the non-stationary diffusion equation with variable diffusion coefficients predicts that the temperature profile during the FIR-NTM event is shifted towards the plasma boundary within 30 μs and during the Sawtooth reconnection within 10 μs. Phenomena of non-complete Sawtooth reconnection in ASDEX Upgrade tokamak are associated with internal kink mode which does not vanish after the crash phase (as would be the case for complete reconnection). It was shown that higher harmonics play an important role during the Sawtooth crash phase. To model incomplete Sawtooth reconnection, we employed the Hamiltonian formalism and reconstructed perturbations. It was demonstrated that stochastization appears due to excitation of low-order resonances. The central safety factor value is always less than unity in case of non-complete Sawtooth reconnection. Stochastic model agrees well with experimental observations and can be proposed for explanation of the Sawtooth reconnection.

The role of stochastization of magnetic field lines in fast reconnection phenomena occurring in magnetized fusion plasma was analyzed *in collaboration with the MPI, Garching, Helsinki University of Technology, and University of Craiova*. A mapping technique was applied to trace the field lines of toroidally confined plasma where the perturbation parameter is expressed in terms of experimental perturbation amplitudes determined from the ASDEX Upgrade tokamak. It was found that fast reconnection observed during amplitude drops of the neoclassical tearing mode instability in the frequently interrupted regime can be related to stochastization. It was also shown that stochastization can explain the fast loss of confinement during the minor disruption. This demonstrates that stochastization can be regarded as a possible cause for different MHD events in ASDEX Upgrade.

GYROTRON DEVELOPMENT FOR ITER

O. Dumbrajs,
B. Piosczyk and G. Dammertz (*Forschungszentrum Karlsruhe, Germany*),
Y. Kominis and K.A. Avramides (*National Technical University of Athens, Greece*),
G.S. Nusinovich (*University of Maryland, College Park, USA*)

The development of high-power high-frequency gyrotrons is strongly driven by the needs of fusion technology. Gyrotrons are superior to other rf sources in the frequency range relevant for electron cyclotron resonance heating (ECRH), or about 170 GHz for ITER. To make an ECRH system cost-effective, the output power of a single gyrotron should be around continuous 2 MW power. Coaxial cavity gyrotrons have the potential to fulfil this requirement as has been experimentally demonstrated within the development program performed as an *ITER task at Forschungszentrum Karlsruhe (FZK)*. In proof of

principle experiments carried out at FZK Karlsruhe on a 165 GHz coaxial cavity gyrotron during the last years, the feasibility of manufacturing a 2 MW, CW coaxial gyrotron at 170 GHz has been demonstrated and information necessary for a technical design has been obtained. Based on these results and on the experience acquired during the development of the 1MW, CW, 140 GHz gyrotron for W7-X, the technical feasibility of a 2 MW, CW, 170 GHz coaxial cavity gyrotron has been studied before EFDA has placed a contract with Thales Electron Devices (TED) for procurement of a first industrial prototype of such a coaxial gyrotron tube. The development work is done in cooperation between European research centers together with TED, the main European tube manufacturer. Experimental operation of the gyrotron could start in summer 2007.

Our laboratory *in collaboration with Forschungszentrum Karlsruhe, National Technical University of Athens, and University of Maryland, College Park,* actively participates in this development. Most recently, the effect of microwave reflections in gyrotrons with radial output and consequences for the ITER coaxial gyrotron was studied, azimuthal instability in gyrotrons with overmoded resonators was investigated, feasibility of coaxial super power (4 MW) was examined, Hamiltonian map description of electron dynamics in gyrotrons was proposed, eigenvalues and ohmic losses in coaxial gyrotron cavity were reexamined by means of a novel method.

UNIVERSAL DESCRIPTION OF ELECTRONIC CORRELATIONS IN DOUBLE QUANTUM DOTS

V. Kashcheyevs,
A. Aharony and O. Entin-Wohlman (*Ben Gurion University of the Negev, Ber Sheeva, Israel*),
A. Schiller (*Hebrew University of Jerusalem, Israel*)

Quantum dots are very important for the optoelectronic applications. *In collaboration with Ben Gurion University of the Negev, Ber Sheeva, and Hebrew University of Jerusalem*, we have put forward a theoretical framework for accurate characterization of strongly correlated states in double quantum dots. Such systems consist of two nanoscale objects with discrete electronic states that are coupled to two leads. In strong magnetic fields only one non-degenerate electronic state dominates the transport in each dot. Strong Coulomb repulsion between the dots can force the two-level system into the regime of a single occupancy, where it effectively becomes a charge qubit. Recently a number of intriguing phenomena in this system have been identified: level population inversion and oscillations, transmission phase lapses and sharp transmission resonances.

