Institute of Physics Polish Academy of Sciences – Warsaw – 2015

Author's Summary of Professional Accomplishments

Attachment nr 2-EN

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I. Name and Surname

Iraida N. Demchenko

II. Academic and Research Career (short version)

- MSc: Donetsk National University, Donetsk, Ukraine, speciality: Solid State Physics and Material Science, 1989-1994;
- Assistant: Donetsk Technical University, Donetsk, Ukraine, Physics Department, 1994-1996;
- Assistant: Donetsk National University, Donetsk, Ukraine, Solid State Physics and Material Science Department, 1996-1999;
- PhD: Institute of Physics, Polish Academy of Sciences, Warsaw, Physics, 01.04.2000 - 23/06/2005.
- France, ESRF (European Synchrotron Radiation Facility), scientific research visit, a week, 2002.
- France, ILL (Institut Laue-Langevin), scientific research visit, a week, 2002.
- France, Atomic Energy Commission, Research Center, scientific research visit, a week, 2002.
- Spain, Universitat de Barcelona, Facultat de Fisica (ECM), scientific research stay, two weeks, 2003.
- Spain, Materials Science Institute of Madrid, scientific research stay, three days, 2003.
- USA, Lawrence Berkeley National Lab (LBNL), Advanced Light Source (ALS), scientific research stay, three weeks, 2003.
- Belgium, University of Antwerp, scientific research stay, a month, 2004.
- USA, University of Nevada, Las Vegas, Nevada (UNLV) and Lawrence Berkeley National Lab (LBNL, Berkeley, California), postdoctoral position, 01.06.2007 - 01.10.2011.
- 2005 -2007, 2011 – present time, Institute of Physics PAS, SL 1.2.

Participation in the scientific projects (mainly as a project leader) at synchrotron radiation facilities: Doris (DESY) in Hamburg and BESSY in Berlin, Germany; ESRF in Grenoble and LURE in Paris, France; ALBA in Barcelona, Spain; ALS in Berkeley, USA, where during 4 years I worked as the beamline 9.3.1 scientist.

III. Bibliometric indicators according to the Web of Science (WoS) database

- total *impact factor* of scientific publications as given by Journal Citation Reports (JCR), for each corresponding publication year (for publications from before 2008, IF2008 was used, while for publications from 2013, IF2012 was used) – **76,203**

- sum of the times publications were cited as given by WoS – **201**

  (without self-citations – **186**)

- Hirsch index of publications as given by WoS – **9**

Iraida Demchenko

IV. Achievement Justifying the Application for Habilitation.

As an achievement, as defined in Art. 16 paragraph 2 of the Act of 14 March 2003 on Academic Degrees and Academic Title and on Degrees and Title in Arts, I am indicating a series of seven monothematic publications entitled:

„Elemental- and orbital-selective characterization of electronic and structural properties of crystalline, non-crystalline, and low-dimensional materials by X-ray spectroscopy"

H-1. "Highly mismatched crystalline and amorphous GaN$_{1-x}$As$_x$ alloys in the whole composition range"

By: Yu, K. M.; Novikov, S. V.; Broesler, R.; Demchenko, I. N., Denlinger, J. D., Liliental-Weber, Z., Luckert, F., Martin, R. W., Walukiewicz, W., Foxon, C. T.

JOURNAL OF APPLIED PHYSICS Volume: 106 Issue: 10 Article Number: 103709 Published: NOV 15 2009

H-2. "An XANES and XES investigation of the electronic structure of indium rich In$_x$Ga$_{1-x}$N films"

By: Demchenko, I. N.; Chernyshova, M.; Piskorska-Hommel, E., Minikayev, R., Domagala, J.Z.,

Yamaguchi, T., Stolte, W.C., Lawniczak-Jablonska, K.

JOURNAL OF ALLOYS AND COMPOUNDS Volume: 509 Issue: 39 Pages: 9528-9535 Published: SEP 29 2011

H-3. "Full multiple scattering analysis of XANES at the Cd L$_3$ and O K edges in CdO films combined with a soft-x-ray emission investigation"

Demchenko, I. N.; Denlinger, J. D.; Chernyshova, M., Yu, K. M., Speaks, D. T., Olalde-Velasco, P., Hemmers, O., Walukiewicz, W., Derkachova, A., Lawniczak-Jablonska, K.

PHYSICAL REVIEW B Volume: 82 Issue: 7 Article Number: 075107 Published: AUG 5 2010

H-4. "Electronic structure of polycrystalline cadmium dichloride studied by X-ray spectroscopies and *ab initio* calculations"

By: Demchenko, I. N.; Chernyshova, M.; Stolte, W. C., Speaks, D.T., Derkachova, A.

MATERIALS CHEMISTRY AND PHYSICS Volume: 135 Issue: 2-3 Pages: 1036-1043 Published: AUG 15 2012

H-5. "Synthesis and Transformation of Zn-Doped PbS Quantum Dots"

By: He, X.; Demchenko, I. N.; Stolte, W. C., van Buuren, A., Liang, H.

JOURNAL OF PHYSICAL CHEMISTRY C Volume: 116 Issue: 41 Pages: 22001-22008 Published: OCT 18 2012

H-6. "XANES: observation of quantum confinement in the conduction band of colloidal PbS quantum dots"

By: Demchenko, I. N.; Chernyshova, M.; He, X.; Minikayev, R., Syryanyy, Y., Derkachova, A., Derkachov, G., Stolte, W.C., Piskorska-Hommel, E., Reszka, A., Liang, H.

JOURNAL OF PHYSICS Conf. Ser. Volume: 430 Article Number: UNSP 012030 Published: 2013

H-7. "Modification of the local atomic structure around Mn atoms in (Ga, Mn) As layers by high temperature annealing"

By: Demchenko, I. N.; Lawniczak-Jablonska, K.; Story, T., Osinniy, V ., Jakiela, R., Domagala, J.Z., Sadowski, J., Klepka, M., Wolska, A., Chernyshova, M.

JOURNAL OF PHYSICS - CONDENSED MATTER Volume: 19 Issue: 49 Article Number: 496205 Published: DEC 12 2007

Iraida Demchenko

IV.I. The context and scientific background of the research.

IV.I.1. Introduction.

The most driving interest in solid state physics is to understand the structure and property of matter. What makes a metal to have metallic properties? Why do silicates in glass become transparent to visible light but other forms of silicates do not? What makes iron a magnetic material? Why is diamond hard but a lump of coal remains fairly soft? They both are made of the same atoms after all. The list of such questions is infinitely long and it is easy to see that striving to fill it with answers is at the same time fascinating and finally potentially rewarding endeavor. The ability to control the physical properties of novel materials, by controlling crystallographic structure, arrangement of atoms inside sample's volume and along the surface taking into account point defects, is of crucial importance nowadays from both fundamental and applied research points of view. In order to understand the nature of matter we need to address ourselves to its building blocks - atoms. These, in turn, consist of nuclei and electrons with the electronic structure ultimately determining all properties of matter. It is, therefore, natural to anticipate that knowing electronic structure of different systems together with the ability to describe and predict electronic structure of new systems will bring progress in science and technology to a new level. Among the ways to reach such information X-ray spectroscopy techniques stand considerably out due to their capabilities to provide detailed information on material electronic structure and thus helping us to construct the informational bridge between the structural and electronic properties of wide class of materials.

This habilitation covers important examples of XAFS[1]/XES[2]/RIXS[3] applications, where the unique features of the photon 'in-/out-' process are exploited. The habilitation is organized as follows. After a short introduction presented in this Section the applicability of soft X-ray spectroscopy (both XANES and XES) for the highly disordered systems, on the example of $GaN_{1-x}As_x$ [H-1], is presented in Section IV.I.2. In Section IV.I.3 the interpretation of the core-hole effect using the real space multiple scattering Green's function (code FEFF8) and knowledge of the underlying mechanisms for 3*d* transition metal systems (based on $In_xGa_{1-x}N$ [H-2]) at metal *L* edge is presented. Sections IV.I.4 and IV.I.5. describe application of joint XANES, XES, and RIXS methods to estimate direct/indirect band gap size of materials (on the examples of CdO [H-3] and $CdCl_2$ [H-4]). The importance of X-ray absorption spectroscopy as a tool for observation of quantum confinement of colloidal quantum dots [H-5, H-6] is discussed in Section IV.I.6. Section IV.I.7 presents usefulness of EXAFS spectroscopy for

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[1] all the fine structures including XANES (X-ray absorption near edge structure) and EXAFS (extended X-ray absorption fine structure) are grouped into one term – XAFS (X-ray absorption fine structure).

[2] XES (X-ray emission spectroscopy).

[3] RIXS (Resonant inelastic X-ray scattering).

spintronic materials taking into account the results for a single substitutional/interstitial Mn impurity, Mn cluster formation and magnetic coupling on the example of $Ga_{1-x}Mn_xAs$ system [H-7]. Short description of the Habilitation candidate's contribution to scientific tasks, which were realized during her scientific career and are presented below, is presented in "Summary of work: own contribution" (Section IV.II). Overall, the examples demonstrated in this habilitation show efficiency of X-ray spectroscopic methods to obtain important information about the electronic structure of wide class of materials confirming the fact that these techniques are relevant to a broad variety of scientific tasks in material science.

Before turning to the main descriptive section of the habilitation, it is important to note that all aspects of researcher's work were covered by the Habilitation candidate in this project: the development of the research idea, which led to organization and realization of synchrotron measurements, interpretation of the obtained experimental data, theoretical analysis, dissemination of the result, allowing the Habilitation candidate to advance in the field of X-ray spectroscopy and to continue obtaining grants for new research topics.

IV.I.2. Application of X-ray spectroscopy to highly disordered systems. [H-1]

Alloying is a commonly accepted method to tailor properties of semiconductor materials for specific applications. However, only a limited number of semiconductor alloys can be easily synthesized in the full composition range. Such alloys are, in general, formed of component elements that are well matched in terms of ionicity, atom size, and electronegativity. In contrast, there is a broad class of potential semiconductor alloys formed of component materials with distinctly different properties in mentioned above terms. In most cases these mismatched alloys are immiscible under standard growth conditions. Opposite to the very extensively studied As-rich GaNAs alloys much less work has been devoted to highly mismatched alloys (HMAs) on the N-rich side of this alloy system. In these studies a highly mismatched $GaN_{1-x}As_x$ alloy system was successfully synthesized in the whole composition range using a nonequilibrium low temperature molecular beam epitaxy (MBE) technique. In addition to other techniques X-ray spectroscopy was utilized to determine the reorganization of electronic (around Fermi level) and atomic structure of novel $GaN_{1-x}As_x$ system in the whole composition range. Examination of atomic structure by XRD for the most part of samples was impossible since obtained films had no long ordering (i.e. had amorphous structure). It is an important fact that crystallinity is not required for X-ray spectroscopy measurements, making it one among a few structural probing techniques available for noncrystalline and highly disordered materials, including solutions. Analysis of X-ray spectroscopy results showed that in As low-doped GaN samples, impurity-like levels display a characteristic blue emission at room temperature, in contrast to samples with higher As doping percentages where an abrupt decrease in the band gap size of obtained $GaN_{1-x}As_x$ alloys was observed. This scientific project proposed by the Habilitation candidate was the first investigation of these materials using X-ray Spectroscopy. Discovered unusual electronic properties and capability for controlling the location of the conductive and valence band edges offer unprecedented opportunity for these alloys to be used in novel solar power conversion devices.

IV.I.2.1. Band gap and electronic structures of $GaN_{1-x}As_x$ over the entire composition.

The optical gaps of the $GaN_{1-x}As_x$ alloys were measured by absorption using a LAMBDA-950 UV/vis/NIR spectrophotometer over the range of 190–3300 nm. It was shown that the films in the composition range of $0.17<x<0.75$ are amorphous while those outside this range are crystalline (either single crystalline or polycrystalline). The band gap of the $GaN_{1-x}As_x$ alloys were estimated by extrapolating the linear part of the α^2 down to the energy axis [H-1]. A strikingly sharp band gap absorption is observed in all films. This is particularly significant for the amorphous films since it suggests that the densities of gap states in the amorphous films are low, consistent with the predicted low number of homopolar bonds in nitride based alloys [1]. Some small features below the band gap were attributed to the Fabry–Perot oscillations indicating uniform film thickness with a smooth surface and of the films with sharp film-substrate interface. Since crystalline and amorphous $GaN_{1-x}As_x$ alloys may be materials with very different properties, similar to crystalline and amorphous silicon, it was interesting to compare their properties directly, especially when very little is known about amorphous nitride materials. Despite the crystalline and amorphous transition the optical absorption results show a continuously monotonic decrease in the band gap as the As content increases. This provides additional support to the claim that the films are single phase with no phase separation in the crystalline state, and no composition nonuniformity in the amorphous state.

The composition dependence of the optical band gap energy for both crystalline and amorphous $GaN_{1-x}As_x$ alloys were compared directly with calculated composition dependence of the band gap. It was shown that the band gap values for the amorphous $GaN_{1-x}As_x$ alloys cannot be explained by the virtual crystal approximation (VCA) or the fitted curve using a single bowing parameter of 16.2 eV. Simultaneously, excellent agreement can be observed between the band gap values for the crystalline alloys and the band anticrossing (BAC) model [2-4, H-1]. The deviation of the experimental optical absorption results from the BAC calculations found for the amorphous alloys is not unexpected as the model has been developed for crystalline materials. Additional uncertainty is introduced by the fact that the band gap has been calculated as a composition weighted interpolation of the BAC model results and is less accurate for the alloys in the middle range of compositions.

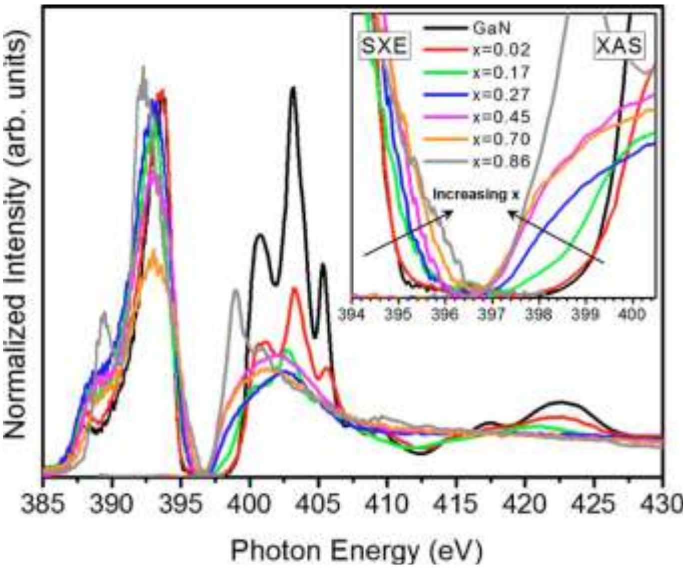

Figure 1

According to the BAC model the observed reduction in the band gap can be attributed to an upward shift of the valence band edge (VBE) and a downward movement for the conduction band edge (CBE) in the N-rich and As-rich $GaN_{1-x}As_x$ alloys, respectively. However, the absolute movement of the conduction band (CB) and valence band (VB) of the $GaN_{1-x}As_x$ alloys cannot be derived from conducted optical measurements.

