INVESTMENTS IN EDUCATION DEVELOPMENT

INTERNATIONAL WORKSHOP

Novel Approaches in condensed matter physics

May 12th to May 13th , 2015 , VŠB – Technical University of Ostrava

THE ABSTRACT BOOKLET

Oral presentations Tuesday May 12th

On the nature of phase transition in GeTe - the parent compound of phase-change materials

U. D. Wdowik
Institute of Technology, Pedagogical University Cracow, Poland

Germanium telluride has attracted an intense renewed interest for the last few years for its relevance and high performance as a phase change material as such and in combination of the form $(GeTe)_m(Sb_2Te_3)_n$ which find useful applications in modern non-volatile data storage devices. Apart from this technological interest, there is a very fundamental issue regarding whether the rhombohedral-to-cubic ferroelectric phase transition in GeTe is order-disorder or displacive type. We present results of the high resolution neutron powder diffraction experiments, inelastic neutron scattering measurements along with the density functional theory calculations that show conclusively the displacive nature of the phase transition rather than the order-disorder type claimed by some authors merely from diffraction data devoid of any dynamical information.

Chemical and Optical tuning of magnetic ordering in multiferroic CuO

J. Hellsvik
Department of Materials and Nanophysics, Royal Institute of Technology, Kista, Sweden

The high Curie temperature multiferroic compound CuO has a quasidegenerate magnetic ground state that makes it prone to manipulation by the so-called “order-by-disorder” mechanism. First principle computations supplemented with Monte Carlo simulations and experiments show that isovalent doping allows us to stabilize the multiferroic phase in nonferroelectric regions of the pristine material phase diagram with experiments reaching a 250% widening of the ferroelectric temperature window with 5% of Zn doping. Our results allow us to validate the importance of a quasidegenerate ground state on promoting multiferroicity on CuO at high temperatures and open a path to the material engineering of multiferroic materials. In addition we present a complete explanation of the CuO phase diagram and a computation on the incommensurability in excellent agreement with experiment without free parameters.

Using CuO as a reference compound, we explore how different optical excitation mechanisms can be used to drive ultrafast phase transitions in insulating antiferromagnets. We estimate the quantum mechanical efficiencies of the mechanisms and how they depend on the characteristics of the femto second laser pulses commonly used as pump pulses in time resolved spectroscopy. The different regimes of off- and on-resonant excitation result in distinctly different dynamics which we investigate in atomistic spin dynamics simulations. Also the influence of electronic and lattice heating and its relevance for the dynamics at the femto- respective pico- second time scales are investigated. Comparisons are done to recently performed experiments on CuO.

[1] J. Hellsvik et al., Phys. Rev. B 90, 014437 (2014)
[2] T. Kimura et al., Nature Mat. 7, 291 (2008)
[3] G. Giovannetti et al., Phys. Rev. Lett. 106, 026401 (2011)

Direct Electromagnetic Excitation and Detection of Ultrasound in Metals

I. Čáp
Faculty of Electrical Engineering, University of Žilina, Slovakia

Ultrasound is widely used in investigation of material properties of condensed matter. It is usually generated and detected by means of attached piezoelectric and similar transducers, which need an acoustic bond with investigated body. The present contribution deals with a special method allowing non-contact generation and detection of mechanical vibrations in a conducting sample by means of direct interaction of electromagnetic field with an electromechanical structure of the sample in presence of a constant magnetic field. Physical model of the interaction of the electromagnetic wave with ionic structure of a metal in the harmonic plane wave representation is analysed. Efficiency of the conversion effect will be derived. Dependence on frequency, temperature and material properties is discussed. Practical utilization of the effect is demonstrated on several examples oriented to bulk and surface wave's generation and detection. Typical shapes of exciting/detecting coils and practical cases of the discussed method application will be described.

Manipulation of spin waves in nanoscale

J. Rychły, J. W. Kłos, P. Gruszecki and M. Krawczyk
Faculty of Physics, Adam Mickiewicz University in Poznan, Poland

Spin waves are coherent disturbances of the magnetization in a magnetic medium, and can propagate in the form of waves over a distance of up to a few centimetres. Their frequency spans the range from hundreds of MHz to a few THz, with the respective wavelengths ranging from micrometers to nanometers. Thus, within these time and space limits spin waves can be used for transferring energy or transmitting and processing information. We present recent advances in manipulation of spin wave dynamic in homogeneous and patterned ferromagnetic film. We propose the new scheme for spin wave beam generation with inhomogeneous microwave transducers and exploit the obtained beam for demonstration new effects in magnonics.