Our work presents a unified quantitative explanation for these phenomena in terms of coherent dynamics of the pseudo-spin, and identifies the relevant physical mechanism, namely competition between the polarizing effect of the effective magnetic field and the Kondo-screening by the coherent environment. By a proper rotation of the quantum-mechanical representation for the charge states on the dots and in the leads, we map the system exactly onto a generalize Anderson impurity model. For the most general case of interest we develop a quantitative pseudo-spin description (Kondo type Hamiltonian), which reveals renormalization of the effective magnetic field and anisotropy of the exchange couplings. Exploiting the exact Bethe *ansatz* solution of the Kondo model, we have put forward very accurate expressions for the occupation numbers and the linear conductance. Our analytical results are in a very good agreement with advanced numerical renormalization group calculations, and call for an experimental test.

REVISITING CLASSICAL GRAIN BOUNDARY DIFFUSION MODELS

D. Gryaznov,
J. Fleig *(Vienna University of Technology, Vienna, Austria),*
J. Maier *(MPI for Solid State Research, Stuttgart, Germany)*

Prediction of transport properties of nanomaterials is of great interest. This study was performed *in collaboration with the Max Planck Institute for Solid State Research, Stuttgart, and Vienna University of of Technology* and completed on 20 September 2006 by a successful defense of PhD Thesis at *Stuttgart University*. The main scope of present study was to analyze limitations of classical grain boundary diffusion models (Fisher's model, Whipple's solution, Le Claire' relation) used to find the grain boundary diffusivity from measured diffusion profiles. The classical grain boundary diffusion models are based on different approximations, supposing sufficiently high temperatures and/or long diffusion times. However, nanocrystalline materials impose new conditions, *i.e.* short diffusion times and low temperatures. To find the grain boundary diffusivity we have established special procedure, which gives accurate values for bi- and polycrystals at short and long diffusion times if orientations of the grain boundaries can be ignored. It was also estimated that the latter effect underestimates the grain boundary diffusivity by using the standard Le Claire relation. The analytical dependence for the maximum of the diffusion profile derivative not only gives an alternative procedure for deducing the grain boundary diffusivity but also sufficiently improves determination of the grain boundary diffusivity in ionic materials.

FIRST PRINCIPLES ATOMISTIC MODELLING OF NUCLEAR FUELS

E. Kotomin, Yu. Zhukovskii, Yu. Mastrikov, and D. Gryaznov,
P. Van Uffelen (*EC Joint Research Center, Institute for Transuranium Elements, Karlsruhe, Germany*)

Actinide nitrides are promising as advanced nuclear fuels for future fast reactors, since they exhibit higher thermal conductivity and higher metal density over the oxides, most commonly used to fabricate commercial nuclear fuels so far. To predict fuel performance under different operation conditions and understand the evolution as spent fuel over long times in a repository, it is necessary to study the defect-induced processes caused by material self-irradiation and the accumulation of fission products. *In collaboration with Institute for Transuranium Elements, Karlsruhe,* we have performed DFT plane-wave calculations on perfect and defective UN *fcc* crystal using VASP computer code. Neutral vacancies were modelled by removing a U (N) atom from the supercell, the Frenkel and Schottky defect pairs were also modeled. Nitrogen Frenkel defects were described by moving a N atom from a regular site into the interstitial position in the cube center. Results of our calculations reproduce quite well the basic properties (lattice constant a_0, bulk modulus and cohesive energy) of pure UN. The calculated effective (Bader) atomic charges indicate the complex chemical bonding, with covalency contributions due to U *5f* and N *2p* orbital hybridization. We calculated defect formation energies, changes of the macroscopic lattice parameter and local lattice distortions. The formation energies for intrinsic Frenkel and Schottky defect pairs inside a 4×4×4 supercells were found to be 4.6 eV and 3.8 eV, respectively.