As it was mentioned earlier, main contribution of the Habilitation candidate to solve the scientific problem described above was to examine electronic structure of investigated system around Fermi level by the combination of soft x-ray emission (SXE) and x-ray absorption (XAS) spectroscopies with the following interpretation of obtained results. XAS and SXE directly probe the partial density of states (DOS) of the CB and VB, respectively [H-1]. Overlapping the SXE and XAS spectra with reference to the core level provides a direct measurement of the energy positions of the VB and CB states in semiconductor materials. For this purpose, the nitrogen K-edge (around 400 eV) was investigated at room temperature at the Advanced Light Source (ALS) on beam line 8.0.1. XAS was detected by the total fluorescence yield detection mode with an energy resolution of about 0.2 eV, and SXE was measured using the Tennessee/Tulane grating spectrometer with a total energy resolution of 0.6 eV.

The absolute positions of the CBE and VBE are directly measured as a function of composition and compared to the results of conventional optical measurements [H-1]. The most striking changes in the spectra are the rapid broadening and suppression of sharp features of the XAS profiles with increasing As content (see Fig. 1). First the three prominent peaks in pure GaN are significantly reduced in amplitude and slightly broadened for alloys with a very dilute amount of As (x=0.02). This behavior is consistent with a small amount of structural disorder and a loss of orientational order of polycrystalline grains of the anisotropic wurtzite structure of GaN. This is confirmed with polarization dependent XAS spectra of these samples obtained by the Habilitation candidate. With increasing As content, the XAS spectra are transformed into very featureless smooth profiles for x=0.17–0.70 consistent with the complete loss of long-range periodicity in the amorphous state. Furthermore, very different XAS threshold lineshapes are observed for crystalline and amorphous alloys. For GaN and dilute As polycrystalline films, we observe a very gradual onset that arises from a single isolated band with light effective mass that disperses down from the main CB DOS and exhibits a quadraticlike DOS profile that is related to nonparabolic dispersion. The amorphous XAS threshold profiles, on the other hand, exhibit an abrupt ~1 eV shift to lower threshold energy but with profile very amenable to linear extrapolation. The increasing slope of this linear onset from x=0.17 to x=0.45 and then relatively constant for alloys with x up to ~0.70 can be understood as a gradually increasing amount of hybridization of N 2p partial density with As conduction states. The strength of this N hybridization with near neighbor As atoms reaches a maximum at 50% As stoichiometry. Despite the large changes in the XAS profile for dilute As (x=0.02), the threshold energy and gradual onset profile were unchanged. Hence the CBE is not responsible for the large ~0.8 eV decrease in the optical band gap observed for dilute As content. Instead, it is possible to observe a weak high-energy foot in the SXE threshold region that develops at the VBE. The VB change is consistent with valence N states hybridizing with an As impurity level just above the GaN valence band maximum (VBM), which is the basis for the BAC model of the band gap reduction in this dilute doping regime. For increasing As content into the amorphous phase, the threshold energy of the this VBE foot increases only by a small amount while the intensity grows steadily due the increasing amount of near neighbor As atoms, which hybridize with the N-p states. Finally, for the As-rich region from the sample with x=0.86, both the SXE and XAS profiles exhibit dramatic changes. The SXE spectrum of this cubic GaAs-like polycrystalline phase develops again a sharp two peak DOS profile but with a lineshape and peak maximum distinctly different from the polycrystalline phase of the hexagonal GaN-like dilute As region. The XAS profiles for the alloy with x=0.86 also exhibit a dramatic new sharp peak just above threshold. Rather than indicative of a structural change, this sharp peak reflects the existence of a localized N impurity level above the GaAs CB minimum. The development of this localized state into a narrow band via hybridization with GaAs conduction states is the source of the rapid band gap reduction from pure GaAs within the BAC model.

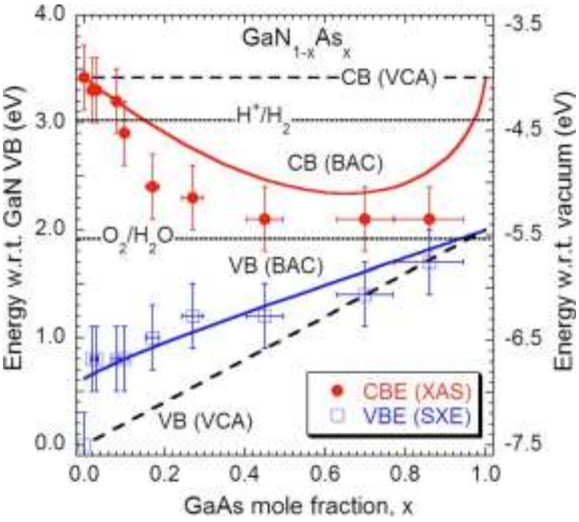

Figure 2

The composition dependence of the CBE and the VBE energies at N sites of $GaN_{1-x}As_x$ alloy as measured by XAS and SXE were displayed together with the BAC predicted values (see Fig. 2). It should be pointed out here that the calculated band movements by an interpolation of the BAC model are included for comparison purposes only. Band movements in the amorphous alloys may vary dramatically from those of crystalline alloys. Both CBE and VBE are observed to shift as x increases. A jump in the VBE to higher energy for dilute As (x~0.10) polycrystalline samples as compared to GaN is observed consistently with the BAC model. A second jump to lower energy is observed in the CBE upon entering into the amorphous phase (x ~0.17). For increasing x in the amorphous phase, both the VBE and CBE are only very weakly shifting to higher and lower energies, respectively. Finally a smaller jump in the VBE yet again to a higher energy is observed for the amorphous to As-rich polycrystalline transition (x~0.70). Not unexpectedly the smooth interpolation of the BAC model from the dilute polycrystalline regions does not explain the discontinuous energy jumps into the amorphous phase. It should be also pointed out that the band gap energies measured by XAS and SXE are lower than the values obtained by optical absorption. This may be attributed to excitonic coupling between the screened core hole and conduction electron [5].

IV.I.3. Interpretation of *L*-shell X-ray absorption spectra for transition metals. Essential aspects. [H-2]

XANES is currently of great interest in many scientific fields due to its promise of providing local chemical information in complex and disordered materials. However, both the calculation and interpretation of XANES have remained challenging problems. Band structure methods [6, 7] are used quite frequently to perform XANES calculations for metals. Although, these calculations are successful in reproducing XANES spectra, they are of limited application because of lattice periodicity requirements for this spectral region. In addition, these calculations often neglect a core hole (CH) as well as self-energy effects, and therefore do not allow direct comparison with experiment. In an attempt to remedy these difficulties the Habilitation candidate examined a SCF real-space multiple-scattering (RSMS) theory of XANES for InGaN system without any requirement of symmetry or periodicity. This method partly avoids the difficulties of large clusters by using full multiple-scattering (MS) calculations to obtain the contribution to the Green's function from a small cluster, typically less than 100 atoms, and a high-order MS expansion for important paths that extend outside this small cluster. The Habilitation candidate's contribution in this topic covered all aspects of research as was explained in the Introduction. Consequently, a detailed analysis of the L_3 edge XANES in transition metals was performed using relativistic, self-consistent real space Green's function code FEFF8 [H-2]. The results of this analysis will be presented in this section. Several recipes for taking into account CH when calculating X-ray absorption spectra are discussed. It was found that for indium rich InGaN films in In-L_3 edge XAS, the initial state (ground state) calculations matched well the experimental data only for InN film instead of excited (modified due to the presence of CH) electron density of states, where for all ternary alloys the opposite agreement was observed.

IV.I.3.1. Electronic structure of indium rich $In_xGa_{1-x}N$ films by XANES investigation.

Despite widespread application in optoelectronic and electronic devices, such as in white light emitting diodes and blue laser diodes, there are still many open questions concerning the basic material properties of group-III nitrides. The ternary (In,Ga)N compound covers the spectral range from the infrared (InN with a bandgap around 0.7 eV) up to the near UV (GaN with 3.42 eV). Unfortunately, this compound is not stable over the whole composition range. Bimodal and spinodal decomposition occurs and the ternary compounds remain stable only for In-contents less than 20% or greater than 80%. This instability range has been also shown to depend upon the strain state of the epitaxial layers. In order to gain more knowledge about this range, the study of $In_xGa_{1-x}N$ layers with a high In content were performed by X-ray spectroscopy.

The fact that the near edge region in the X-ray absorption reflects the electronic structure of the corresponding final state band was understood long time ago. The white line peaks in the $L_{2,3}$ edge XAS were first correctly interpreted by Mott [8] as being due to transitions from 2*p* to unoccupied *d*-like states near the Fermi level. Intensity of the white-line depends on the number of unoccupied states in the *d* band of the metal. The white lines are quite intense for the early transition metals of each transition series, but almost absent in case of metals with have almost filled *d* band such as Cu or In. In most cases, L_3 and L_2 edges have relatively similar spectral shapes. It is the reason why Habilitation candidate proposed to consider L_3 edge in the following interpretation. The main contribution of the Habilitation candidate in this project was to conduct a detailed analysis of the obtained XANES spectra and their subsequent theoretical interpretation while taking into account core-hole effect.

In [H-2] comparison of the calculated In-L_3 XANES spectra and PDOS for InN and $In_{0.23}Ga_{0.77}N$ alloy with the experimental results is presented (see Fig. 3). For both samples the main features in the L_3 spectra closely follow a mixture of the In *d*-PDOS with insignificant amount of In *s*-PDOS. By taking into account either transitions to $l-1$(s) or to $l+1$(d) states symmetry in the FEFF8 code for calculations of the “unpolarized” XANES In L_3 edge spectra, one can discriminate the contribution to different symmetry states. It is commonly accepted that contribution from transitions to the final *s* states is negligible. The density of *s*-symmetric final states is relatively small and spread over an extended energy range. As a result, the radial part of dipole transition matrix element for *s* states is approximately an order of magnitude smaller than for *d* states, and the *d* density of final states is larger and narrow. It was shown in [H-2] that the estimated contribution of metal *s* states into the InN spectrum is about 30 times weaker than that of *d* states. It agrees with the results obtained in [9] for the L_3 edge of Re, where the calculated ratio of the absorption cross sections corresponding to the transitions into *d* and *s* final states is about 50:1. However, we should emphasize that close to the CBM metal, *s* orbitals are involved into hybridization with N 2*p* states and could not be neglected since they influence on modification of the low energy region of In L_3 spectrum. It was also demonstrated by *ab initio* study (WIEN2k code) of electronic and optical properties of InN in wurtzite and cubic phases [10].

Since the final state in the soft X-ray emission process contains a hole in the valence band (VB) rather than the core level, the emission spectra reflect the ground-state PDOS provided that final state rule is valid. In case of X-ray absorption process, in the absence of a core hole (the initial state rule), both the initial and the final states in FEFF are represented by the ground-state single electron wave functions. The transition of an electron from a deep core level into the unoccupied orbital results in the creation of a core hole in X-ray absorption process. Therefore, the initial (ground state) and the final state Hamiltonians are different. A fully quantitative treatment of the core hole effect on XANES is not yet developed. Within the independent particle approximation calculations are typically carried out at two extreme cases, namely for static initial and final state potentials. The 'final state rule' says that in the one-electron approximation the photoelectron states should be calculated in the presence of a core hole. On the other hand, the 'initial state rules' says that the calculations should be done with a fully screened core hole (no core hole, NH). In the FEFF8 code, the core hole effect can be taken into account by putting a frozen core hole in the given core level. The SCF procedure then automatically screens the core hole. This approach yields a SCF treatment of core hole relaxation analogous to the Z+1 impurity approximation used by Zeller et al [11] in the Korring–Kohn–Rostoker (KKR) formalism. As an approach intermediate between the final state rule (full core-hole) and the initial state rule (no core hole), one can calculate the photoelectron states in a potential that has a half of electron removed from its core level, i.e. the so-called transition state rule suggested by Slater [12]. One can go even further and consider any fraction of an electron removed from the core level. Since all prescriptions described above are 'ad hoc', the choice between the initial and final state rule is somewhat arbitrary and is usually made by comparing the results of calculations with experimental data. In many cases, for example in case of K-shell absorption in insulators such as BN [13], or in semiconductors [14], the final state rule gives a better agreement with experiment. However, in case of the L-shell absorption in transition metals the situations is opposite and the initial state rule is favorable.

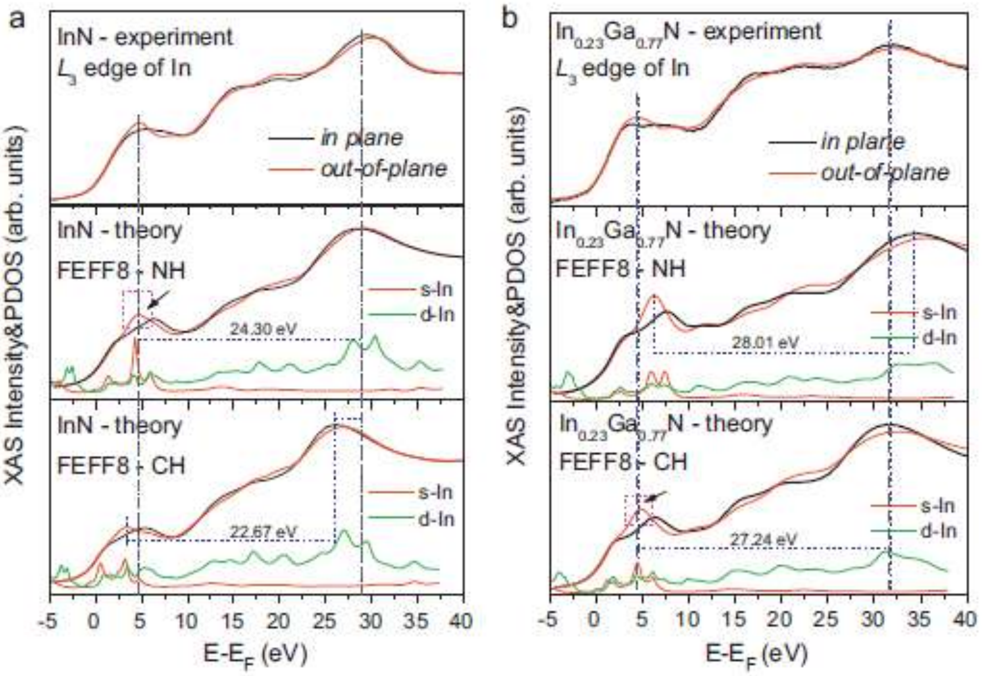

Figure 3.

