Vita Summary

1. Name: **Lukasz Plucinski**

2. Holder of: MSc and Engineering Diploma, Warsaw University of Technology, Warsaw (1999).

   PhD Diploma (Doktor der Naturwissenschaften), Hamburg University, Hamburg, Germany (2002), thesis ”Bulk and Surface Electronic Structure of Gallium Nitride and Zinc Selenide”.

3. Employment: Hamburg University, Germany, postoctoral appointment from November 2002 to June 2003.
   Boston University, USA, Research Associate from June 2003 to May 2005.
   University of Connecticut, Storrs, USA, Research Associate, from May 2005 to May 2006.
   Materials Science Department, Lawrence Berkeley Laboratory, USA, Scientific Engineering Associate, from June 2006 to November 2006.
   Forschungszentrum Jülich GmbH, Peter-Grünberg Institut PGI-6, Scienfitic Staff (Wissenschaftlischer Mitarbeiter), since November 2006.

4. Scientific achievement according to the “Art. 16 ust. 2 ustawy z dnia 14 marca 2003 r. o stopniach naukowych i tytule naukowym oraz o stopniach i tytule w zakresie sztuki (Dz. U. nr 65, poz. 595 ze zm.)”:

a) Title of the scienfitic achievement:

“Electronic structure of spintronic materials measured using the spin- and angle-resolved photoemission”

b) Composed of the following papers:

[H1] **L. Plucinski**, Yuan Zhao, E. Vescovo, and B. Sinkovic, *MgO/Fe(001) interface: A study of the electronic structure*, Phys. Rev. B 75, 214411 (2007), IF(impact factor): 3.172[1], doi: 10.1103/PhysRevB.75.214411.

My contribution was in performing most of the measurements included in the paper, preparing all the figures, and writing the text of the manuscript. Furthermore, I was the corresponding author interacting with the editor. I evaluate my “percentage contribution” at 60%[2].

[1] I used the “Impact Factor” values according to the Journal Citation Reports (JCR) database for the year, in which the paper was published. For papers published in 2013 I used the values from the year 2012.

[2] The “percentage contribution” of the co-author in a scientific article is difficult to evaluate and carries a large uncertainty, because the criteria which would have been used to evaluate it are practically impossible to define. It

[H2] **L. Plucinski**, Yuan Zhao, C. M. Schneider, B. Sinkovic, and E.Vescovo, *Surface electronic structure of ferromagnetic Fe(001)*, Phys. Rev. B 80, 184430 (2009), IF: 3.475, doi: 10.1103/PhysRevB.80.184430.

My contribution was in performing most of the measurements included in the paper, preparing all the figures, and writing the text of the manuscript. Furthermore, I was the corresponding author interacting with the editor. I evaluate my "percentage contribution" at 60%.

[H3] J.-S. Lee, E. Vescovo, **L. Plucinski**, C. M. Schneider, and C.-C. Kao, *Electronic structure and Magnetic Properties of Epitaxial FeRh(001) ultra-thin films on W(100)*, Phys. Rev. B 82, 224410 (2010), IF: 3.774, doi: 10.1103/PhysRevB.82.224410.

My contribution was in performing the calculations of the electronic band structure of FeRh using the DFT LAPW method and in participation in editing the manuscript. I evaluate my "percentage contribution" at 25%.

[H4] **L. Plucinski**, G. Mussler, J. Krumrain, A. Herdt, S. Suga, D. Grützmacher, and C. M. Schneider, *Robust surface electronic properties of topological insulators: Bi_2Te_3 films grown by molecular beam epitaxy*, Appl. Phys. Lett. 98, 222503 (2011), IF: 3.844, doi: 10.1063/1.3595309.

My contribution was in performing most of the measurements included in the paper, preparing all the figures, and writing the text of the manuscript. Furthermore, I was the corresponding author interacting with the editor. I evaluate my "percentage contribution" at 60%.