Handling and disposal of new nuclear materials, including uranium nitride, require a deeper knowledge of the surface reactivity. *In collaboration with Institute for*

Transuranium Elements, Karlsruhe, we have performed DFT calculations of the atomic and electronic structure of perfect and defective UN substrate as well as the early stages of surface oxidation. We have focused on a study of (*i*) (001) substrate relaxation, (*ii*) basic properties of surface point defects and adsorbed oxygen (including dissociation of O_2 molecules at surface), and (*iii*) modification of substrate properties as a result of defect formation or oxygen adsorption. The lattice relaxation energy of 1.35 eV calculated for the surface N vacancies (V_N) at the 0.25 ML concentration is twice as larger as that in the bulk (0.7 eV) whereas the formation energy of the surface vacancy is smaller than in the bulk. This indicates that vacancies should segregate to the UN grain boundaries. Due to metallic-covalent chemical bonding in UN, we observe high affinity of atomic oxygen towards the (001) substrate: the *binding energies* are found to be 8.1 and 7.1 eV *per* adatom atop surface U or N atoms, respectively. We found also that O adatom atop surface U and N ions transforms into O^-_{ads} ion, which determines an initiation of the oxidation process.

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

E.A. Kotomin, Yu. Zhukovskii, S. Piskunov, R. Eglitis, and Yu. Mastrikov
R.A. Evarestov (*St. Petersburg University, Russia*)
D.E. Ellis (*Northwestern University, Evanston, Illinois, USA*)
E. Heifets (*California Institute of Technology, Pasadena, USA*)
J. Felsteiner (*Technion, Haifa, Israel*) and A. Gordon (*Haifa University, Tivon, Israel*)
G. Borstel (*Osnabrück University, Germany*)
J. Maier (*MPI for Solid State Research, Stuttgart, Germany*)

Understanding perovskites surface properties of is important for catalysis, growth of high T_c materials, and optoelectronics. *In collaboration with Northwestern University, Evanston, and California Institute of Technology, Pasadena,* we have studied the atomic and electronic structures as well as thermodynamic stability of three double-layered (DL) $SrTiO_3$(001) surfaces: (*i*) SrO-terminated, (*ii*) TiO_2-terminated, and (*iii*) TiO_2-terminated with (2×1) substrate reconstruction. A thermodynamic stability diagram obtained from our DFT calculations using hybrid B3PW exchange-correlation functional have shown that regular TiO_2- and SrO-terminated surfaces are the energetically most stable. Due to nearly perfect agreement of calculated and experimental formation energies we have determined boundaries of stability for different crystals very well. The stability regions of (2×1) DL TiO_2- and DL SrO-terminated surfaces lie beyond the precipitation lines of SrO and TiO_2 compounds and, thus, are less stable than regular $SrTiO_3$(001) surfaces. Precipitation of strontium and titanium oxides occurs much earlier, than any of studied DL terminations can be formed. We suppose that the SrO or TiO_2 oxide films would grow preferably on $SrTiO_3$ perovskite through cluster formation rather than layer-by-layer deposition. When partial pressure of O_2 gas decreases at a constant temperature, either TiO_2 precipitation or Ti atom reduction occurs, which precipitate to metallic particles. Sr precipitation on $SrTiO_3$ surface will not occur. Increase of Sr chemical potential leads to SrO precipitation.

In collaboration with Osnabrück University and California Institute of Technology, Pasadena, we have also calculated relaxation of $BaTiO_3$ and $PbTiO_3$ perovskite (001) surfaces and surface rumpling for two different terminations (BaO&PbO and TiO_2) as well as relaxation of $BaTiO_3$ and $PbTiO_3$ (110) surfaces for three different terminations (Ba&Pb, TiO_2, and O). The O-terminated A-type $BaTiO_3$(110) polar surface possesses a surface

energy close to that for the (001) surface, which indicates that both (110) and (001) $BaTiO_3$ surfaces can exist simultaneously in perovskite ceramics. The energetically most unfavorable, and thereby most unstable are found to be metal (Ba or Pb) terminated $BaTiO_3$ (3.24 eV) or $PbTiO_3$ (2.03 eV) (011) surfaces. The surface energies for the O terminated, *A* type $BaTiO_3$ and $PbTiO_3$ (011) surfaces practically coincide (1.72 eV).