Magneto-Optical Reflection-Spectroscopy from the XUV to the Soft X-ray Regime: An Analysis of Linear and Quadratic Effects in Crystalline Thin Films

M. Tesch
Institute of Methods for Material Development, Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany

Magneto-optical spectroscopy techniques with synchrotron radiation are a powerful tool to exploit magnetic materials. In contrast to magneto-optics in the visible regime the use of XUV and soft x-rays allows for an exploration of magnetic properties on an element selective level when tuning the photon energy to the binding energies of the core electrons. Techniques like the well-known x-ray magnetic circular dichroism (XMCD) allow e.g. for the detection of individual magnetic moments of different elements. However, this technique requires circular polarized light. Linear polarized synchrotron radiation, however, is easier to generate but nevertheless magneto-optical techniques using linear polarized light are not so frequently used, although these techniques can reveal valuable information about magnetic materials.
In the talk magneto-optical effects based on linear polarized light will be presented. In particular the transverse magneto-optical Kerr effect, which is linear in magnetization and the X-ray magnetic linear dichroism (XMLD) which is quadratic in magnetization and highly sensitive to the crystalline structure will be illuminated. Based on measurements at the 2p and 3p edges of Fe, Co, and Ni the advantages of the different techniques will be discussed and the experimental results will be compared to calculated spectra.

Oral presentations Wednesday May 13th

Theoretical strength under multiaxial loading

M. Černý
Faculty of Mechanical Engineering, University of Technology, Brno, Czech Republic
Institute of Physics of Materials, Academy of Sciences of the Czech Republic, Brno, Czech Republic
Central European Institute of Technology, CEITEC VUT, Brno, Czech Republic

The theoretical strength represents an upper limit to the envelope of attainable stresses and its knowledge enables us to assess the gap remaining to upper strength values of advanced engineering materials. Most of the theoretical strength calculations were performed for simple loading modes, given by a single non-zero stress (or strain) tensor component as uniaxial or isotropic tension or simple shear. On the other hand, materials used in the industrial exploitation are usually subjected to multiaxial loading.

This talk will focus on two particular examples of a superposition of simple loading modes: an axial loading of cubic crystals under superimposed transverse stresses and a shear loading under superimposed normal stress. Typical examples of the former case are stress states at the crack tip, in DAC experiments or those induced by the matrix/reinforcement incompatibility strain on the reinforcing single crystal fibers (or whiskers) in composite materials. The influence of a stress applied perpendicularly to slip planes during shear deformation of a crystal on the shear strength is also important in many deformation processes. As an example, one can consider a nanoindentation process as a combination of shear and compressive deformations in the vicinity of an indenter. Results of the aforementioned studies were obtained from atomistic modeling using first principles computational codes.

Magnetocrystalline anisotropy of adatoms: role of the spin orbit coupling and of the position of the Fermi level

O. Šipr, H. Ebert and J. Minář
Institute of Physics AS CR, v. v. i., Prague, Czech Republic

Even though it has been known for decades that the magnetocrystalline anisotropy is linked to the spin orbit coupling (SOC), the specific mechanism how does it arise for concrete systems is still subject to debate. It has been widely accepted that for uniaxial systems such as thin films or layered compounds the magnetocrystalline anisotropy energy (MAE) can be accounted for within the second order perturbation theory. This is because of the small magnitude of SOC energy when compared to the electron band width of such systems. However, the situation can be different in the case of single atoms deposited on a surface because then the width of electronic bands becomes comparable to the SOC-induced changes in the orbitally-resolved density of states upon the rotation of the magnetization. Our fully relativistic KKR-Green's function calculations demonstrate that if there is an orbital degeneracy of adatom-related states close to the Fermi level, the magnetocrystalline anisotropy may contain a significant contribution due to pushing of the SOC-split states above or below the Fermi level. As a result of this, the MAE crucially depends on the position of the energy bands of the adatom with respect to the Fermi level of the substrate.