To estimate the influence of the CH on the XANES spectral profile, additional calculations were performed assuming a completely screened core hole (NH) [H-2]. By detail comparison of calculations and experimental In-L_3 XANES spectra, it was found that, by taking the CH into account, the experimental spectrum for the $In_{0.23}Ga_{0.77}N$ is more closely reproduced, whereas for the InN the NH approach should be applied. The experimental spectrum for the InN is blue-shifted as compared to the CH calculated spectrum (the inclusion of a core hole leads to an energy shift of the *d* density of states due to electron – core hole interaction), and for the region around 29.3 eV after the edge, it more closely resembles the simulated spectrum without taking into account CH. The distance between the main resonances for NH model is 1.6 eV larger compared to CH model and agrees well with the experimental one. Therefore, for the InN a CH potential seems to be effectively screened by mobile electrons. Such an effect was not observed for the $In_{0.23}Ga_{0.77}N$ alloy where the accounting for CH provides better agreement with the experiment in the considered region. Let us remind that XANES spectra were collected by means of a surface sensitive detection mode (total electron yield, TEY). Thus, considering the results in [15], where the existence of an electron accumulation layer at the InN surface was quantitatively confirmed, we hypothesize that the screening of the core-hole potential for InN is more effective due to the extra free surface electrons, what does not appear to be the case for the $In_{0.23}Ga_{0.77}N$ film. Additionally, in [16] a notable difference between the X-ray absorption edge onsets for the total fluorescence yield (TFY, which is bulk sensitive) and the TEY modes was observed for nitrogen K edge of InN. The onsets were found to occur at approximately 0.8 eV and 1.4 eV above the valence band maximum, respectively. The Habilitation candidate attributed the shift of the absorption threshold for the TEY XAS by pinning the Fermi level at the surface high above the conductive band minimum, due to the intrinsic electron accumulation. These results confirm our assumption about screening of CH potential for indium L_3 edge of InN. Thus, the results presented here and in [H-2] demonstrate that it is indeed the case, at least for the transition metals with almost filled *d* band.

IV.I.4. Potential of combined soft X-ray emission and absorption spectroscopies for estimation of direct and indirect bandgaps size in semiconductors. [H-3]

With the arrival of high-brilliance third-generation synchrotron sources, a new approach to study the bulk band structure has been established, namely to utilize resonant inelastic X-ray scattering (RIXS). In RIXS, an electronic Raman scattering process is used to select specific excitations of valence electrons into unoccupied conduction band states. In other words, a core electron is resonantly excited into an unoccupied state at a certain *k* value, and the resonant fluorescence decay of a valence electron with the same *k* value into the core hole is detected. The observed RIXS spectrum thus contains momentum-resolved information about the occupied and unoccupied electronic states, which can be analyzed based on the Kramers-Heisenberg formalism [17]. Since the reachable information depth is typically of the order of a few hundred nanometers, study of systems with poorly defined surface properties or protective cap layers becomes possible.

Starting from the first resonant X-ray emission spectra gathered using synchrotron radiation a vivid discussion of resonance effects in RIXS has been occurring. Today it is widely accepted that band structure effects can be readily observed, and that this conclusion is true also for materials with core excitons. The purpose of the work presented in [H-3] was to demonstrate that RIXS indeed excellently describes the band structure of semiconductor (by the example of CdO) and the experimental spectra agree very well with *ab initio* DFT calculations based on band structures derived with various functionals.

IV.I.4.1. Analysis of O K-edge XANES for CdO films combined with a soft-x-ray emission investigation.

In order to probe the bulk-sensitive occupied valence band electronic structure, near-threshold excitation X-ray emission spectra were recorded for CdO films for excitation energies at the O K absorption threshold. Main contribution of the Habilitation candidate during realization of the project described in [H-3] was to demonstrate that the XES experiments are unique since they can provide direct evidence to the band structure of a semiconductor, in particular whether a semiconductor has direct or indirect band gap,

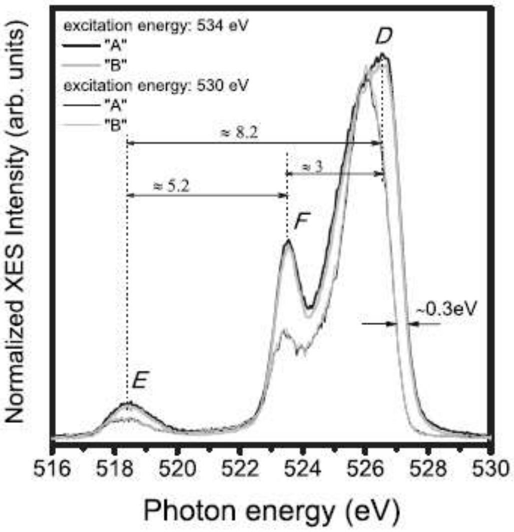

Figure 4

without further theoretical input. In a XES experiment the band-gap type can be determined by observing the emission spectra as a function of excitation energy. In case of a direct energy gap material, emission at the highest energy is expected for an excitation energy in the vicinity of the absorption threshold (into the conductive band (CB) minimum, CBM). As the excitation energy increases the emission should shift to a lower energy. For indirect band-gap materials the opposite behavior is expected, i.e., a shift of the emission spectrum (namely, top of the valence band (VB) maximum, VBM) to higher energy with increasing excitation energy. In another words, as the excitation energy increases, the probing transitions get closer, in *k* space, to the top of the VB. Our XES/RIXS data clearly show this tendency [H-3]. Fig. 4 presents the O K-edge XES spectra recorded with two different excitation energies which demonstrate that increasing the excitation energy from 530 (excitation energies just below the absorption threshold) to 534 eV (slightly above the first absorption resonance) shifts the top of the VB to higher energies at about 0.3 eV. This behavior results from a well-established *k*-selectivity effect, whereby restrictions on the intermediate state relaxation enhance the emission at the *k* point of the CB minimum relatively. Consequently, the selective appearance of a peak at 526 eV below the top of VB is a clear signature of an indirect band gap in CdO as opposed to a direct band-gap semiconductor which would have the opposite relative enhancement of spectral “weight” at the VBM.

As mentioned in this work, the size of CdO energy gap was controversial. The experimental direct band gap values, accepted in literature, are around 2.3–2.4 eV. The experimental values of indirect band gap represented in the literature vary from 0.55 and 0.84 eV (Refs. [18-20]) to the higher ones of about 1.2 and 1.9 eV (Refs. [21] and [22-24]). The same level of ambiguity exists in the reference data concerning the theoretical prediction of the indirect gap values, where the different ones are obtained using different approaches: linear combination of atomic orbitals (1.18 eV (Γ-L) and 1.12 eV (Γ-Σ); augmented plane wave (0.8 eV (Γ-L) and 1.2 eV (Γ-Σ) and 1.11 eV (Γ-L) and 0.95 eV (Γ-Σ); local density approximation (1.7 eV); GGA+U+Δ and HSE03 +GW (0.68 eV). Up to publishing of our article, we had not found any reports about the immediate evaluation of indirect gap values for CdO directly from combination of X-ray emission and absorption spectroscopy, except some attempts to indirectly estimate it [25]. To make up for this deficiency Habilitation candidate performed RIXS measurements to probe

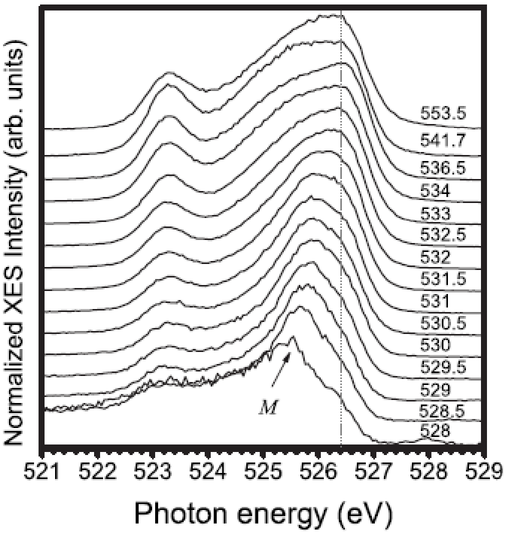

Figure 5

transitions at different points in the Brillion zone in the CdO film. In resonant excitation, the core electron is promoted to a bound state in the CB, so, the generated core hole recombines with the electrons from the higher electronic level (according to dipole transition rule), giving rise to the emission of a photon with the energy hv’ less than the energy of incident radiation, hv. For comparison, nonresonant excitation occurs when the incoming radiation promotes a core electron to the continuum. When a core hole is created in this way, it could recombine through one of the several different decay paths. Since the core hole is refilled from the sample’s high-energy free states, the decay and emission processes must be treated as the separate dipole transitions. It is in contrast to RIXS, where the events are concerned with each other and must be treated as a single scattering process.

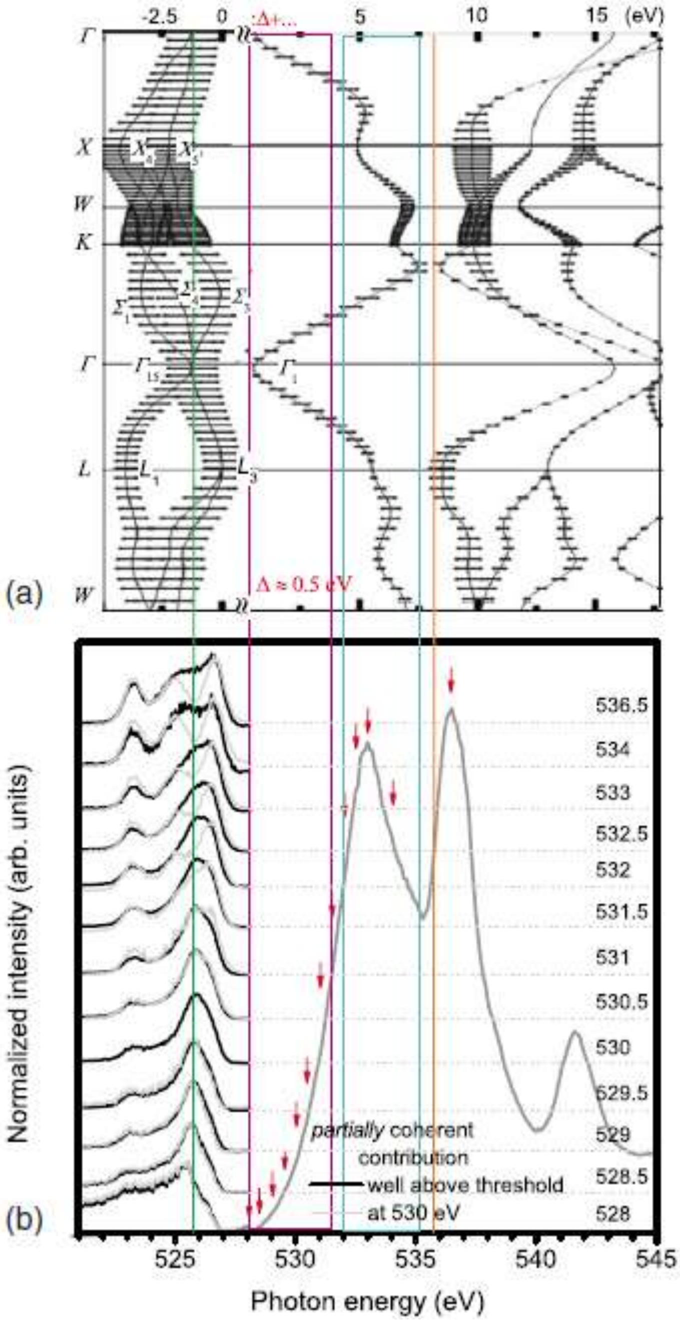

Figure 6

The RIXS spectra (see Fig. 5) were recorded in 0.5 eV step through the threshold region up to the first absorption peak at about 533 eV, as indicated by arrows on the XAS spectrum (see Fig. 6(b)), and then for the resonances: 536.51, 541.7, and 553.5 eV. An elastic emission peak in the threshold-excited XES is used for correspondence with the XAS photon energy scale. The key experimental observation is the relative loss of intensity near the VB maximum and apparent shifts to lower energy as excitation energy is tuned closer to the CB minimum threshold (at about 528 eV). Nonlinearity of the VBM profile (see region 525–527 eV) in comparison with peak positioned at around 523.2 eV is clearly seen on the intensity map (see Fig. 7(a)).

To understand the energy shifts and RIXS line shape changes, a procedure for subtracting the residual "incoherent" fraction component of the RIXS spectra has been proposed and used for enhancing the band-structure effects of the coherent fraction component [26]. This involves usage of a high-energy excited spectrum well above threshold as a representative of the incoherent X-ray emission with *k* mixing via intermediate state relaxations and scattering processes. This incoherent spectrum is then scaled and subtracted from the closer-to-threshold excited spectra with the restriction that remaining intensities must be positive. We call such a procedure as a standard one. For indirect band-gap materials such as silicon and BeTe, this procedure has been applied with clear and understandable results [27, 28]. However, for CdO the leading energy shift of the VBM above threshold (see Fig. 4) is problematic for these data analysis procedure (namely for a few first excitation energies spectra) since even with different scaling either a negative intensity dip above the 527 eV VBM results from subtraction of a high energy XES spectrum or subtraction has no effect on the spectra profile (an incoherent contribution is still there). Hence, there is a quandary that while there is 0% incoherent fraction between 527 and 527.5 eV in the 528 eV threshold spectrum, there is still clearly an incoherent shoulder from 526.2–527 eV extending above the 525.5 eV peak that one would like to subtract off. It is still visible after any type of subtraction taken for the estimation of pure coherent fraction. We propose that the CdO data set is showing a progressively varying partial *k* mixing of initial and final states near the threshold and thus a varying incoherent line shape. The failure to find a single