Due to its antiferroelectric behavior, $PbZrO_3$ (PZ) is technologically important for many applications including actuators and high-energy storage devices. $PbZrO_3$ is also a parent compound of $PbZr_{1-x}Ti_xO_3$ solid solutions, which are of high technological interest for their ferroelectricity and piezoelectricity, observed over a wide range of compositions. The structural and electronic properties of pure cubic and low-temperature orthorhombic $PbZrO_3$ (antiferroelectric phase), as well as cubic PZ containing single *F* centers (neutral oxygen vacancies) have been simulated *in collaboration with Northwestern University, Evanston.* The band gap obtained for PZ bulk (cubic phase) is in good agreement with the experimental data (3.7 eV). The electronic charge redistribution calculated for a cubic PZ bulk confirms a notable Pb-O bond covalency, which considerably increase in the orthorhombic phase. We have also found a strong increase of the Zr-O bond covalency near the ZrO_2-terminated (001) surface as compared to the PZ bulk. Formation of an *F* center in cubic PZ is accompanied by a substantial displacement (0.25 Å) of the nearest Pb atoms towards the vacancy. The *F* center forms a defect level in the middle of the band gap (1.72 eV below the conduction band bottom) unlike the shallow *F* level found in $SrTiO_3$ (0.5 eV). Thus, the point defects affect both atomic polarization in PZ and its ferroelectric properties.

Understanding and control of surface properties of pure and Sr-doped $LaMnO_3$ is important for applications in fuel cells, magnetoresistive devices, and spintronics. We have compared the atomic, electronic, and magnetic structures of $LaMnO_3$ bulk as well as the (001) and (110) surfaces calculated *in collaboration with Max Planck Institute for Solid State Research, Stuttgart, and St. Petersburg University,* using two *ab initio* approaches – hybrid B3PW functionals with optimized LCAO basis set and GGA-PW91 functional with plane wave basis set. Combination of non-local exchange and correlation used in hybrid functionals allows us to reproduce the experimental *magnetic coupling constants* J_{ab} and J_c as well as the optical gap much better than using other methods. Calculations performed by both methods using slab models show that the anti-ferromagnetic (AFM) and ferromagnetic (FM) (001) surfaces have lower *surface energies* than the FM (110) surface. Both AFM and FM surfaces reveal considerable atomic relaxations, up to the fourth plane from the surface, which reduce the surface energy by about a factor of two, being typically one order of magnitude larger than the energy difference between different magnetic structures.

FIRST-PRINCIPLES CALCULATIONS AND THERMODYNAMIC STUDY ON SURFACE REACTIVITY OF LIGHT METAL OXIDES AND FLUORIDES

Yu. Zhukovskii, E. Kotomin, and R. Eglitis
D. Fuks (*Ben Gurion University of the Negev, Ber Sheeva, Israel*),
D.E. Ellis (*Northwestern University, Evanston, Illinois, USA*)
P. Balaya and J. Maier (*MPI for Solid State Research, Stuttgart, Germany*)
G. Borstel (*Osnabrück University, Germany*)

Understanding the metal adhesion and growth mode of thin metallic films is important for micro- and nanoelectronics. In collaboration with *Northwestern University, Evanston*

and Ben Gurion University, Ber Sheeva, we have performed *ab initio* calculations (using hybrid B3LYP method) and thermodynamic study of Ag and Cu adhesion onto defective MgO(001) substrate. We observe a strong change of the bonding between the metal adatoms and substrate in the vicinity of the surface F_s centers (neutral O vacancies), which affects the thermodynamic conditions and the morphology of the growing metallic layer. For a perfect MgO surface we confirm the experimentally observed submonolayer growth of *metallic islands*. However, the surface F_s centers weaken the trend toward metal atom aggregation and above some critical surface concentration lead to formation of *disordered* 2D metallic films; *i.e.*, the island formation mode is changed for the layer-by-layer growth mode. For silver films, the effect of the F_s centers is less pronounced than for copper: substantially higher atomic fraction of defects (at least 35-40 per cent) is needed for the growth of uniform Ag film, which is substantially larger than that for Cu (<10 per cent).

Ab initio calculations on H_2O and O_2 molecules adsorbed on different Al_2O_3 substrates, namely the Al terminated (0001) surface of crystalline corundum, and amorphous-like $(Al_2O_3)_n$ clusters with n=2-7 formula units, have been performed *in collaboration with Osnabrück University*. Two types of first-principles computer codes, CRYSTAL and SIESTA, have been used for the calculations on periodic slabs and clusters, respectively. We have performed complementary research of adsorption and dissociation of water on $(Al_2O_3)_n$ amorphous-like clusters with n = 2-7. We have also calculated the binding energy of an O_2 molecule on α-Al_2O_3 (0001) substrate. Our results point to a large contribution of Coulomb correlations and relaxation effects for the energies of H_2O and O_2 molecule adsorption on alumina surfaces and clusters.