[H5] A. Herdt, **L. Plucinski**, G. Bihlmayer, G. Mussler, S. Döring, J. Krumrain, D. Grützmacher, S. Blügel, and C. M. Schneider, *On the nature of the spin polarization limit in the warped Dirac cone of the Bi_2Te_3*, Phys. Rev. B 87, 035127 (2013), IF: 3.767, doi: 10.1103/PhysRevB.87.035127.

My contribution was in performing part of the measurements included in the paper, preparing part of the figures, and significantly contributing to the writing of the text of the manuscript. Furthermore, I was the corresponding author interacting with the editor. I evaluate my "percentage contribution" at 40%.

[H6] **L. Plucinski**, A. Herdt, S. Fahrendorf, G. Bihlmayer, G. Mussler, S. Döring, J. Kampmeier, F. Matthes, D. E. Bürgler, D. Grützmacher, S. Blügel, and C. M. Schneider, *Electronic structure, surface morphology, and topologically protected surface states of Sb_2Te_3 thin films grown on Si(111)*, J. Appl. Phys. 113, 053706 (2013), IF: 2.210, doi: 10.1063/1.4789353.

concerns for example the balance between the hour-time and the evaluation of the innovative ideas contributed by each of the co-authors.

My contribution was in performing part of the measurements included in the paper, preparing part of the figures, and writing the text of the manuscript. Furthermore, I was the corresponding author interacting with the editor. I evaluate my "percentage contribution" at 50%.

[H7] **L. Plucinski** and C. M. Schneider, *The Electronic Structure of Spintronic Materials as Seen by Spin-Polarized Angle-Resolved Photoemission*, invited review paper to the topical issue of the Journal Electron Spectroscopy and Related Phenomena 189, 137 (2013), IF: 1.706, doi: 10.1016/j.elspec.2013.05.001.

This publication contains the summary of my contributions to the field of spin- and angle-resolved photoemission spectroscopy. My contribution was in writing the text of the manuscript, taking into account both the selected scientific highlights published in previous articles and the contributions to the development of the instrumentation. Furthermore, I was the corresponding author interacting with the editor. I evaluate my "percentage contribution" at 70%.

c). Scientific goal of the above contributions and obtained results, including their possible applications.

c1). Introduction

Technologies related to the fast digital data transfer have dominated the modern electronic industry. Since many decades the vast majority of devices is based on traditional silicon-based integrated circuits, however, these devices have limitations related to the power consumption and heat dissipation, the limit in the ultimate data transfer speed, and miniaturization. For example, since 2005 the frequency of the most efficient desktop processors stays in the range between 3.5 and 4 GHz, which has popularized the multi-core designs, as an alternative method to increase the efficiency.

However, in commercial production there also exist circuits which are based on materials other than silicon. Read-write heads in computer hard drives were traditionally based on layered nanometer-scale devices, where the two ferromagnetic layers are separated by the paramagnetic layer, where the resistance of the of circuit depends on the mutual directions of the magnetization of the magnetic layers (the giant magnetoresistance, GMR[3]). Since 2005 read-write heads in commercially produced drives are based on the tunneling magnetoresistance (TMR) effect, where the two ferromagnetic layers are separated by an insulator. Such devices are based on the prototypical Fe/MgO/Fe epitaxial junction, where the integrated layers are monocrystalline. The operation principle takes into account exchange-splitted electronic band structure dispersions, and the explanation of the effect requires taking into account interband transitions in the reciprocal space.

Popularization of the devices based on the TMR effect shows, that the miniaturization of the modern electronics is tied to the monocrystalline structures and their electronic band structure. The most direct method of measuring the electronic band structure is angle-resolved photoemission (ARPES), and the majority of current ARPES investigations focuses on the

[3] The Nobel Prize in Physics 2007 was awarded jointly to Albert Fert and Peter Grünberg for the discovery of GMR effect.

details of band dispersions near the Fermi level, since these electronic states are responsible for the transport properties. The most relevant range near the Fermi level can be defined by taking into account the temperature broadening, explained by the Fermi-Dirac statistics, which for the room temperature is in the range of 0.1 eV[4]. Therefore, the most relevant binding energy range lies within the several hundreds of meV around the Fermi level, although measurements in the wider binding energy range can also provide interesting information related to the details of the band structure and electron-electron correlations.