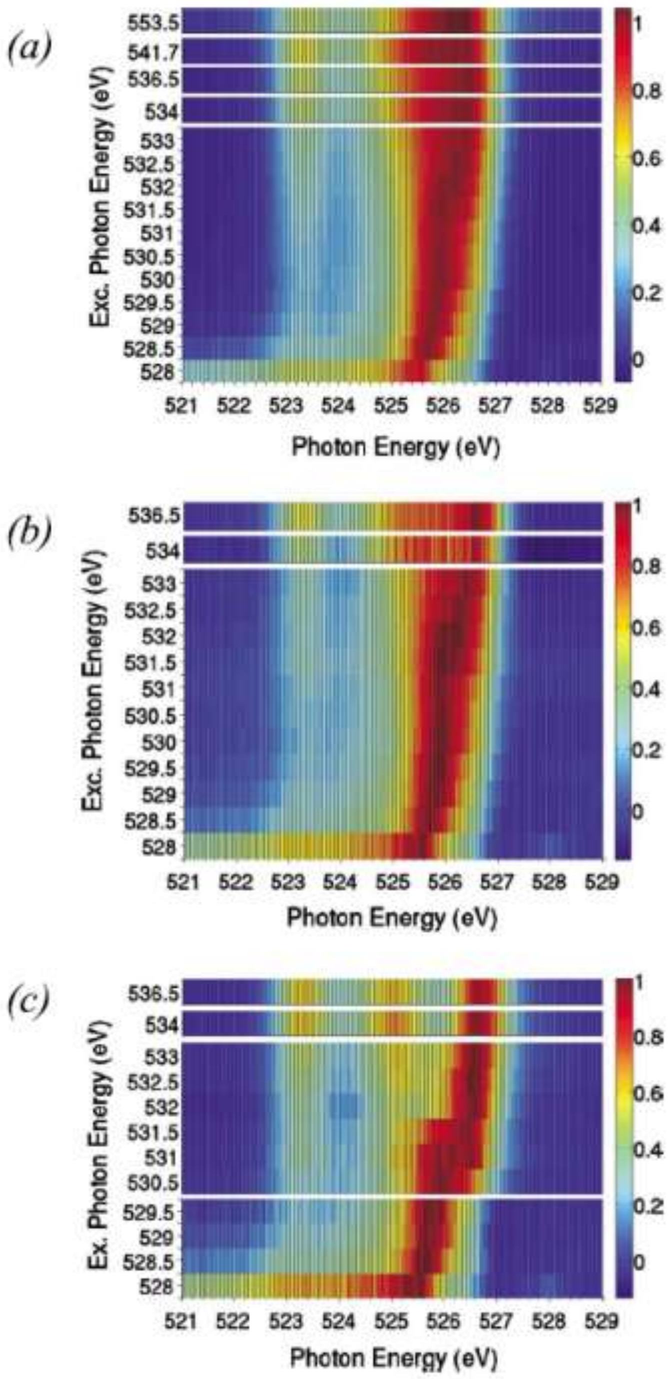

Figure 7

representative experimental incoherent line shape results from an over-simplified approximation that breaks down, probably, for the very large 4 eV CB dispersion of CdO. The single incoherent line shape subtraction works well for Si and BeTe where the CB lowest branch dispersion is <1 eV (Refs. 27 and 28) and complete *k* mixing is easier even near the threshold. From this scenario, we then claim from Figs. 6 and 7 that the VB-CB gap in the XES-XAS threshold spectrum has no special meaning due to partial *k* mixing. Since the standard incoherent subtraction procedure could not result in completely removing the incoherent fraction and could not give fully a demonstration of the band structure of (Γ_{15}-L and Γ_{15}-Σ) branching effect (see Fig. 6(a)), it was decided, then, in parallel to the standard approach described above, how to arbitrarily enhance the excitation energy line shape changes by subtracting off an intermediate XES spectrum at 530 eV. In Fig. 6(b) we present the resulting, partially coherent, emission spectra with comparison to the band structure (Fig. 6(a)) taken from Ref. [29]. The partially coherent contributions corresponding to standard procedure are denoted by black lines, whereas light gray lines correspond to subtraction off an intermediate XES spectrum at 530 eV excitation energy (called here as an intermediate). In Fig. 7 we present intensity maps corresponding to standard and intermediate partially coherent fraction of XES along with RIXS for a better visualization of band dispersion branches away from the (Γ_{15} point (see Fig. 6(a)). To align the calculated band structure with respect to the experimental data the VB Γ_{15} high-symmetry point was matched with the VBM of XES corresponding to excitation energy at 528.5 eV, so, the CBM was shifted from the theoretical value of 1.9 eV to the optical experimental value at about 2.4 eV.

The estimated direct band gap value for CdO films, from our own optical absorption measurements, by an extrapolation of the square of the absorption coefficient comes to ~2.4 eV. Qualitatively, the aligned band structure agrees quite well with our results. This comparison highlights the low-energy and high-energy dispersions of the VB intensity with a good correspondence to the X and L high-symmetry points that lie at about 0.6 eV below and at about 1.0 eV above the Γ-point Γ_{15} energy. The Cd 5*s* orbital with even symmetry and the O 2*p* orbital with odd symmetry cannot mix at the Γ point, so, the translation symmetry constraints are such that the Cd 5*p*-O 2*p* interaction is fully antibonding. Taking this into account and comparing our PDOS distribution (see H-3) with the presented band structure (Fig. 6(a)) we are able to conclude that the orbital character of the lowest energy CB branch is mostly of Cd 5*s*-O 2*p* σ*. As is well known, the VB upper bands have predominantly O 2*p* character.

IV.I.4.2. Estimation of band-gap values.

In Fig. 8 the overlapping of selected XES and XAS spectra (with the excitation energies equal to 528.5, 534, and 553.5 eV) in photon energy scale is presented. Two curves corresponding to partially coherent contributions (standard ones) are added to the plot (at 528.5 and 534 eV of excitation energy, curves of the smaller intensity) for more precise estimation of energy gap. Starting from the excitation energy of 534 eV the edge of VB remains at the same energy and only the high energy tail increases its intensity. It should be noticed that the VB maximum (labeled as "M" in Fig. 5) movement occurs without any constant energy separation from the elastic peak position when the excitation energy increases. This suggests that the VBM for excitation energy of 528 eV cannot be associated with a constant (Raman-type) loss feature. To be firmly convinced, the 528.5 eV excitation energy spectrum was assumed to be a determinative one during our estimation of band-gap value. Taking into account that the CB minimum lies at 528.1 eV (point where absorption starts, obtained by taking the first nonzero values of the XAS spectrum first derivative), and the maximum of XES spectrum with the lowest excitation energy (528.5 eV) lies at 525.7 eV, we can evaluate the band-gap value to be 2.4 eV (Γ_1-Γ_{15} gap on the band structure). This is in good agreement with the direct band gap value presented in the literature and coincident with our own optical results.

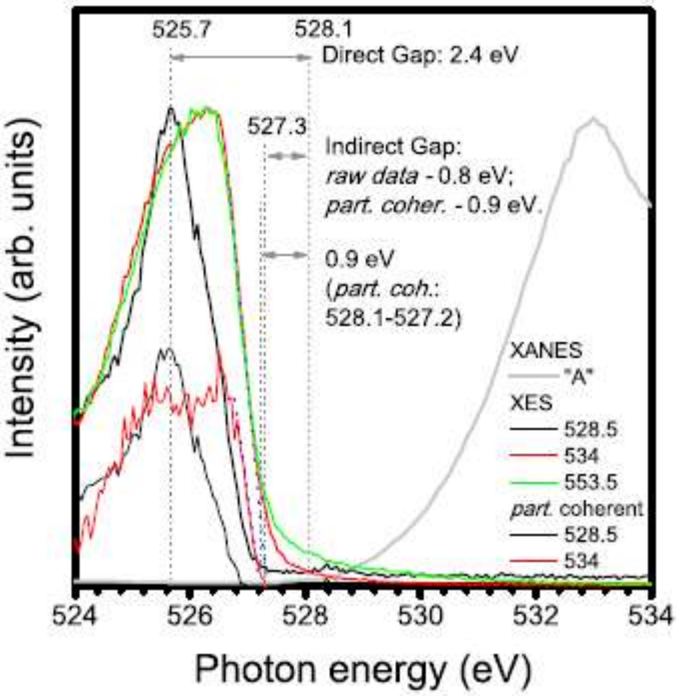

Figure 8

Next, the difference between the CBM and the top of VB (at about 527.2 eV close to the L point) with the highest excitation energy is equal to about 0.9 eV which is in quite good agreement with the reported indirect band gap of 0.84 eV. Moreover, as is well known, the procedure of the indirect band-gap value estimation in case of thin CdO films by means of optical absorption spectra faces essential difficulties in view of weak signal and influence of Fabry-Pérot oscillations on the pre- and near-edge region. In order to directly measure the indirect gap of CdO by optical absorption we grew, then, a thick CdO film (0.6 μm) so the indirect gap absorption is more significant. Electrical property of this thick CdO film is comparable to the thin CdO studied here. Linear extrapolation of the square root of the absorption coefficient gave a value of indirect band gap at about 0.95 eV which agrees well with our results discussed above.

Thus, combination of Figs. 6 and 8 allows us to conclude that for investigated CdO thin films—(i) the direct energy gap at the Γ point is $\approx$2.4 eV, (ii) an indirect gap of $\approx$0.9 eV which implies dispersion along Γ-L and Γ-K, and (iii) lower energy dispersion along Γ-X. Furthermore, the overall theoretical VB bandwidth is in good agreement with the lower energy XES peak at about 518 eV and overall 4–5 eV band width. Such clear and distinct indirect band gap and valence band dispersion signatures in CdO RIXS were not observed in previous X-ray emission studies, in part, because of the worse energy resolution and since the threshold excitation region down to 528 eV was not probed.

IV.I.5. X-ray spectroscopies and *ab-initio* calculations in studies of electronic structure of polycrystalline cadmium dichloride. [H-4]

Similar to the approach presented in Sec. IV.I.4., the analysis of cadmium dichloride RIXS spectra measured around the chlorine K core threshold was performed in another study with the details to be found in [H-4]. Two dominant contributions in the RIXS data were distinguished, namely, the resonant and the excitonic contributions. It was shown that the dispersion relation below the absorption threshold follows Raman Stokes law, whereas, dispersion above the threshold splits into two qualitatively different relations. Only the high-energy edge of the excitonic sideband follows a linear dispersion. This dispersion is shifted relative to the Raman-Stokes linear one below the absorption threshold by about 0.85 eV. The constant features below absorption threshold were attributed to the excitation of a valence electron into the CB with the energy of 6.6 ± 0.15 eV. The Raman features above absorption threshold occur presumably from splitting of core and valence excitons contribution (see Fig. 9). To make this supposition completely clear further theoretical investigations were needed.

As the excitation increases well above the core binding energy, non-linear dispersive effects were observed. The experimentally determined direct band gap of $CdCl_2$ came to ~5.7 ± 0.05 eV at the Γ high symmetry point, which was in good agreement with the fundamental optical absorption energy gap. Good agreement between experimental XES, XANES spectra and calculations using WIEN2k code was also obtained. Conducted by the Habilitation candidate investigations were among the first ones where RIXS was utilized for $CdCl_2$ band structure exploration.

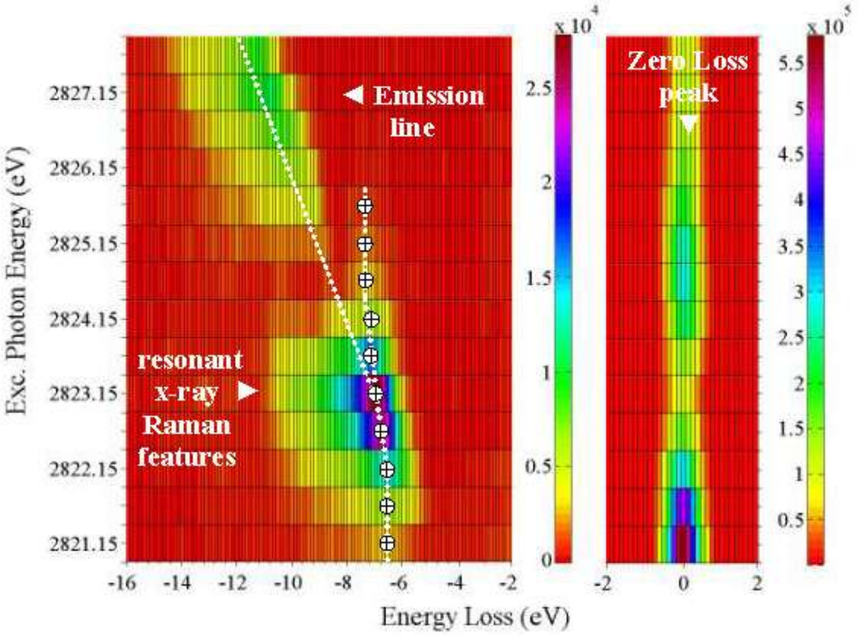

Figure 9.

IV.I.6. Quantum confinement effect manifested by XANES for the conduction band of colloidal quantum dots. [H-5, H-6]

The first appearance of semiconductor nanocrystals as the building blocks of nanotechnology has opened up new ways to utilize them in next generation solar cells. In this field, low-dimensional structures have recently provoked an increasing interest. Due to the decreased size of nano-particles (NPs) down to the nanometer scale, quantum effects occur, thus some physical (e.g. mechanical, electrical, optical, etc.) properties change compared to those of bulk materials. For example, the quantum confinement effect can be observed once the diameter of the NP is of the same magnitude as the wavelength of the electron wave function. Along with the decreasing size of NPs, the energy levels of NPs turn from continuous states to discrete ones, resulting in a widening of the bandgap apparent as a blue shift in the absorption and photoluminescence spectra. There is common agreement in the literature that it can be useful for photo-voltaic (PV) applications. The results presented in this Section are based on [H-5, H-6] and aimed to contribute to the research and development of alternative energy sources which our civilization would be forced to use in the nearest future. Namely, it presents the preliminary research of electronic local structure of unoccupied states under quantum dots (QDs) size modification with supporting investigations of XRD and TEM. To our knowledge these were the first X-ray absorption investigations on these materials, which revealed the detailed local electronic structure of QDs in comparison to the bulk one. That kind of in-depth knowledge of the properties of such materials would be invaluable for their prompt application in solar energy conversion devices.

IV.I.6.1. Confinement by example of PbS QDs.

According to the synthesis procedure described in [H-5], nano-particles of different sizes, ~50 nm (NPs) and ~5 nm (QDs), were grown as was manifested by TEM. A narrow size distribution of QDs is observed. The high resolution (HR)TEM investigations confirmed the monocrystalline PbS QDs formation. In accordance with synchrotron XRD result [H-6], three main fcc diffraction patterns, i.e. 200, 111, and 220, were identified. These investigations confirmed PbS QDs single-phase character with NaCl structure.

XANES measurements were devoted to directly evaluate the eventual modification of conductive band position/profile of bulk PbS versus PbS QDs. Fig. 10 shows the bonding symmetry for the bulk and QDs of PbS along with $PbS(VI)O_4$, $Na_2S(IV)O_3$ standard samples near the sulfur K edge spectra recorded in total fluorescence yield (TFY), total electron yield (TEY), and transmission (TR) detection modes. The transitions from an atomic-like S 1*s* state to the unoccupied S 3*p* σ* antibonding orbitals are probed.