To clarify the mechanism of lithium storage anomaly in LiF nanocomposites in the context of lithium batteries, we have performed comparative DFT hybrid calculations on the atomic and electronic structure of the non-polar Cu/LiF(001) and model Li/LiF(001) interfaces, *in collaboration with Max Planck Institute for Solid State Research, Stuttgart*. For this aim, we have modeled the extra Li atoms incorporated at several possible sites of the Me/LiF interface, including the free surface of the substrate slab and interstitial sites inside a slab. Increase of Li concentration at the substrate side of interfaces is accompanied by an increased electron charge transfer from the extra Li atoms towards the transition metal adlayers, in agreement with a proposed mechanism of interfacial charge storage. Interfacial stability and charge transfer depends on the number of extra Li atoms and Me adatoms *per* LiF(001) surface unit cell. The Li diffusion on the interface is found to be energetically much easier than Li penetration into the bulk.

FIRST PRINCIPLES SIMULATION OF ELECTRONIC STRUCTURE FOR PERFECT AND DEFECTIVE BaF_2 AND CaF_2: BULK AND SURFACE

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

In collaboration with *Osnabrück University,* we have performed *ab initio* calculations on technologically important barium and calcium fluorides (perfect and defective bulk and densely-packed surfaces). BaF_2 is important as a candidate material for high-temperature batteries, fuel cells, chemical filters and sensors. CaF_2 has been identified as a prime candidate for windows operating at chemical laser wavelengths due to very low bulk absorption and exceptionally small thermal tensing coefficients. The hybrid B3PW method was used as implemented into the *CRYSTAL'03* code, which provides the best agreement

with experiment for the band gap. When comparing the results of calculations on CaF_2 (111), (110), and (100) surfaces, we have confirmed that the CaF_2(111) surface is the most stable one, in agreement with the experiment, the same is true for the BaF_2(111) surface. The charge density map of the *F* center in CaF_2 shows that the charge is well localized inside the vacancy: the spin density on the *F* center has been found to be 0.716 *e*. The relaxation of atoms around defect is rather small. Our results for defect level position suggest a possible mechanism for absorption in CaF_2. We also calculated the aggregates of two *F* centers (*M* center) for both BaF_2 and CaF_2.

EXPERIMENTAL AND THEORETICAL STUDIES OF NANOSTRUCTURED MATERIALS

A. Popov and Yu. Zhukovskii,
C. Balasubramanian, S. Bellucci, M. Cestelli Guidi, A. Grilli, M. Piccinini, and A. Raco,
(*National Laboratory of Frascati, Italy*)
V. Baranov, V. Biryukov, Yu. Chesnokov, and V. Maisheev
(*Institute for High Energy Physics, Protvino, Russia*)
I. Bolesta, S. Velgosh, and I. Karbovnyk (*National University of Lviv, Ukraine*)

In collaboration with Laboratori Nazionali di Frascati (LNF) at Synchrotron Radiation Facility using both XANES (X-ray absorption near edge spectroscopy) and FTIR (Fourier transform infrared spectroscopy) techniques, we have studied different AlN nanosystems using spectroscopic methods, in order to investigate both tribological and electronic properties of nanostructured materials. III group nitrides nanostructures attract enhanced attention of both experimentalists and theorists, due to numerous technological applications in nanoengineering. Comparison has been performed between measurements by standard X-ray diffraction (XRD) and X-ray absorption spectroscopy (XAS) at the K-edge of Al, sensitive to the local order and correlated to the local and empty density of states of wide band-gap semiconductor. Preliminary XAS simulations were also performed. Correlations between XRD and XAS have been drawn. Using infrared (IR) absorption both in the mid- and in the far-IR ranges we have compared parameters of different AlN samples: powders, nanoparticles and nanotubes. Our results clearly show difference between their electronic properties and optical phonon modes.

In collaboration with LNF, Frascati, we have also analyzed the effect of N vacancies created on AlN single-walled (SW) nanotubes (NT), on both the electronic and structural properties of NTs. For this aim, we construct 1D periodic models of armchair- and zigzag-type chiralities and perform their DFT calculations using the *CRYSTAL-03* code taking into account structural reconstruction around each point defect on AlN NTs. To achieve the limit of single vacancy for both nanotube chiralities, we have considered three sets of inter-defect distances repeated along the axes of these nanotubes. The Mulliken charges on the *F* centers are found to be -2 *e*, close to the effective charges on N ions. However, the electron charge density re-distributions around the *F* center are substantial for both chiralities. They remain well localized along NT axis and disturb the electron density on the nearest atoms across NTs. N vacancies results induce one-electron energy levels in the NTs band gaps with main contributions from 3*p* and 3*s* atomic orbitals of the nearest Al atoms. The larger is the inter-defect distance on AlN SW NTs, the smaller dispersion of defect levels.