Conventional ARPES measurements are performed using the radiation of the energy hν=20-100 eV, because at these energies the photoemission cross section is relatively high and it is possible to construct high resolution spectrometers. At these energies the mean free path of the photoelectron excited from the Fermi level region is in the order of 10Å, which means that only electrons localized at the surface are emitted elastically. Moreover, it means that photoemission experiments must be performed under ultra-high vacuum (UHV) conditions using carefully prepared atomically clean surfaces, because outside of the vacuum every surface is being rapidly covered by the layer of impurities, typically thicker than the probing depth of the conventional photoemission measurement. When the photon energy is larger, in the order of 2-6keV, then the mean-free path of the electrons emitted from the region near the Fermi level reaches several nm, and it is possible to measure the bulk electronic band structure, however, at a slightly compromised energy resolution, due to the low cross section and number of challenges in optimizing the efficiency of such a measurement system [35] [5].

Above arguments indicate that present-day technological challenges require comprehensive studies of the electronic band structure near the Fermi level. In order to obtain the complete characterization of the electronic states responsible for the electronic transport, such measurements should also include the spin resolution and the possibility to manipulate the surface sensitivity of the photoemission experiment.

The “Scientific Achievement” listed in this *Vita Summary* is related to the research on the spin electronic structure of number of model spintronic materials. It includes papers related to the Fe/MgO interface [H1-H2], material which undergoes ferromagnetic-paramagnetic phase transition [H3], and topological insulators [H4-H6]. The list of papers given in the “Scientific Achievement” is concluded with an invited review article on the spin- and angle-resolved photoemission, published in the special topical edition of the ”Journal of Electron Spectroscopy and Related Phenomena” [H7].

c2). Scientific achievements for the Habilitation

According to the Juelliere’s model[6] the magnetoresistance (MR) ratio in an TMR device can be expressed as $MR = 2P_1P_2/(1 - P_1P_2)$, where P_1 and P_2 are spin polarizations of the two electromagnetic electrodes. These polarizations are defined as $P = (N_\uparrow(E_F) - N_\downarrow(E_F))/(N_\uparrow(E_F) + N_\downarrow(E_F))$, where $N_\uparrow(E_F)$ and $N_\downarrow(E_F)$ are electronic densities of states (DOS) at the Fermi level respectively for the spin-majority and spin-minority bands. Explanation of the

[4] Fermi level broadening due to the temperature is described by the Fermi-Dirac distribution $I(E) = (e^{(E-E_F)/(k_BT)} + 1)^{-1}$, where k_B is the Boltzmann constant. Conventionally the broadening of the Fermi level width is taken as $4k_BT$, which at T = 300K equals approx. 103.4 meV.

[5] The number concerns my full list of publications provided in a separate attached document “Summary of Scientific Publications”.

[6] M. Julliere, Phys. Lett. 54A, 225 (1975).

coherent tunneling in the monocrystalline epitaxial junctions requires to complement Julliere's model by taking into account the dependence of the density of states $N(E_F)$ on the reciprocal wave vector ***k***. The operation principle of the TMR device based on Fe/MgO/Fe junction has been theoretically predicted in 2001[7] and is based on the tunneling between the electronic states of Δ_1 symmetry which effectively couple into the MgO barrier. This indicates that the TMR effect should be stronger for the thinner MgO barriers, and the realistic thickness of the electrically isolating MgO layer is in the range of several atomic layers. However, for very thin MgO layers, such as approx. 4 atomic layers, strongly localized interface states start to have an influence on the effectivity of the junction functionality. For these reasons it is necessary to investigate and understand the *k*-space resolved spin electronic structure of Fe/MgO(001) interface.