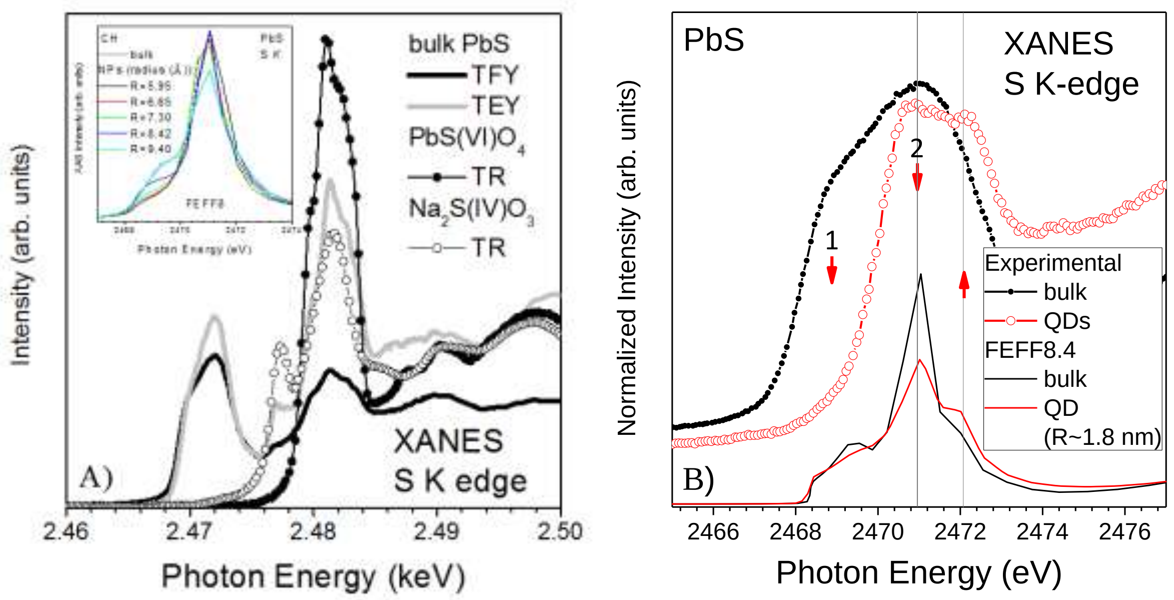

Figure 10

For bulk PbS target the self-absorption (SA) effect [30, 31] was visible in experimental data (intensity damping of the first resonance, see Fig. 10 A)). The differences in the spectral profiles for bulk PbS XANES spectra collected in TFY and TEY detection modes in the higher energy region, 2.476-2.486 keV, definitely indicate on the surface oxidation. From comparison of investigated here XANES spectra to $PbSO_4$ and Na_2SO_3 standards and the literature data [32], the feature at ~2.478 keV can be attributed to the absorption of sulfur in the form of sulfite ($S(IV)O_3$), whereas the second resonance at ~2.482 keV mainly in the form of sulfate ($S(VI)O_4$), Fig. 10 A.

A blue shift, visible for the absorption threshold (inflection point), is about 1.67 eV for PbS QDs with respect to the bulk one in consequence of decreasing the conductive band minimum p-S states contribution, antibonding orbital of t1u symmetry, at about 2.470 keV (see the shoulder marked as 1), Fig. 10 B. Whereas the absorption onset positions for bulk and QDs PbS obtained under the technique mentioned in [33], so called extrapolation and arctangent subtraction data analysis methods, make possible to conclude that this shift is less than 1 eV.

As it is well known, the energy gap of semiconductor separating the conduction and valence energy bands is its defining feature. In semiconductors of macroscopic sizes the gap width is a fixed parameter determined by the material's peculiarity. It is changed in the case of nano-scale semiconductor particles smaller than ~10 nm. This size range already corresponds to the regime of quantum confinement, when the spatial extent of the electronic wave function is comparable with the quantum dot size. As a result of such "geometrical" constraints, electrons "feel" the presence of the particle boundaries and respond to the particle size changes by adjusting their energy. This phenomenon is known as the quantum-size effect and it plays an important role in QDs. Here we assume that a blue shift of the absorption threshold (Fig. 10 B) occurs due to quantum confinement.

Our suggestion is bolstered up by the fact that contrary to Si, Cu_2S, $CuInS_2$, $CuInGaSe_2$ and $CuZnInS_2$ having small Bohr exciton radii and generally preserving their bulk properties, PbS has large Bohr exciton radius, ~ 20 nm [34]. Since the QDs radius of PbS investigated here is much smaller than the Bohr radius of the exciton in the initial bulk material, optical and electronic properties of PbS QDs may exhibit their great enhancement allowing the wide tunability, even producing bandgaps that can reach the red edge of the visible light. It was shown that the optical absorption onset of PbS QDs can be tuned from 3000 nm to < 600 nm as a function of QD size [35]. Precise examination of the TEM data shown in [H-5] reveals the dimension of the smaller PbS QDs to be of order of 5 nm. If these QDs are the main contributor to the aggregate, they will account for the blue shift in the XANES spectrum of PbS QDs.

Other noticeable differences in XANES spectra were found comparing the above edge regions, around ~2.480 keV, Fig. 10 B. The sharp features around ~2.480 keV in colloidal PbS QDs can presumably be attributed to the absorption of sulfur in the form of thiosulfate [36] versus sulfate/sulfite revealed at the surface of bulk PbS.

As observed there are no differences in TFY and TEY XANES of QDs spectra profiles, except a small discrepancy in the resonances intensity (data are not presented here). As particles become smaller, a bigger fraction of the atoms is located on the surface, resulting in the increased surface sensitivity (we are considering here the influence of "surface atoms" on the final XANES spectral profile) often visible in TEY measurements compared to TFY. As it is shown the investigated QDs have the average size of about 5 nm. For such small objects the contribution of surface component from each QD is hardly distinguishable within the differences between TEY and TFY spectra, since even for the soft X-rays the probing depths for TEY and TFY are of about 5 and 100 nm, respectively [37]. These values are larger for semi-hard X-rays. It makes clear why TFY and TEY XANES spectra for the sample with QDs provide similar profiles.

Finally, the XRD analysis of PbS QDs does not expose the existence of other, than cubic, phases of PbS with the rock-salt structure [38], whereas all standards, discussed under XANES qualitative analysis, have low-symmetry crystallographic structure, like orthorhombic or monoclinic, which was not detected by the XRD. It is likely that the surface of PbS QDs is oxidized, forming a thin structurally disordered in macro-scale, thus invisible to XRD, passivated layer of SO_x. We cannot exclude the possibility that the thiosulfate comes from the oxidation of unreacted S^{2-} in the system.

Qualitative analysis of PbS QDs and thiosulfate [31] XANES spectra allows us to preliminarily conclude, that the surface sulfur atoms in the state of thiosulfate have a minor contribution into the spectrum profile close to conduction band minimum. To conclusively determine a measure of the surface oxidation and to estimate precisely its eventual influence on the observed blue shift, in comparison to the quantum-size effect, further photoelectron spectroscopy and high resolution TEM measurements with the following advanced analysis are necessary and are currently ongoing.

IV.I.6.2. Size effect in FEFF calculations.

The calculations of PbS cluster of increasing size were done by FEFF8 by adding the successive coordination shells to the central S atom until radius (R) of 9.4 Å. It was found that the S p unoccupied states form a shoulder at the absorption edge enhancing its intensity (inset in Fig. 10 A) until cluster radius 9.4 Å, where no further modification of near-structure profile was found. Next, the calculations for cluster of fixed diameter of 3.6 nm were repeated taking into account a different number of inequivalent sites of S close to the surface region, defined as sites with different coordination numbers. Such an approach was previously described in details in [39]. It concerned the relation between the total number of atoms in full shell cluster and the percentage of surface atoms. The result is presented in Fig. 10 B at the bottom. A significant effect of decreasing the shoulder intensity (marked as 1) and increasing the states marked as 2 was observed for the sample with QDs compared to unoccupied states of bulk PbS. Similar dependence is clearly visible in the experimental XANES spectra, establishing, thus, that electronic structure of unoccupied states close to the absorption threshold is very sensitive to size effect and surface atoms contribution in the final XANES profile.

IV.I.7. EXAFS studies for spintronic materials. [H-7]

Recently, there has been a rapid development in the field of research called spintronics, a new paradigm of electronics which utilizes not only the charge of electron but also its spin. Addition of such an extra degree of freedom could potentially lead to a creation of electronic devices which, besides being much faster and having much lower power consumption, possess nonvolatile properties as compared to contemporary ones based on conventional semiconductor. To achieve this it is necessary to fabricate effective injectors of polarized spins, learn how to manipulate and detect spin polarization, and to integrate magnetic materials with the conventional semiconductor technology. All of this requires fabrication of suitable materials with appropriate properties at room temperature and manufacture of a reliable spin based device.

This Section presents the results of the study of $Ga_{0.95}Mn_{0.05}As$ film before and after annealing at temperatures of 500 and 600◦C [H-7]. EXAFS spectra were examined to determine the average local atomic structure around Mn atoms. These investigations performed by the Habilitation candidate were among the first ones for GaMnAs system. The EXAFS technique is sensitive to the local structure around a selected element, what makes it an effective tool for studying multicomponent materials. To characterize the films, SIMS and XRD methods were used to evaluate the content of Mn and quality of the grown film. Measurements of the magnetic moment for the same samples were also performed to relate the structural properties with the magnetic ones.

IV.I.7.1. Modification of the local atomic structure around Mn atoms in (Ga, Mn)As layers by high temperature annealing.

Out of all of the reported structures for as-grown films, EXAFS data indicate that Mn atoms are the most likely substitute for Ga in a GaAs matrix. Dramatic structural changes were reported at a high annealing temperature (around 450◦C), e.g. [40]. The Habilitation candidate suggested that this was probably due to initial stages of precipitation of an MnAs phase. To verify this hypothesis we have performed detailed studies of $Ga_{0.95}Mn_{0.05}As$ single layers annealed at 500 and 600◦C.

SIMS and XRD methods were used to evaluate the content of Mn and quality of the grown layer. Measurements of the magnetic moment for the same samples were also performed to relate the structural properties with the magnetic ones. The influence of high temperature annealing on the structural and magnetic properties of GaMnAs layers grown by MBE was investigated by EXAFS, HRXRD, and SQUID techniques. It was shown that annealing at 500◦C introduces large disorder in the zinc-blende GaMnAs structure with Mn concentration of 0.05 and causes the relaxation of the matrix from highly compressively strained in the 'as-grown' sample to only slightly strained. Simultaneously, the structure around Mn atoms becomes more disordered as compared to the reference sample and the distance between Mn–As atoms in the first coordination sphere becomes much longer and is close to that predicted for MnAs cubic structure (~2.55 Å). No evidence for the formation of Mn dimers or small clusters was found. The annealing at 600◦C leaves small tensile strain in the GaAs host matrix but results in the formation of hexagonal MnAs inclusions, which still have large structural disorder and clearly form hexagonal structure. The MnAs inclusions are ferromagnetic with Curie temperature of about 300 K. TEM studies performed for the same sample, studied by EXAFS and described in this paper, revealed that the hexagonal inclusions of MnAs had a spherical shape with diameter around 20 nm. Most of the MnAs clusters were coherent with the GaAs matrix. The annealing of (Ga, Mn)As at 600◦C is a suitable method to form small hexagonal MnAs inclusions in the GaAs host matrix, exhibiting ferromagnetic properties at room temperature.

Knowing the atomic structure of a sample, let us relate it to its magnetic properties. The magnetic properties of $Ga_{1-x}Mn_xAs$ as-grown samples, within wide limits of x, have been actively studied, e.g. [41]. The Curie temperature for the $Ga_{1-x}Mn_xAs$ layer with $x = 0.053$ was reported to be about 110 K [42]. The magnetic properties of annealed samples were examined and their ferromagnetic contribution clearly evidenced by magnetization hysteresis loops. For sample annealed at the highest temperature the ferromagnetic state exists up to room temperature. The saturation value of magnetization M_s found experimentally in this layer is about 20 emu cm^{-3} at T = 10 K. It agrees well with the results of previous magnetic studies of $Ga_{1-x}Mn_xAs$ layers annealed at high temperatures: $M_s = 17$ emu cm^{-3} was observed in [43] in the layer with $x = 0.05$, while $Ms = 40$ emu cm^{-3} was found in [44] in the layer with $x = 0.06$. Assuming the expected magnetic moment of 5 Bohr magnetons per Mn ion and the technological data for Mn content and layer thickness, one can estimate the magnetization saturation value $M_s = 50$ emu cm^{-3} for an ideal ferromagnetic $Ga_{1-x}Mn_xAs$ layer with $x = 0.05$. Taking into account the unavoidable reduction of the magnetization expected due to non-collinear spins at the surface of nanoclusters and magnetic blocking effects, one can conclude that a large portion of Mn ions present in the layer belongs to the ferromagnetic nanocluster phase. It strongly supports the conclusion of the structural analysis of annealed at 600°C layer, evidencing the presence of hexagonal MnAs inclusions for which Curie temperature of about 310 K is expected [43, 44]. The magnetic properties of the layer annealed at lower temperature show about 10 times smaller ferromagnetic contribution characterized by much smaller coercive field. Based on the results of the EXAFS and XRD analysis, we attribute this behavior to the formation stage of Mn-rich zinc-blende clusters within the GaMnAs layer exhibiting strong magnetic disorder and a broad ferromagnetic transition region. The largest portion of Mn ions in annealed at 500°C GaMnAs layer is in the paramagnetic state.

Consequently, the EXAFS investigation proved that after thermal treatment, the local structure transition around Mn atoms takes place from the chemically homogeneous 'as-grown' layer to the chemically inhomogeneous layer (with cubic Ga(Mn)As clusters), and further to the material with well-developed MnAs hexagonal clusters [H-7]. This points out that the investigated structure is unambiguously placed in the groups described in [45]. It is worth emphasizing that high temperature annealing (600◦C) results in a dramatic modification of the magnetic properties of the layer with Curie temperature of about 300 K, which is the crucial point for spintronic materials applications.

IV.II. Summary of work: own contribution.

To understand the mechanism for changes of material properties, we must understand the local environment and electronic structure of the investigated elements at the atomic scale. Theoretically, the changes in the electronic structure caused by the presence of trace elements (dopants), point defects, quantum effects, etc. are difficult to discuss even qualitatively and hardly possible to discuss quantitatively within the framework of conventional solid state physics, as opposite to the case of defect-free crystals. Luckily, there are several experimental methods for analyzing the local environment of atoms and/or ions along with their electronic structure reorganization. Among these methods, X-ray spectroscopy, which uses synchrotron radiation, occupies a special place. The most significant achievements of the representative examples of the Habilitation candidate's research enclosed in this habilitation, which added both to the improvement of the technique itself as well as to the growth of the scientific knowledge about each particular system, are:

- Effective use of soft X-ray spectroscopy (XAS vs XES) for materials with a high level of structural disorder in order to determine the size of the band gap by tracking the dynamics of top of the valence and bottom of the conduction bands and following comparison of obtained data with theoretical VAC and BAC models [H-1]. For the $Ga_{1-x}N_xAs$ films in the whole composition range chosen as an example, it was shown that the reduction in the band gap can be attributed primarily to the downward movement of the conduction band (CB) minimum for alloys with $x>0.2$, and to the upward movement of the valence band (VB) maximum for alloys with $x<0.2$. The unusual electronic structure and capability for controlling the locations of the CB and VB edges offer unprecedented opportunity to use these alloys for novel solar power conversion devices. It was the first investigation applying X-ray Spectroscopy for these materials.
- The importance of considering the core-hole (CH) during calculations of XANES spectra and their following comparison to experiment. XANES calculations often neglect core-hole effect and therefore do not allow direct comparison with experiment. A detailed analysis of the In-L_3 edge XANES in transition metals (shown on the example of $Ga_{1-x}In_xN$ films in whole composition range) was performed using relativistic, self-consistent real space Green's function code FEFF8 [H-2]. For pure InN the no-hole approach describes better the experimental XANES data, which is due to an accumulative layer effect causing a higher concentration of free carriers in InN that fully screen the core level with a hole. For all ternary alloys the opposite approach (with CH) better fits the experimental data. The results presented here demonstrate that it is indeed the case, at least for the materials containing transition metals with almost filled *d* band.
- Estimation of semiconductor band gap size and type by combination of RIXS and XANES. These were pioneering works where it was demonstrated how to estimate the direct/indirect band gap

size of semiconductor materials using X-ray Spectroscopy [H-3]. Presented RIXS CdO data set shows a progressively varying *partial* ***k*** mixing of initial and final states near the threshold and thus a varying incoherent line shape. Overlapping of XAS spectrum with RIXS ones makes possible to estimate both direct and indirect bandgap values. The obtained results are consistent with the theoretical/experimental ones presented in the literature and our own optical absorption results.