INVESTMENTS IN EDUCATION DEVELOPMENT

Dynamical Mean-Field Modeling of Electronic Structure of Light Actinide Dioxides

J. Kolorenč
Institute of Physics AS CR, v. v. i., Prague, Czech Republic

A correlated band theory implemented as a combination of the local density approximation with the dynamical mean-field theory (LDA+DMFT) is applied to UO_2, NpO_2 and PuO_2. The calculated band gaps and valence-band spectra are in very good agreement with optical absorption experiments as well as with photoelectron spectra. The relatively large hybridization of the actinide 5f shell with the 2p states of oxygen causes a sizable increase of filling of the 5f orbitals from the nominal ionic configurations with two, three and four electrons to fractional values 2.5, 3.4 and 4.4. This enhancement is found to be compatible with 4f core-level photoelectron spectra but in the same time it appears to disagree with recent synchrotron experiments that employ X-ray absorption spectroscopy (XAS) and resonant X-ray emission spectroscopy (RXES), and suggest fillings much closer to the nominal integers. The discrepancy is analyzed in the LDA+DMFT framework by an explicit calculation of the XAS and RXES spectra at the actinide L absorption edge.

Reliability of calculated energies and measured enthalpies of interfacial segregation

P. Lejček[1] and M. Šob[2,3,4]

[1] Laboratory of Nanostructures and Nanomaterials, Institute of Physics, Academy of Sciences of the Czech Republic, Praha 8, Czech Republic
[2] Central European Institute of Technology, CEITEC MU, Masaryk University, Brno, Czech Republic
[3] Institute of Physics of Materials, Academy of Sciences of the Czech Republic, Brno, Czech Republic
[4] Department of Chemistry, Faculty of Science, Masaryk University, Brno, Czech Republic

Intergranular brittle fracture is closely related to the chemistry of grain boundaries and to the difference of the segregation energies of the grain boundaries and the free surfaces (Rice–Wang model). To elucidate the effect of individual solutes on embrittlement of various base materials such as steels and nickel-base superalloys, grain boundary and surface segregation was extensively studied in many laboratories. As a result, numerous data on surface and grain boundary segregation have been gathered in literature. They were obtained in two main ways, by computer simulations and from experiments. These results are frequently applied to quantify the embrittling potency of individual solutes. Unfortunately, the values of the segregation energy of a solute at grain boundaries as well as at the surfaces obtained by various authors sometimes differ by more than one order of magnitude: such a difference is unacceptable as it cannot provide us with representative view on the problem of material temper embrittlement. In some cases it seems that these values do not reflect physical reality or are incorrectly interpreted. Here we summarize the available data on interfacial segregation and embrittlement of various solutes in nickel and bcc iron and critically discuss their reliability, assessing also limitations of individual approaches employed to determine the values of segregation and strengthening/embrittling energies. We demonstrate that theoretical approaches are limited by the size of the computational repeat cell used for the calculations of the segregation energy. On the other hand, even when using repeat cells that are not sufficient for reliable evaluation of the segregation energy, the change in the grain boundary cohesion (strengthening/embrittling energy) may be obtained with a reasonable accuracy. For many impurities, there is lack of experimental segregation data. Therefore, many calculated results are theoretical predictions which may motivate future experimental work.

INVESTMENTS IN EDUCATION DEVELOPMENT

Ab initio and CALPHAD modelling of Laves and sigma phases

J. Pavlů[1,2,3], J. Vřešťál[1,2,3], P. Brož[1,2,3], M. Mazalová[2] and M. Šob[1,3,2]

[1] Central European Institute of Technology, CEITEC MU, Masaryk University, Brno, Czech Republic
[2] Department of Chemistry, Faculty of Science, Masaryk University, Brno, Czech Republic
[3] Institute of Physics of Materials, Academy of Sciences of the Czech Republic, Brno, Czech Republic

Systems containing intermetallic phases such as Laves or sigma phases play an important role in modern materials. Some systems with Laves phases are used in thermoelectric coolers (Mn-Ta) or are considered as prospective hydrogen storage material (Mn-Ti). On the other hand, sigma phase causes degradation of mechanical properties of steels and of resistance to various corrosive media.

Therefore, a good knowledge of phase relations, stability and magnetism of these phases is crucial for prediction of their behaviour under industrial conditions. Some of these properties can be determined by means of the first-principles calculations in the frame of Density Functional Theory (DFT) [1]. Further progress in phase modeling is achieved by the combination of ab initio approaches with semiempirical CALPHAD method which enables us to calculate phase diagrams of complex systems [2,3]. In addition to it, thermodynamic modelling at low temperatures can be accomplished using the results of phonon spectra calculations [3,4].