In the year 2004 two groundbreaking articles on the realization of the TMR devices based on the interface between iron and magnesium oxide have been published[8]. They have experimentally demonstrated approximately 200% tunnel magnetoresistance in highly crystalline epitaxial junctions based on Fe/MgO/Fe. The combination of Fe and MgO seems to be ideal for these types of junctions due to the small lattice mismatch (3.8% taking into account growth in the [001] direction) and large difference between the free surface energies for Fe (approx. 2.9 J/m) and MgO (approx. 1.1 J/m). This allows pseudomorphic growth of the nanometer epitaxial layers with a minimal interface mixing.

Fascinated by the new opportunities related to the TMR devices, in 2005 I started a collaboration with Dr. Elio Vescovo from NSLS/BNL to conduct thorough investigations of the spin electronic structure of the interfaces between the ferromagnetic and electrically insulating epitaxial layers. Measurements were performed at the U5UA endstation at the NSLS synchrotron laboratory using undulator-produced synchrotron radiation in the energy range of $h\nu$ = 15-150eV and the mini-Mott type spin polarimeter mounted behind the hemispherical electron energy analyzer. Epitaxial layers of Fe and MgO were evaporated on (001) surfaces of molybdenum or tungsten substrates using molecular beam epitaxy (MBE) under UHV conditions.

In the first decade of the XXI century, investigations of the Fe/MgO interface have focused on number of challenges, related for example to the formation of the interface FeO layer[9], formation of the localized interface states, which can have negative influence on the parameters of the TMR device, or the existence of the magnetic dead layer of Fe near the interface. My research published in articles [H1] and [H2] provides insight into these issues from the point of view of the photoemission experiment.

In the article [H1] epitaxial layers of MgO(001), evaporated on the Fe(001) surface using the direct evaporation from a stoichiometric magnesium oxide target under the ultra-high vacuum, were investigated using spin-resolved photoemission from the valence band and using the magnetic linear dichroism in the core level spectroscopy. Negligible photoemission spectral weight for the kinetic energies above the valence band maximum of MgO confirmed the stoichiometry of the MgO layers prepared in this way. Epitaxial Fe(001) layers of 40Å which were used as a substrate were evaporated on the surface of Mo(001) crystal.

[7] Butler et al. Phys. Rev. B 63, 054416 (2001) and Mathon and Umerski, *ibid.* page 220403(R).
[8] Parkin et al., Nature Materials 3, 862 (2004), Yuasa et al., *ibid*. page 868.
[9] Tusche et al., Phys. Rev. Lett. 95, 176101 (2005).

A comparison of the spectra from the Fe(001) oxidized using one Langmuir (1L = 10^{-6} Torr·s) of the molecular oxygen under ultra-high vacuum to the spectra of the single MgO layer evaporated on Fe(001) indicates that the interfacial FeO layer was missing in the measured MgO/Fe(001) samples. Annealing the investigated layers at temperatures below 400ºC lead to relatively small changes in the photoemission spectral weight, most likely related to the structural ordering of the interface. Annealing at the temperature of 500ºC lead to the more pronounced changes in spectra, in my interpretation caused by the desorption of MgO or forming of the MgO clusters on the surface, which lead to the partial uncovering of the metallic Fe(001) surface.

All measured results clearly indicate the lack of the magnetic dead Fe layer at the interface to MgO. Spin-resolved photoemission spectra have shown, that the spin polarization of the valence band electrons of Fe does not decrease between one and two monolayers of MgO evaporated on Fe(001). In accord, linear magnetic dichroism from the Fe 3p states have shown, that ferromagnetism in the interfacial region prevails after evaporation of the single MgO monolayer, however, for the thicker layers the measurement of the dichroism is not possible due to the overlay between Fe 3p and Mg 2p core level features.

Furthermore, on the course of the measurements I noticed interesting effects in the photoemission of the Mg 2p core level. Kinetic energy of the photoemission feature related to that state decreases with the increasing thickness of the MgO evaporated on Fe(001). This is due to the multi-electron correlation effects, and fast screening of the photohole created in MgO by the Fe(001) metallic substrate. Moreover a small feature, which is a satellite of the Mg 2p peak, has been observed for the thin MgO layer of approx. a single monolayer thickness. It's kinetic energy is 10.7 eV smaller than the energy of the Mg 2p peak, and it is related to the surface plasmon in the Fe(001) substrate.