Further, it was shown that the position of the RIXS band in $CdCl_2$ follows a linear dispersion according to the Raman Stokes law if the excitation energy is tuned below the absorption threshold [H-4]. The situation changes for core excitation above the photoabsorption threshold where the dispersion relation is split into two branches. The position of the resonant contribution does not depend on the excitation energy, while the excitonic sideband follows the Raman Stoke law. Combined XANES and RIXS measurements compared to the calculated band structure (by Wien2k code) allowed determining the direct band gap of $CdCl_2$.

- Observation of quantum confinement effect manifested by XANES [H-5, H-6]. In case of PbS system it is generally agreed that quantum confinement caused by the restricted size of the nanometer scale PbS particles is essential for the light-emitting properties. A prediction of the quantum confinement model is that the energies of the valence band and conduction band edges are shifted relative to the bands of bulk PbS, leading to an increased energy gap. To date the change in the VB and CB edges as a function of the nanocrystal PbS size has not been experimentally determined.
- Application of EXAFS spectroscopy to examination of structure changes. This was among the first investigations of modification of the local structure around Mn atoms in (Ga, Mn)As layers after high temperature annealing by EXAFS and relation of the results to their magnetic properties [H-7]. The qualitative and quantitative analysis of EXAFS spectra gives unambiguous evidence for the transition from a cubic to a hexagonal phase around Mn atoms as a result of annealing at temperatures of 500 and 600 °C. It was concluded that the annealing of (Ga, Mn)As at 600 °C is a suitable method to form small hexagonal MnAs inclusions in the GaAs host matrix, exhibiting ferromagnetic properties at room temperature. These investigations performed by the Habilitation candidate were among the first ones for GaMnAs system.

Acknowledgements

I would like to express deep thanks to Advanced Light Source synchrotron facility (Berkeley, USA) for allowing me time and access to the equipment to perform XANES/XES/RIXS measurements of the considered above systems during my postdoctoral stage. In addition, I deeply appreciate the allocated time and access to the equipment provided by Hasylab synchrotron (Hamburg, Germany) to conduct EXAFS measurements supported by European project ELISA. Finally, I would like to express my gratitude to the code developers and user-support community of FEFF, FDMNES, and Wien2k software codes which were used myself to theoretically interpret the obtained experimental data.

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V. Discussion of the other research activities.

V.1. Academic and Research Career.

1989 – 1994: student at the Donetsk State University (Ukraine), Department of Physics;

1994 – 1996: lecturer of physics at the Donetsk State Technical University (Ukraine).

Assistant Professor of Physics teaching undergraduate courses in engineering physics . Instructor and mentor of small groups of students for theoretical physics course and for practical laboratory training

1996 – 1999: scientist at the Donetsk State University (Ukraine), Solid State Physics and Material Science Department.

Research area in the field of materials science, more specifically, analysis of the physical nature of reversible inelastic deformation and of the possibilities of practical application of the materials having shape memory property.

1.04.2000 – 21.06.2007: Ph.D. student at the Institute of Physics, Polish Academy of Sciences in Warsaw; after defense of PhD thesis in 2005 - adjunct.

As a Ph.D. student I prepared a Ph.D. thesis titled "X-Ray absorption for characterization of low-dimensional Si/Ge/Si structures". It was devoted to characterizing Ge structures buried in Si by X-ray absorption spectroscopy using TEM microscopy and PL as additional tools. There was shown that the local atomic structure of GeSi self-assembled islands buried in a silicon matrix strongly influenced the optical properties of such systems. Derived structures were investigated by X-ray absorption fine-structure (XAFS) spectroscopy and high resolution transmission electron microscopy (HRTEM). Obtained results were used to build a schematic description of the band structure model [A-18]. Quantitative analysis of the EXAFS spectra was performed for three coordination shells around the Ge absorbing atom with multiple scattering taken into account [A-18, A-19, A-24, A-29, A-32, A-35]. It was proved that the coordination number of elements in an alloy resulting from EXAFS analysis for all three coordination spheres (introduced by author as 'mixing degree' parameters) could not be taken as the concentration of alloy but could be used together with a proper model of the alloy unit cell to calculate a realistic concentration. The fraction of Ge calculated in such a way was consistent with HRTEM results. The found model of the unit cell was used to generate an X-ray absorption near edge structure spectrum by *ab initio* calculations. This approach yielded spectra which were in good agreement with the experimental ones. The information gained from XAFS and HRTEM was, then, used for calculation of the band structure diagram and compared with the experimental photoluminescence spectra. Good agreement between proposed approximation and the experimental data led to a conclusion that XAFS technique was an excellent tool to describe the optical properties of SiGe systems.

Moreover, during my Ph.D. studies, after the defense of the Ph.D. thesis and before my postdoctoral stage in USA, I familiarized myself with different techniques like XPS, PL, HRTEM and EPMA and worked with a wide class of materials, namely, ceramics (TiN, TiC, Ti3SiC$_2$ [A-23, A-28, A-30], NaNbO$_3$ based ceramics doped with Mn and Bi ions [A-22, A-27]), alloys (Ge$_x$Si$_{1-x}$), GaN compounds [A-33], single crystals (Ge, Si), low-dimensional structures (with single and multilayers of Ge$_n$/Si$_m$) [A-34], semiconductor magnetic structures (MnTe, EuS/PbS, (Eu,Gd)Te) [A-25, A-26, A-31], malarial pigment complexes with iron [21], raw materials used in pigments production [39].

For the purpose of the popularization of X-ray absorption techniques I was a co-organizer and leading lecturer at the scientific workshop entitled "Application of X-ray Absorption for Determination of the Local Atomic and Electronic Structure of Materials" (13 - 15 November, 2006, Warsaw). Series of my lectures included: explanation of XAFS experiment (possibilities, advantages, limitations); theoretical/practical interpretation of EXAFS data using numerical code FEFF8; practical examples of EXAFS data processing on the example of SiGe systems [C-4].

21.06.2007 – 01.10.2011: post-doctoral research associate at UNLV/ALS (Las Vegas/Berkeley, USA).

Realization of work connected with X-ray spectroscopy experiments (XANES, XES, RIXS) for a wide range of materials: from gas phase to solid state at different ALS beamlines. In collaboration with Bremen University, The University of Nottingham and LBNL, examinations of materials related to solar cell industry were made at different beamlines of ALS. Interpretation of obtained data with their following publishing [A-5 - A-14, B-54, B-55, B-60 - B-74]. Great part of my work was devoted to carrying-out tests with a new equipment and electronics aiming to be used at UNLV beamline 9.3.1 at ALS. Additionally, my work was associated with UNLV chemical department projects which were based on non-dipole effects, drag current measurements and mass spectroscopy for a gas phase.

During this period, I was a co-author of the chapter titled "X-ray absorption spectroscopy," in a review book entitled "Synchrotron radiation spectroscopy and structural studies" [A-47], edited by B.J. Kowalski, W. Paszkowicz, and E. A. Görlich. The main goal of this book was to popularize the synchrotron techniques for Polish young scientists and students, that has been an important point in context of the Polish Synchrotron (SOLARIS) construction.

01.10.2011 – present:

After returning from the postdoctoral fellowship in USA, I was appointed a head of the SL1.2 group at IP PAS and held this position until the autumn of 2014. In parallel to the above until present time I am acting as a Head of Statute project entitled "Characterization of new inorganic and organic materials: atomic arrangement, chemical bonding and the elemental composition". Since 2012, I have been being also the scientific tutor of the IP PAS PhD student P. Konstantynov [C-14]. Summarizing the conducted management work it should be noticed that it has been focused, among other things, on development of promising research directions for future investigations. As a result of that, currently I am continuing scientific projects which are a part of this habilitation, with emphasis on the usage of X-ray spectroscopy as a dominant technique in materials investigation. Below I present a short summary from some of these projects which are not mentioned above.

Characterization of (Ga, Mn) N layers

Room temperature stable ferromagnetism is one of the most desirable states for diluted magnetic semiconductor (DMS). This might be achieved by growing homogeneous DMS materials of high-quality with high concentrations of substitutional metal ions. For this project, homogeneous layers of (Ga, Mn) N with a high content of Mn were grown using MBE at the Solid State Institute of Bremen University (Germany). For preliminary characterization of these layers, a number of complementary methods were used: TEM, XRD, SIMS, and RBS. TEM and XRD studies demonstrated the high quality of the grown layers and showed a homogeneous distribution of manganese ions in the matrix of GaN. RBS measurements revealed that Mn ions are located at substitutional positions of GaN matrix. To confirm this observation and to estimate the valency of manganese in (Ga, Mn) N, XAFS study was carried out at the Mn K edge. Quantitative analysis of XAFS spectra based on first principles calculations confirmed that manganese occupies substitutional positions of gallium. Moreover, all test samples (with the content of Mn from 5 to 9 at.%) exhibit similar valency of manganese which was estimated to be between 2+ and 3+ (closer to 2+). These results, together with the data of magnetic measurements were presented at the international conference [B-77] and were accepted for publication in Journal of Applied Physics at the end of 2014 [A-46].

Changes in the local structure of (Ga, Mn) As at the medium-temperature annealing

Understanding the evolution of the sample microstructure during the growth and then after annealing of DMS semiconductors is one of the key issues for spintronic materials possessing magnetic properties at room temperature. The microstructure of such layers and its heterogeneity determines strongly the properties of the material, including the basic points of the phase transition (for instance from high-temperature superconductors to DMS). The aim of this project, carried out initially at MaxLab [A-45] in collaboration with MaxLab researchers, involves checking the effectiveness of XAFS (especially EXAFS) as probing tool in the study of local structure reorganization around doped transition metal in GaAs matrix due to medium temperature annealing (up to about 400 °C). The XAFS data on the initial set of samples contained a desired extended fine structure but also imposed diffraction peaks resulted from the massive GaAs substrate and, therefore, proper estimation of the radial function of EXAFS turned out to be extremely difficult. To solve this issue, we have developed a method of physical separation of the studied layers and the substrate (so called lift-off procedure). Our preliminary tests indicated that the mentioned above problem disappeared leading to a correct interpretation of the EXAFS data. The study will be continued in other research center - the ALBA synchrotron (proposal is accepted for realization in March of 2015). The results of these investigations will be helpful in understanding the mechanisms of microstructure modification around manganese atoms leading to formation of Mn-rich cubic and hexagonal precipitates in GaAs matrix.

Preliminary studies: Silicon implanted by rhenium

Rhenium doped silicon belongs to one of the widely studied classes of DMS materials, which includes semiconductors of group III-V, II-VI and IV or transition metal oxides. Admixtures are usually 3*d* elements, the most exploited are Mn, Fe, and Cr. Rhenium is an element of the 5th group of Mendeleev's table. Preliminary theoretical studies show that the Re electrons should create strongly hybridized states with the states of Si matrix. This fact has not been yet verified experimentally, mainly because of the difficulty of implanting Re into the Si matrix. In collaboration with the Institute of Plasma Physics and Laser Microfusion in Warsaw rhenium atoms were successfully implanted into c-Si wafer using plasma-focus device. In order to determine the range of diffusion of Re in the silicon matrix SIMS measurements were carried out at IP PAS. Analysis of SIMS profiles shows a high content of Re in the silicon matrix and continuous constant concentration of Re from the surface to a depth of at least 7 microns (further depth was not tested). The samples tested using microprobe revealed the presence of rhenium in addition to copper and trace amounts of chromium in silicon matrix (both elements are present in the material of implantation chamber). XRD measurements allowed concluding that the original structure of single crystal of Si after implantation changes predominantly toward the phase of the polycrystalline $ReSi_2$. Studies using SQUID showed that after implantation the sample manifests a weak ferromagnetic signal at room temperature. At present time the nature of the signal is not clear and requires further investigation to determine the source of the ferromagnetism. Followed SQUID measurements revealed a reduction of ferromagnetism in the samples over time. This result gives us hope that the source of ferromagnetism in the samples could come from rhenium, because it is well known that, with the time it is energetically more profitable for atoms of rhenium to be grouped into clusters and thus, similar to (Ga, Mn) As systems to deteriorate the magnetic properties. Presumably, if the source of ferromagnetism would come from chromium only, the authors expected quite stable ferromagnetism as a function of time. The research of this subject is continued.

Examination of niobium layers buried in amorphous silicon

Transition metal silicides with their wide range of structures and electronic properties at the present time are a subject of a big interest mainly because of their intensive exploitation in microelectronics. In cooperation with IPC PAS in Warsaw and ON2.4 we started to investigate the niobium thin films of different thicknesses buried in an amorphous silicon matrix. Studies of Hall effect on Nb layers as a function of the thickness displays change of the carrier type . So far, the cause of these changes is not known. Knowledge of local/electron structure is required for understanding the physical properties of these materials. Consequently, preliminary measurements of XPS data for selected samples were performed. Since Nb 4*d* and Si 3*p* electrons play a major role in the chemical bonds of Si-Nb solutions, usage of the XPS analysis for identification of bonds type (especially at interfaces a-Si/Nb/a-Si) in the investigated samples allows separation and identification of bands derived from Si 3*s*, 3*p* and Nb 4*d* electrons. Preliminary analysis of the XPS studies demonstrates usefulness of these techniques in solving the tasks we are faced with. Obtained results will be published soon.

Other activities

Among my other activities it should be noted that I was an active participant in the preparation of the European project in the framework of FP7 program (EAgLE, FP7-REGPOT-2012-2013-1: http://www.eagle-regpot.eu/) which was accepted for realization for 2013-2016 at IP PAS, Warsaw. Currently, I am a head of tasks 2.4, 3.2 and 3.9 [D-15] - (i) "Enhancing of human potential through exchange of know-how and twinning activities": the organization of trips within the scientific exchange of experienced staff of ALBA synchrotron and IP PAS workers; (ii) "Enhancement of IP PAS human resources through recruitment of experienced researchers and trainings": organization and coordination of the work of an experienced specialist in the field of theoretical physics; (iii) organization of scientific workshop on WIEN2k code, based on DFT.