In this talk we present new ab initio results for selected systems containing Laves and/or sigma phases which can be included in thermodynamic assessment of these systems and in calculations of phase diagrams by CALPHAD method. Comparison of calculated results with recent experimental data is presented.

References:

[1] Pavlů J, Vřešťál J, Šob M: Intermetallics 18(2010)212
[2] Pavlů J, Vřešťál J, Šob M: CALPHAD 34 (2010) 215
[3] Štrof J, Pavlů J, Wdowik U D, Buršík J, Šob M, Vřešťál J: CALPHAD 44 (2014) 62
[4] Vřešťál J, Štrof J, Pavlů J: CALPHAD 37 (2012) 37

INVESTMENTS IN EDUCATION DEVELOPMENT

Nano-to-macro-scale modeling of hierarchical biocomposites

M. Friák[1,2,3], M. Petrov[2], C. Sachs[2], H. O. Fabritius[2], P. Hemzalová[2,4], D. Ma[2], B. Wu[2], G. Pfanner[2], J. Fikar[1], L. F. Zhu[2], L. Lymperakis[2], M. Šob[3,4,1], M. Všianská[3,4,1], S. Nikolov[5], A. Ziegler[6], D. Raabe[2]and J. Neugebauer[2]

[1] Institute of Physics of Materials, Academy of Sciences of the Czech Republic, Brno, Czech Republic
[2] Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany
[3]Central European Institute of Technology, CEITEC MU, Masaryk University, Brno, Czech Republic
[4] Department of Chemistry, Faculty of Science, Masaryk University, Brno, Czech Republic
[5] Institute of Mechanics, Bulgarian Academy of Sciences, Sofia, Bulgaria
[6] Central Facility for Electron Microscopy, University of Ulm, Ulm, Germany

Biological structural materials receive increasing attention by material scientists because they have been optimized during evolution and they are therefore ideally suited to study the efficiency of nature's design principles. These materials differ fundamentally from most man-made structural materials in being structurally heterogeneous by combining different in/organic constituents into composites with hierarchical organization. We propose a hierarchical model for the prediction of the elastic properties of a mineralized arthropod cuticle using quantum-mechanical calculations to find the elastic properties at the nanoscale and employing hierarchical homogenization to find the cuticle properties at all hierarchy levels. Based on our results we suggest that the mineral-protein matrix possesses a microstructure (so-called symmetric cell material) which exhibits extremal properties in terms of stiffness. We also discuss the role of chitin and the multifunctional optimization of the cuticle in terms of a trade off between stiffness and transport capacity of the pore canal system (Nikolov et al., Advanced Materials 22 (2010) 519; Nikolov et. al., Journal of the Mechanical Behavior of Biomedical Materials 4 (2011) 129; Petrov et. al., Biopolymers 99 (2013) 22). Recently, we have further extended our study to analyze the stiffening impact of magnesium additions on Mg-containing calcite particles (Zhu et al., Journal of the Mechanical Behavior of Biomedical Materials 20 (2013) 296).

Posters Tuesday, Wednesday during the Coffee breaks

An ab initio study of the phonon vibrations of Co_3O_4

A. Titov[1], D. Legut[2,3] and L. Obalová[3]
[1]Nanotechnology Centre, VSB–TU Ostrava, Ostrava, Czech Republic
[2]IT4Innovations Centre, VSB–TU Ostrava, Ostrava, Czech Republic
[3]Inst. Env. Techn., VSB–TU Ostrava, Ostrava, Czech Republic

Co_3O_4 belong to the party of the catalyst for N_2O decomposition. Since this reaction has oxidation-reduction mechanism, the electronic properties of Co_3O_4 represent important feature. Electronic structure and lattice dynamics, i.e. atomic vibrations were calculated using first-principles calculations. We determined Raman and infra-red frequencies of the phonon modes. Our results were calculated using single electron framework within the density functional theory. The general gradient approximation as parameterized by Perdew–Burke–Ernzerhof [1] was used for the electronic exchange correlation. To obtain the correct description of the insulating behaviour the Hubbard U technique was used. The anti-ferromagnetic ordering and spin-orbit interaction were also considered. For the lattice vibrations calculations Phonopy package was used [2]. The dependences of the band gap, infra-red and Raman frequencies on the Coulomb interaction (Hubbard U) were revealed. Calculated results are compared with experimental data measured at the VSB-TU Ostrava.