In collaboration with National University of Lviv and LNF, Frascati, we have studied an influence of $(Cd_i)_n$ metallic clusters on the optical absorption and phonon spectra of CdI_2

crystals, to understand a role of Cd nano&micro-clusters in context of CdI_2 crystal application as possible scintillator material and very promising materials for second harmonic generation. Metallic clusters of spherical shape were formed during the growth of non-stoichiometric crystals. Radii of clusters fall in the range from 10 to 500 nm, according to scanning electron microscopy (SEM) data. The density of clusters was estimated from fractal dimension calculations. Both spectral and size dependencies on extinction coefficients have been calculated using Mie theory. The experimentally obtained spectra show that metallic clusters are responsible for the bands in the transparency region of CdI_2 crystals (360–430 nm) and peaks in mid-infrared absorption spectra, which are not present in those for cadmium iodide. The nature of this additional optical and infrared absorption is concerned with bulk and surface plasmons and surface phonon modes of metallic clusters, respectively. Transmittance in the far-IR (50 to 600 cm^{-1}) and mid-IR (600 to 1300 cm^{-1}) regions was measured at the infrared station of the Synchrotron Radiation facility of LNF. The activation of crystals by diffusion during/after growth does not have any significant effect on their far IR spectra. Relative intensity of IR peaks varies depending on the impurity. This result is in a good agreement with SEM analysis and optical data.

Recently invented technique of crystal bending has been applied to produce samples with a high curvature. *In collaboration with LNF, Frascati, and Institute for High Energy Physics, Protvino,* we have investigated the deflection of a positron beam with energies of 400–700 MeV, available in the beam test facility (BTF) of LNF, by means of bent silicon crystals. This technique was successfully applied for crystal undulator production. We have observed positron bending by a crystal lattice, presumably being guided by a channeling phenomenon, deflecting the beam by about 10 milliradian over a 1 mm length of silicon. This technique may result in the use of the channeling effect for steering particle beams at energies below 1 GeV for the purpose of producing beams of low emittance with enhanced stability for medical and biological applications. By giving to nanotubes a controlled bending of a few milliradian, we could deflect the channeled particles out of the incident beam. Carbon nanotubes (CNT) proposed for particle channelling have been synthesized at LNF and then have been characterized there by SEM, TEM and AFM to obtain ratio and dimensions of the CNTs. SEM images show that the ratio of NTs is very high (more than 70%). Single-wall-CNTs have an average diameter 1.3 nm and a length of several microns.

QUANTUM CHEMICAL INTERPRETATION OF X-RAY ABSORPTION SPECTRA IN ABO_3 COMPOUNDS

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X-ray absorption spectroscopy (XAS) provides experimentalists with unique information on electronic, atomic and dynamic structure of materials. At the same time, quantum chemistry allows us to simulate reactivity, chemical properties, atomic and electronic structure of crystalline solids. In this work, we have interpreted experimental O K-edge XAS in perovskite-type WO_3 and AWO_3 compounds (A is the first group ion: H, Li, Na, K, Rb, Cs) using both DFT method as implemented in *CRYSTAL-2003* code and conventional multiple-scattering approach realized in *FEFF-8.2* code. Our calculations performed using both codes show qualitative agreement with available experimental data.

FEFF multiple-scattering calculations of XANES region allow us to obtain spectra qualitatively close to experimental ones. Calculated XAS have energy scale, which is non-

linearly compressed. The position of the Fermi level was estimated with an accuracy of about ±2-4 eV. Since XAS is sensitive to the position of the Fermi level, its correction is required to achieve reasonable agreement with the experiment. A cluster size of 6.5-7.5 Å around absorbing oxygen atom allows one to reproduce qualitatively experimental curves. The accuracy of *CRYSTAL* program for description of unoccupied electron states was tested for AWO_3 systems. Several optimized basis sets give similar results for our compounds in the region up to 15 eV above the Fermi level, whereas strong deviation of calculated results for higher energies indicates *CRYSTAL* code limitations. Our calculations make it possible to estimate bonds covalency in AWO_3 compounds: O-H bond is strongly covalent, W-O may be described in terms of both ionic and covalent contributions whereas O-A bonds are either pure ionic (A = K, Cs, Rb) or ionic with almost negligible covalency.

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