In addition, I have been taking an active participation in the realization of the tasks 4.1 and 4.2 (being a part of work package 4 "Capacity building of the EAgLE laboratories through purchase and upgrading of research equipment") in order to prepare the specifications required by the IP PAS specialists of XPS/UPS spectrometer, and, consequently, the organization of 'X-ray photoelectron' research laboratory at IP PAS.

In the framework of realization of EAgLE project I organized the Wien2k workshop entitled „WIEN2K and SPECTROSCOPY: HANDS-ON WORKSHOP" [C-12] in Warsaw during 29.09-02.10.2014. Details of the workshop are presented at http://www.eagle-regpot.eu/info/Wien2k/index.html.

Moreover, I am a member of scientific teams that currently work on design and construction of the 'X-ray spectroscopy' experimental stations (for soft and semi-hard regions) at Solaris light source in

Poland: (i) “RIXS station at the wiggler” is developed by the team consisting of prof. dr hab. K. Jablonska (SL1.2 IP PAS), myself, and specialists from ICP PAS (Warsaw); (ii) “The bending magnet beamline for X-ray absorption” was proposed by SL1.2 IP PAS specialists, namely, prof. dr hab. K. Jablonska, myself, dr M. Klepka, and dr hab. A. Wolska.

I am a Member of the Polish Society for Synchrotron Radiation and the International X-ray Absorption Society.

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V.2. Scientific publications in journals listed in Journal Citation Reports (JRC) database.

[A-1] Experimental observation of quantum confinement in the conduction band of PbS quantum dots
By: Demchenko, I. N.; Chernyshova, M.; He, X.; et al.
X-RAY SPECTROMETRY Volume: 42 Issue: 4 Special Issue: SI Pages: 197-200 Published: JUL-AUG 2013

[A-2] XANES: observation of quantum confinement in the conduction band of colloidal PbS quantum dots
By: Demchenko, I. N.; Chernyshova, M.; He, X.; et al.
Journal of Physics Volume: 430 Article Number: UNSP 012030 Published: 2013

[A-3] Synthesis and Transformation of Zn-Doped PbS Quantum Dots
By: He, Xingliang; Demchenko, Iraida N.; Stolte, W. C.; et al.
JOURNAL OF PHYSICAL CHEMISTRY C Volume: 116 Issue: 41 Pages: 22001-22008 Published: OCT 18 2012

[A-4] Electronic structure of polycrystalline cadmium dichloride studied by X-ray spectroscopies and ab initio calculations
By: Demchenko, I. N.; Chernyshova, M.; Stolte, W. C.; et al.
MATERIALS CHEMISTRY AND PHYSICS Volume: 135 Issue: 2-3 Pages: 1036-1043 Published: AUG 15 2012

[A-5] An XANES and XES investigation of the electronic structure of indium rich $In_xGa_{1-x}N$ films
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[B-34] “X-ray absorption study of Fe ions in metal-chitosan complexes”

By: M. Klepka, K. Lawniczak-Jablonska, I.N. Demchenko, N. Nedelko, A. Slawska-Waniewska, M. Walczak, C.A. Rodrigues, C. Bordini, 8th International School and Symposium on Synchrotron Radiation in Natural Sciences 5, 1-2, 65 (2006).

[B-35] “XAFS studies of the local structure of Mn doped magnetic semiconductors”

By: I.N. Demchenko, K. Lawniczak-Jablonska, J. Sadowski, M. Klepka, A. Wolska, European Conference on X-Ray Spectrometry, Paris, France – June 19-23, 190 (2006).

[B-36] “Determination of composition, size and orientation of Ge-Si islands buried in silicon matrix by XAFS and HRTEM analysis”

By: I.N. Demchenko, K. Lawniczak-Jablonska, S. Kret, M. Zak, A. Novikov, konserwatorium krystalograficzny, Wroclaw (2006).

[B-37] „Deposition of nanolayers by means of dense plasma focus”

By: M. Chernyshova, I. Ivanova-Stanik, L. Karpinski, M. Scholz, B. Ulejczyk, I.N. Demchenko, J.K. Lee, 22nd symposium on plasma physics and technology, 26-29 June, Prague, Czech Republic (2006).

[B-38] “Thin layer deposition using plasma focus device”

By: M. Chernyshova, L. Karpinski, M. Scholz, B. Ulejczyk, I.N. Demchenko, M. Klepka, J.K. Lee, 29-31 May, symposium on plasma physics, Gdańsk, Poland (2006).

[B-39] “Influence of Mn nanoinclusions on magnetic properties of MBE grown GaMnAs”

By: I.N. Demchenko, K. Lawniczak-Jablonska, J. Domagala, A. Wolska, M. Klepka, J. Sadowski, Workshop on Properties of Ultrathin Magnetic Films, 7-9 September, Bialowieza, Poland (2006).

[B-40] “XAS investigation of Fe in metal-chitosan complexes”

By: M. Klepka, K. Lawniczak Jablonska, I.N. Demchenko, N. Nedelko, A. Slawska Waniewska, M. Walczak, C.A. Rodrigues, C. Bordini, European Conference on X-Ray Spectrometry (EXRS 2006), 19-23 June, Paris, France (2006).

[B-41] “X-ray Absorption Study of Fe Ions in Metal-Chitosan Complexes”

By: M. Klepka, K. Lawniczak Jablonska, I.N. Demchenko, N. Nedelko, A. Slawska Waniewska, M. Walczak, C.A. Rodrigues, C. Bordini, 8th International School and Symposium on Synchrotron Radiation in Natural Sciences (ISSRNS-8), 12-17 June, Zakopane, Poland (2006).

[B-42] „Metody rejestracji widm absorpcyjnych”

By: I.N. Demchenko, warsztaty p.t.: „Zastosowanie Absorpcji Rentgenowskiej do Określania Lokalnej Struktury Atomowej i Elektronowej Materiałów” 13-15 of November, Warsaw, (2006).

[B-43] „Demonstracja programów Athena i Atoms”

By: I.N. Demchenko, warsztaty p.t.: „Zastosowanie Absorpcji Rentgenowskiej do Określania Lokalnej Struktury Atomowej i Elektronowej Materiałów” 13-15 of November, Warsaw, (2006).

[B-44] „Program FEFF – modelowanie widm EXAFS”

By: I.N. Demchenko, warsztaty p.t.: „Zastosowanie Absorpcji Rentgenowskiej do Określania Lokalnej Struktury Atomowej i Elektronowej Materiałów” 13-15 of November, Warsaw, (2006).

[B-45] „Zastosowanie EXAFS do wyznaczania składu atomowego w niskowymiarowych strukturach pod przykrywką na przykładzie Ge w Si”

By: I.N. Demchenko, warsztaty p.t.: „Zastosowanie Absorpcji Rentgenowskiej do Określania Lokalnej Struktury Atomowej i Elektronowej Materiałów” 13-15 of November, Warsaw, (2006).

[B-46] "Influence of high temperature annealing on the local atomic structure around Mn atoms and magnetic properties of (Ga,Mn)As layers"

By: I.N. Demchenko, K. Lawniczak-Jablonska, T. Story, V. Osinniy, R. Jakiela, J.Z. Domagala, J. Sadowski, M.T. Klepka, A. Wolska and M. Chernyshova Fall meeting of the European Materials Research Society (E-MRS 2007), Warsaw, Poland (17-21.09.2007) Book of Abstract p 232.

[B-47] "High temperature annealing modification of the local atomic structure around Mn atoms in (Ga,Mn)As layers"

By: I.N. Demchenko, K. Lawniczak-Jablonska, T. Story, V. Osinniy, R. Jakiela, J.Z. Domagala, J. Sadowski, M.T. Klepka, A. Wolska and M. Chernyshova 7th Polish Meeting of Synchrotron Radiation Users (KSUPS-7), Poznan, Poland (24-26.09.2007) Biuletyn PSRS, Vol 6 No1-2 p41

[B-48] "X-ray absorption spectroscopy investigation of Fe in metal chitosan complex"

By: Klepka M., Ławniczak-Jabłońska K., Demchenko I., Nedelko N., Rodrigues C.A., Bordini C., , 7 KSUPS, The 7th Polish Meeting of Synchrotron Radiation Users, Poznań, Polska, 24-26/09/2007, Biuletyn PSRS, Vol 6 No1-2 p 20.

[B-49] “Atomic order of magnetic inclusion in semiconductors”

By: K. Lawniczak-Jablonska, I.N. Demchenko, A. Wolska, J. Sadowski, M. Klepka 4th Int. Workshop on Functional and Nanostructured Materials and the 8th Conference on Intermolecular and Magnetic Interactions in Matter (FNMA'07), Gdansk, Poland (09/01/2007-09/06/2007), Book of abstract p 41.

[B-50] "XANES studies of Mn K and L3/2 edges in the (Ga,Mn)As layers modified by high temperature annealing"

By: A. Wolska, I.N. Demchenko, K. Lawniczak-Jablonska, M.T. Klepka, J. Sadowski, E. Holub-Krappe, A. Persson, D. Arvanitis 7th Polish Meeting of Synchrotron Radiation Users (KSUPS-7), Poznan, Poland (24-26.09.2007), Bulletin PSRS, Vol 6 No1-2 p79.

[B-51] "Electronic structure of Mn atoms in (Ga,Mn)As layers modified by high temperature annealing"

By: A. Wolska, I.N. Demchenko, K. Lawniczak-Jablonska, M. Klepka, J. Sadowski, E. Holub-Krappe, A. Persson, D. Arvanitis Fall meeting of the European Materials Research Society (E-MRS 2007), Warsaw, Poland (17-21.09.2007) Book of Abstract p 238.

[B-52] "Identification of Mg based phases in ilmenites by x-ray absorption spectroscopy"

By: Klepka M., Ławniczak-Jabłońska K., Demchenko I., Minikayev R., Jabłoński M., E-MRS 2007 Fall Meeting, Symposium I, Warszawa, Polska, 17-21/09/2007, Book of Abstracts p 234.

[B-53] "XAS study of Mg based phases in ilmenites"

By: Klepka M., Ławniczak-Jabłońska K., Demchenko I., Minikayev R., Jabłoński M., 7 KSUPS, The 7th Polish Meeting of Synchrotron Radiation Users, Poznań, Polska, 24-26/09/2007, Bulletin PSRS, Vol 6 No1-2 p 39

[B-54] “The local environment around the In atoms in InGaN layers grown by MBE”

By: I.N. Demchenko, W.C. Stolte, E. Piskorska-Hommel, D. Hommel, K. Lawniczak-Jablonska and O. Hemmers Advanced Light Source Users' Meeting, October 13-15, 2008, Berkeley, California.

[B-55] "XANES studies of newly synthesized nanostructured manganese oxides"

By: I.N. Demchenko, K. Lawniczak-Jablonska, T. Tyliszczak, N.R. Birkner, W.C. Stolte, M. Chernyshova, and O. Hemmers, , Advanced Light Source Users' Meeting, October 13-15 2008, Berkeley, California.

[B-56] "Natural minerals - the major and minor elements chemical bonding"

By: M.T. Klepka, R. Minikayev, K. Lawniczak-Jablonska, A. Wolska, I.N. Demchenko, M. Jablonski, 9th International School and Symposium on Synchrotron Radiation in Natural Sciences, 15-20 June 2008, Ameliówka, Bulletin of the Polish Synchrotron Radiation Society, 7 (2008) 148.

[B-57] “XAFS determination of local atomic arrangement of iron in Fe-chitosan complexes“
By: M.T. Klepka, K. Lawniczak-Jablonska, I.N. Demchenko, , 9th International School and Symposium on Synchrotron Radiation in Natural Sciences, 15-20 June 2008, Ameliówka, Bulletin of the Polish Synchrotron Radiation Society, 7 (2008) 94-95.

[B-58] “Local atomic structure of iron in Fe-chitosan complexes determined by XAFS“
By: M.T. Klepka, K. Lawniczak-Jablonska, I.N. Demchenko, , XXI Congress of the International Union of Crystallography, 23-31 August 2008, Osaka, Acta Cryst. (2008) A64, C204.

[B-59] “Phase composition of natura ilmenites used In white pigment production“
By: M. Jablonski, M.T. Klepka, R. Minikayev, K. Lawniczak-Jablonska, A. Wolska, I.N. Demchenko, , XXI Congress of the International Union of Crystallography, 23-31 August 2008, Osaka, Acta Cryst. (2008) A64, C502-503.

[B-60] “X-ray Absorption Studies on Cadmium Selenide Thin Films”
By: Selma Erat, Artur Braun, Hulya Metin, Iraida N. Demchenko, Wayne C. Stolte and Thomas Graule, MRS, Symposium M: Thin-Film Compound Semiconductor Photovoltaics, April 13 - 17, San Francisco, CA, USA - 2009.

[B-61] “The Effect of the Annealing Temperature on XANES of Cadmium Sulphide Thin Films”
By: Selma Erat, Artur Braun, Hulya Metin, Feride Sat, Iraida N. Demchenko, Wayne C. Stolte and Thomas Graule, MRS, Symposium O: Compound Semiconductors for Energy Applications and Environmental Sustainability, April 13 - 17, San Francisco, CA, USA – 2009.

[B-62] “Non-Equilibrium $GaN_{1-x}As_x$ Alloys with Band Gap Ranging from 0.8-3.4 eV”
By: K. M. Yu, S. V. Novikov, R. Broesler, C. R. Staddon, M. Hawkridge, Z. Liliental-Weber, I.N. Demchenko, J.D. Denlinger, V. M. Kao, F. Luckert, R. W. Martin, W. Walukiewicz, and C. T. Foxon, 8th International Conference on Nitride Semiconductors, October 18 - 23, ICC Jeju, Korea – 2009.

[B-63] “Full multiple scattering analysis of X-ray absorption near edge structure at the O K- and Cd L_3- edges in CdO thin layer combined with X-ray emission spectroscopy investigation”
By: I.N. Demchenko, ALS User's meeting, October 15-17, Berkeley, CA – 2009.

[B-64] “Soft X-ray Spectroscopy of $GaN_{1-x}As_x$ in the Full Composition Range”
By: K. M. Yu, S. V. Novikov, R. Broesler, I.N. Demchenko, J.D. Denlinger, Z. Liliental-Weber, F. Luckert, R. W. Martin, W. Walukiewicz, and C. T. Foxon, ALS User's meeting, October 15-17, Berkeley, CA – 2009.

[B-65] “Polarization dependent studies of InGaN layers by means of XANES”
By: E. Piskorska-Hommel, I.N. Demchenko, T. Yamaguchi, W.C. Stolte, W. Yang, O. Hemmers, XAFS 14 Conference: Camerino (ITALY) July 26-31, 2009.