References:

[1] J. P. Perdew, K. Burke, M. Ernzerhof Phys. Rev. Lett. 77, 3865 (1996).
[2] A. Togo, F. Oba, I. Tanaka, Phys. Rev. B 78, 134106 (2008).

Ideal strength and magnetic properties of ∑5 (210) grain boundaries in FCC cobalt with segregated sp-impurities

P. Šesták[1,2], M. Černý[1,2], P. Řehák[1,2], M. Všianská[3,1] and M. Šob[3,1,4]
[1] Institute of Physics of Materials, Academy of Sciences of the Czech Republic, Brno, Czech Republic
[2] Faculty of Mechanical Engineering, Brno University of Technology, Brno, Czech Republic
[3] Central European Institute of Technology, CEITEC MU, Masaryk University, Brno, Czech Republic
[4] Department of Chemistry, Faculty of Science, Masaryk University, Brno, Czech Republic

Grain boundaries (GB) predetermine mechanical properties of polycrystalline materials, in particular, their strength. Moreover, the impurities contained in the material tend usually to segregate at the GB and thus they can have a strong negative or positive influence on its mechanical characteristics. In this first-principles study we present the uniaxial tensile strength and magnetic properties of Σ5 (210) tilt GB in FCC cobalt with segregated sp-impurities. The uniaxial deformation was performed along an axis perpendicular to the GB. The impurities Al, Ga, In, S, Sb, Sn and Te were considered in substitutional positions at the GB and As, Ge, P, S, Se, Si in interstitial positions. The strength of clean GB was compared with that of GB containing segregated impurities. The uniaxial deformation was realized using two different approaches. In the first one the computational supercell was continually optimized during the entire deformation path and in the second one the deformation corresponds to a rigid separation of grains along a defined plane without any cell optimization. It was also found that magnetic moments of atoms in atomic layers close to the GB change rapidly when strain is applied.

INVESTMENTS IN EDUCATION DEVELOPMENT

Magnetism in selected Fe-Pd and Fe-Pt nanostructured systems from ab initio calculations

M. Zouhar[1] and M. Šob[2,3,4]
[1]Central European Institute of Technology, CEITEC MU, Masaryk University, Brno, Czech Republic
[2]Central European Institute of Technology, CEITEC MU, Masaryk University, Brno, Czech Republic
[3]Institute of Physics of Materials, Academy of Sciences of the Czech Republic, Brno, Czech Republic
[4]Department of Chemistry, Faculty of Science, Masaryk University, Brno, Czech Republic

We present an ab initio study of ordered nanocomposite Fe-X systems, X being Pd or Pt, extending the analysis of the Mn-Pt system performed in [1]. The considered structures are based on face-centered-cubic (FCC) supercell (up to 3x3x1) and contain Fe nanowires (NW) in the matrix of X. The composition varies from elemental FCC X through FeX_{15}; FeX_8; FeX_7; FeX_3 (L12 structure), FeX (L10 structure) to FCC Fe. The Fe NWs are oriented along the [001] direction, except for the FeX structure that contains alternating atomic planes of Fe and X.

The equilibrium structural parameters are determined using the Vienna Ab initio Simulation Package (VASP). Generalised gradient approximation as parametrised by Perdew-Burke-Ernzerhof is employed without spin-orbit coupling. We examine the effect of ferromagnetic (FM), nonmagnetic (NM) and selected antiferromagnetic (AFM) orderings on structure stability, structural parameters, bulk modulus and values of magnetic moments. We display these quantities as functions of Fe content and comment on trends these functions exhibit.

It turns out that FM configurations are the most favourable except for FCC Fe, $FePt_3$ and $FePd_{15}$ that prefer the AFM state. The trends of quantities calculated for Fe-X FM configurations match better the FCC Fe high-spin (HS) state, rather than the FCC Fe low-spin (LS) state. With increasing Fe content, atomic volume decreases almost linearly in all the FM, NM and AFM configurations. Also the magnetic moment of Fe atoms decreases with increasing Fe concentration. The trends of (absolute value of maximum) induced magnetic moment on atoms of the matrix are more complex due to different symmetries of the Fe-X structures. In case of the FM arrangement, this induced magnetic moment increases with increasing Fe content and reaches a maximum either at FeX_3 or at FeX.

References:

[1] T. Káňa and M. Šob, Phys. Rev. B 85, 214438 (2012)

Investigation of cerium titanates from first principles

B. Kačerovská[1], L. Sojka[1], D. Legut[2,3] and L. Matejová[3]
[1]Nanotechnology Centre, VSB-TU Ostrava, Ostrava, Czech Republic
[2]IT4Innovations Centre, VSB-TU Ostrava, Ostrava, Czech Republic
[3]Institute of Environmental Technology, VSB-TU Ostrava, Ostrava, Czech Republic

Cerium titanate structures offer broad range of technological applications because of their optical and catalytic properties. Cerium titanate can form various phases, which depend on the oxidation state of cerium. In $CeTiO_4$ and $CeTi_2O_6$ compounds cerium is in the oxidation state Ce^{4+}. We have investigated electronic structure of these compounds as well as CeO_2 using ab-initio calculations. For $CeTiO_4$ we considered both orthorhombic and monoclinic phases. Furthermore, the influence of pressure applied to Ce titanate phases on various properties was revealed. Electronic structure, thermodynamical and optical properties were calculated using the single-electron framework of density functional theory employed in VASP code [1,2]. For the exchange-correlation term the generalized gradient approximation was considered [3].

References:

[1] G. Kresse, J. Furthmueller, Phys. Rev. B 54, 11169 (1996).
[2] G. Kresse, J. Furthmueller, J. Comput. Mater. Sci. 6, 15 (1996).
[3] J.P. Perdew, K. Burke, M. Ernzerhof, Phys. Rev. Lett. 77, 3865 (1996).

Ab-initio study of cerium-doped anatase and brookite phases

L. Sojka[1], B. Kačerovská[1], D. Legut[2,3] and L. Matejová[3]
[1]Nanotechnology Centre, VSB-TU Ostrava, Ostrava, Czech Republic
[2] IT4Innovations Centre, VSB-TU Ostrava, Ostrava, Czech Republic
[3] Institute of Environmental Technology, VSB-TU Ostrava, Ostrava, Czech Republic

TiO_2 is a well-known catalyst [1]. There is a number of ways howto improve its efficiency in visible-light spectrum further. One way is to create oxygen vacancies or Ti^{3+} defects. Another way how to induce visible-light photoactivity is by doping by lanthanides. Here we consider cerium doped TiO_2 in the anatase and brookite phases. Our results were obtained using ab-initio calculations. The electronic structure and thermodynamical properties (enthalphy of formation) of Ce doped TiO_2 phases were investigated under pressure as motivated by experimenal studies at VSB-TUO. Two valences, i.e. Ce^{3+}/Ce^{4+} were considered. The calculations were perforemd using the VASP code [2,3] and the generalized gradient approximation [4] was used to account for exchange-correlation effects. The thermodynamical stability with respect to the Ce concentration and Ce valence states are revealed in both anatase and brookite phases.

References:

[1] D. O. Scanlon et al., Nature Mater. 12, 798 (2013).
[2] G. Kresse, J. Furthmueller, Phys. Rev. B 54, 11169 (1996).
[3] G. Kresse, J. Furthmueller, J. Comput. Mater. Sci. 6, 15 (1996).
[4] J. P. Perdew, K. Burke, M. Ernzerhof, Phys. Rev. Lett. 77, 3865 (1996).

The interface nonplanarity investigated by the surface plasmon resonance imaging.

P. Ľalík[1,2], D. Blažek[1,3] and M. Lesňák[4]
[1]IT4Innovations Centre, VSB-TU Ostrava, Ostrava, Czech Republic
[2]Faculty of Electrical Engineering, University of Žilina, Žilina, Slovakia
[3]Nanotechnology Centre, VSB-TU Ostrava, Ostrava, Czech Republic
[4]Departmet of Physics, VSB-TU Ostrava, Ostrava, Czech Republic

Surface plasmon resonance imaging (SPRi) sensors realize highly sensitive, real-time, quantitative, label-free, high-throughput biological interaction monitoring and the binding profiles from multi-analytes. Further provide the binding kinetic parameters between different biomolecules. With such a sensitive method it is very important to point the need for planarity and homogeneity of the entire biochip for a correct output data.

This paper is inspired by experimental SPRi data from our commercial device GenOptics SPRI-Lab+ measured at biochip with Kretschmann configuration. Initial processing of calibration data shows significant variations in the resonance angle across the active layer of the biochip. Here we analyze in detail the possible reasons for observed inhomogeneity, which has a great influence on the operation of the device.