[B-66] “Nondipole photoemission from chiral enantiomers of camphor”
By: K.P. Bowen, W.C. Stolte, J.A. Young, I.N. Demchenko, R. Guillemin, O. Hemmers, M.N. Piancastelli, D.W. Lindle, The 37th International conference on Vacuum Ultraviolet and X-ray Physics, University of British Columbia, Vancouver, Canada, July 11-16, 2010.

[B-67] “Electronic structure of CdO studied by soft X-ray spectroscopy”
By: I.N. Demchenko, J.D. Denlinger, M. Chernyshova, K.M. Yu, D. Speaks, P. Olalde-Velasco, W.C. Stolte, O. Hemmers, W. Walukiewicz, A. Derkachova, K. Lawniczak-Jablonska, The 37th International conference on Vacuum Ultraviolet and X-ray Physics, University of British Columbia, Vancouver, Canada, July 11-16, 2010.

[B-68] “Full multiple scattering analyses of XANES and X-ray emission studies of AgCl near the Cl K-edge”

By: W.C. Stolte, I.N. Demchenko, O. Hemmers, The 37th International conference on Vacuum Ultraviolet and X-ray Physics, University of British Columbia, Vancouver, Canada, July 11-16, 2010.

[B-69] “Polarization study of the electronic structure at the InGaN quantum dots”

By: E. Piskorska-Hommel, I.N. Demchenko, T. Laurus, C. Tessarek, A. Wolska, W.C. Stolte, O. Hemmers, J. Falta, D. Hommel, The 7th International conference on Synchrotron Radiation in Materials Science, Oxford , UK, July 11-14, 2010.

[B-70] “Modification of the local structure of oxygen in CdO under irradiation”

By: I.N. Demchenko, T. Tyliszczak, M. Chernyshova, K.M. Yu, J.D. Denlinger, D. Speaks, P. Olalde-Velasco, O. Hemmers, W. Walukiewicz, G. Derkachov, K. Lawniczak-Jablonska, The 10th jubilee International School and Symposium on Synchrotron Radiation in Natural Science, Szklarska Poreba, Poland, June 6-11, 2010.

[B-71] “Cationic and anionic photodissociation of thionyl chloride following deep-core level excitation”

By: A.F. Lago, J.Z. Dávalos, W.C. Stolte, I.N. Demchenko, The 37th International conference on Vacuum Ultraviolet and X-ray Physics, University of British Columbia, Vancouver, Canada, July 11-16, 2010.

[B-72] "Electronic structure of polycrystalline cadmium dichloride"

By: I.N. Demchenko, M. Chernyshova, W.C. Stolte, The International Workshop on Resonant Inelastic X-ray Scattering (RIXS), Las Vegas, Nevada, USA, May 25-27, 2011.

[B-73] "Characterization of galena thin films deposited by PLD on different type of substrates"

By: I.N. Demchenko, M. Chernyshova, W.C. Stolte, K.M. Yu, D.T. Speaks, W. Walukiewicz, The International Workshop on Resonant Inelastic X-ray Scattering (RIXS), Las Vegas, Nevada, USA, May 25-27, 2011.

[B-74] "XAS/RIXS investigation of indium rich $In_xGa_{1-x}N$ films"

By: I.N. Demchenko, M. Chernyshova, E. Piskorska-Hommel, R. Minikayev, J.Z. Domagala, T. Yamaguchi, W.C. Stolte, and K. Lawniczak-Jablonska, ALS user meeting, Berkeley, California, USA, October 3-5, 2011.

[B-75] “Experimental observation of quantum confinement in the conduction band of PbS quantum dots”

By: I.N. Demchenko, M. Chernyshova, R. Minikayev, A. Derkachova, G. Derkachov, O. Volnianska, H. Liang, European Conference on X-ray Spectrometry, oral presentation, Vienna, Austria, June 18-22, 2012.

[B-76] “Electronic structure of irradiated CdO thin films”

By: I.N. Demchenko, R. Minikayev, T. Tyliszczak, M. Chernyshova, K.M. Yu, J.D. Denlinger, D. Speaks, W. Walukiewicz, Synchr. Rad. in Nat. Scien., Cracow, Poland, May 20-25, 2012.

[B-77] „XAFS analysis of (Ga,Mn)N layers”

By: E. Piskorska-Hommel, G. Kunert, A. Wolska, I.N. Demchenko, T. Li, A. Bonnani, M.T. Klepka, J. Falta, D. Hommel, Intern. Worksh. on Nitr. Semicon., Sapporo, Japan, October 14-19, 2012.

[B-78] „Investigation of PbS nanoparticles by XANES and RIXS”

By: I.N. Demchenko, M. Chernyshova, X. He, R. Minikayev, G. Derkachov, O. Volnianska, A. Derkachova, E. Piskorska-Hommel, The 15th Intern. Conf. on X-ray Abs. Fine Struct., Beijing, China, July 22-28, 2012.

[B-79] "Investigation of PbS nanoparticles by XANES and RIXS"

By: Demchenko I., Konstantynov P. , Chernyshova M. , He X. , Liang H. , Minikayev R., Derkachov G. , Derkachova A. , Stolte W., XLVIII Zakopane School of Physics (Zakopane, Poland, 2013-05-20), p.50, 2013.

[B-80] "Badania strukturalne i chemiczne katalizatorów dimetalocyjankowych"
By: Dynowska E. , Ławniczak-Jabłońska K., Demchenko I., Lisowski W. , Sobczak J.W., Chruściel A., Janik J., 55 Konwersatorium Krystalograficzne (Wrocław, Poland, 2013-06-27), p.139, 2013.

[B-81] "Badania strukturalnych uwarunkowań właściwości katalizatorów dimetalocyjankowych"
By: Chruściel A. , Dynowska E., Ławniczak-Jabłońska K., Reszka A., Demchenko I., Flisak Z., Czaja K., Janik J., Sacher-Majewska B., 55 Konwersatorium Krystalograficzne (Wrocław, Poland, 2013-06-27), p.32, 2013.

[B-82] "Complementary studies of the structural properties of highly disordered materials by x-ray absorption and diffraction"
By: Ławniczak-Jabłońska K., Demchenko I., Dynowska E., Chruściel A., Janik J., Synchrotron Radiation in Natural Science (Bulletin of the Polish Synchrotron Radiation Society), vol.12, p.33, 2013.

[B-83] "Photoelectron spectroscopy studies of double metal cyanide catalysts"
By: Ławniczak-Jabłońska K., Lisowski W., Sobczak J.W., Demchenko I., Chruściel A., Janik J., Synchrotron Radiation in Natural Science (Bulletin of the Polish Synchrotron Radiation Society), vol.12, p.43, 2013.

[B-84] "XAFS investigations of local structural changes in (Ga,Mn)As thin layers at low temperature postgrowth annealing"
By: I.N. Demchenko, P. Konstantynov, M. Chernyshova, J. Domagala, Y. Melikhov, and J. Sadowski, 12th International School and Symposium on Synchrotron Radiation in Natural Science (ISSRNS), Book of abstracts, p. 81, June 15-20, Warsaw, Poland, 2014.

[B-85] "Complementary XRD and XAS Studies of Double Metal Cyanides Catalysts"
By: K. Lawniczak-Jablonska, I.N. Demchenko, E. Dynowska, A. Chruściel, W. Hreczuch, International Union of Crystallography (IUCr) Congress and General Assembly, Montréal, Canada, August 5-12, 2014.

[B-86] "Wyznaczenie lokalnego uporządkowania atomowego wokół centrum aktywnego w katalizatorach dimetalocyjankowych"
By: K. Ławniczak-Jabłonska, I.N. Demchenko, E. Dynowska, A. Chruściel, oraz J. Janik, 56 Polish Crystallographic Meeting, Book of abstracts, p. 12, Wrocław, 26-28 June, Poland, 2014.

V.5. Organizational, Teaching and Other Activities

[C-1] In 1994-96, in the framework of my professional obligation, I conducted practical and laboratory studies, along with lectures for students on elementary physics (mechanics, molecular physics, optics, electrostatics, and magnetism) at the Donetsk Technical University (Ukraine).

[C-2] In the academic year 1994/95 I worked as a teacher of physics in the secondary school # 59 in Donetsk (Ukraine).

[C-3] Participation in the Festival of Science: presentation of the principles of the X-ray apparatus (microprobe), fall 2004.

[C-4] Co-organizer and leading lecturer of scientific workshop entitled "Application of X-ray Absorption for Determination of the Local Atomic and Electronic Structure of Materials", 13-15 of November, Warsaw, (2006) delivering the following lectures:

(a) „Metody rejestracji widm absorpcyjnych”
(b) „Demonstracja programów Athena i Atoms”

(c) „Program FEFF – modelowanie widm EXAFS”
(d) „Zastosowanie EXAFS do wyznaczania składu atomowego w niskowymiarowych strukturach pod przykrywką na przykładzie Ge w Si”

[C-5] delivery of a seminar entitled: “Okreslanie składu atomowego zagrzebanych kropek kwantowych – badania EXAFS”, IP PAS, 08.02.2005.

[C-6] invited lecture: „EXAFS as a tool for investigation of the local environment of Ge atoms in buried low-dimensional structures”, Workshop on Advanced Methods for Interpretation of TEM, X-Ray and SIMS Measurements in Nano and Atomic Scale, IP PAS, 3.06.2005.

[C-7] invited lecture: „Complementary Studies of the Structural Properties of highly disordered materials by x-ray spectroscopy and diffraction”, The 2014 Workshops, Conference, and Exhibition, Program&Abstracts Book, p. 38, Perth, Australia, 9 - 13 February 2014.

[C-8] invited lecture: “Experimental observation of quantum confinement in the conduction band of PbS quantum dots”, EXRS 2012, Book of Abstracts, p. 51, Vienna, Austria, June 18-22.

[C-9] delivery of a seminar entitled: “Investigation of electronic structure of materials by x-ray spectroscopies - part 1”, IP PAS, Warszawa, 10.01.2012.

[C-10] delivery of a seminar entitled: “Investigation of electronic structure of materials by x-ray spectroscopies - part 2”, IP PAS, Warszawa, 17.04.2012.

[C-11] preparation of three communications to „Synchrotron light news” pp. 163-165, Bulletin ISSRNS, 2012.

[C-12] chairing and organization of workshop entitled: ”Wien2k and spectroscopy: hands-on workshop”, IP PAS, Warsaw, 29/09-02/10/2014.

[C-13] organization of seminars in SL1 2013/2014 academic year.

[C-14] the scientific tutor of the IP PAS PhD student P. Konstantynov (2012-present).

V.6. Participation in Research Projects

It is worth to noticing that since costs of the mentioned below projects for realization are very high, acceptance for their implementation as well as for providing financial support by certain European project/funds is under consideration for every project. For instance, 1 h of synchrotron time costs about 300 euros. Typically, the scientific project takes minimum three full days (at least 21,600 euros) just for the experimental time. Taking into account provisions for accommodation, meals and trip for two scientists (what could cost even up to 2200 euros) the above costs would be increased at least to about 23,800 euros per project. Depending on the timing of the project, the Habilitation candidate sought and received funding from the Calypso and Elisa European funds.

- *participation as a Principal Investigator*

[D-1] Proposals ID: I-02-051 EC, I-02-052 EC - “*Ge atoms buried in silicon matrix*”, Hasylab, Hamburg, Germany, 2003- PI.

[D-2] Proposal ID: PS-050-03 EC - “*Study of strains of Ge atoms bonds in* Ge_n/Si_m *superlattice by XAFS exploring polarization of SR*”, Lure, Orsay, France, 2003- PI.

[D-3] Proposal ID: I-03-062 EC - “*Ge atom surrounding in Ge/Si heterostructures*”, Hasylab, Hamburg, Germany, 2004 - PI.

[D-4] Proposal ID: II-05-056 EC - “*XAFS studies of the local structure of Mn doped dilute magnetic semiconductors*”, Hasylab, Hamburg, Germany, 2004- PI.

[D-5] Proposal ID: HS-2973 - *“Study of the stress field and structural defects in LT-MBE grown Si(n)/Ge(m) superlattices with ultra small quantum dots*”, ESRF, Grenoble, France, 2005 - PI.

[D-6] Proposal ID: II-05-056 EC - “*XAFS studies of the local structure of Mn doped dilute magnetic semiconductors*”, Hasylab, Hamburg, Germany, 2006- PI.
[D-7] Nevada Renewable Energy Consortium (NVREC) - "*Synthesis and characterization of novel (IV,II)VI group materials for solar energy utilization*", UNLV, Nevada, USA - 2010/11 - PI.
[D-8] Proposal ID: 20130112 – „*New EXAFS investigations of local structural changes in (Ga,Mn)As thin layers at low temperature pos..."...*” MaxLab, Lund, Sweden, 2013 – PI.
[D-9] Proposal ID: 20140298 – „*XAS measurements of the ambient Zn ions in up-converting* $Gd_2O_3:Er^{3+}, Yb^{3+}$ *nanoparticles doped by tran...*” MaxLab, Lund, Sweden, 2014 - PI.
[D-10] Proposal ID: 2013100637 - "*XAFS investigations of local structural changes in (Ga,Mn)As thin layers at low temperature postgrowth annealing*", ALBA, Barcelona, Spain, 2014-2015 - PI.
[D-11] Proposal ID: 20150152 – *„Zinc oxide films implanted with Rare Earth for optoelectronic applications”*, ELETTRA, Trieste, Italy, 2015 – PI.

- *participation as a co-Principal Investigator*

[D-12] Proposal ID: ID.06.2.344 EC - “*XANES study of Mg based phases in ilmenites*”, BESSY, Berlin, Germany, 2006- co-PI.
[D-13] Proposal ID: ID.07.1.873 EC - “*XANES study of Mg based phases in ilmenites*” - continuation, BESSY, Berlin, Germany, 2007- co-PI.
[D-14] “An Approved Program” ALS2012-37 – „*Photon in/out spectroscopy for material Science*” accepted for realization in 2012-2014 at ALS (USA) – co-PI.
[D-15] Proposal ID: EAgLE project (FP7-REGPOT-2012-2013-1), 2013-2016 – co-PI, Head of tasks 2.4, 3.2, 3.9, and associated work package 2 leader.

- *participation as a Principal Investigator*

[D-16] PhD grant No. 2 P03B 055 24 - "X-ray absorption study of low-dimensional semiconductor structures", KBN (State Committee for Scientific Research), implementation in 2003-2006.

V.7. Reviewing Activity

I have refereed manuscripts for the following peer-reviewed scientific journals:

- The Journal of Physical Chemistry
- Journal of Physics B: Condenced matter
- Chemistry Central Journal
- Radiation Physics and Chemistry
- J. of Elect. Spect. And Rel. Phenom.
- Act. Phys. Pol.
- Phys. Rev. B
- J. of Alloys and Comp.

Iraida Demchenko