In summary, the publication [H1] has shown, that the electronic structure of the MgO/Fe(001) interface, as observed in the photoemission experiment, matches the conditions defined by the theories which describe the operation of the TMR devices. Taking into account that in this publication I did not focus on the interface states, which can have influence on performance of the TMR devices, this subject has been extended in the subsequent publication [H2] dedicated to the surface spin electronic structure of the clean and oxidized Fe(001).

Although low index surfaces of Fe are important as prototypical ferromagnetic surfaces, the details of the electronic structure of Fe(001) still require thorough investigations. Furthermore, the Fe(001) surface is important also from the point of view of the spin-polarimetry, because the operation principle of the most efficient spin detector is based on the "exchange scattering" from the oxidized Fe(001) [S2]. In the article [H2] I have focused on the details of the electronic structure of the Fe(001) surface. Measurements were performed on samples cooled to approx.100K by the liquid nitrogen cooled cryostat, and the total energy resolution of the spin-polarized photoemission measurement was below 120 meV. The spin-resolved photoemission results for normal emission and along the $\overline{\Gamma X}$ direction have shown that the polarization of the bulk electronic states does not change after the oxidation of the surface using 1L O_2. Respectively, the minority surface state along the $\overline{\Gamma X}$ at energies near the Fermi level, which is of the d_{xz+yz} orbital character, disappears after the oxidation. Moreover, in this publication I have presented calculations performed using the WIEN2k[10] program package for the 30 atomic layer slab, where adjacent surfaces were separated by almost 30 Å of vacuum. These calculations

[10] P. Blaha, K. Schwarz, G. Madsen, D. Kvasnicka and J. Luitz, www.wien2k.at.

have shown that the minority surface state near the Fermi level along the $\overline{\Gamma X}$ direction is composed of the two separate energy bands. One of the bands, located exclusively near the $\overline{\Gamma}$ point approx. 200meV above the Fermi level is of the d_{z2} orbital character, while the second band, which spreads along most of the $\overline{\Gamma X}$ and is partly filled, is of the d_{xz+yz} character. According to various calculations performed by the different research groups, it is this second band, now as an interface state between the Fe and MgO, which is responsible for the compromising of the performance of the TMR devices based on the Fe/MgO(001) interface. My research on the Fe/MgO interface has been appreciated by the experts by invitation to publish the report in *2007 NSLS Science Highlights*.[11]

Ordering of the spin polarization vectors in magnetic materials is typically related to the relatively small energy differences, therefore number of materials undergo phase transitions related to the temperature, pressure, doping, or the strain of the crystalline structure due to thin film growth in the pseudomorphic regime. One of the important compounds which undergoes the temperature phase transition between the low temperature antiferromagnetic (AF) phase and the ferromagnetic (FM) phase is FeRh. Experience gathered during the investigations of Fe/W(001) allowed to pursue this research and measurements on FeRh films evaporated on W(001), with the results presented in the publication [H3]. For the FeRh thickness of approx. 10 monolayers the phase transition appears between 315K and 356K, while the Curie temperature of such film is approx. 535K.

The phase transition for the layers investigated in the publication [H3] has been characterized using linear magnetic dichroism in the spectroscopy of Fe 3p core levels. This dichroism has shown a sizeable difference between the magnetic moments of Fe and Rh, which is in accordance with theoretical predictions (approx. 3μB for Fe and 1μB for Rh), and the parallel alignment of these moments. Simultaneously, only small difference in the electronic structure of the valence band have been measured between the AF and FM phases, which means that the phase transition is not related to the significant reordering of the charge density within the crystal structure. Low energy electron diffraction (LEED) has shown pseudomorphic growth for 10 monolayers of FeRh/W(001). The difference between lattice constants of W and FeRh is approx. 5%, so these types of FeRh layers are certainly subjected to the lattice strain. The phase transition has been observed for similar temperatures for FeRh single crystals and polycrystals, therefore one can suppose that it is relatively independent on the crystalline strain. However, one should note that there exist publications which show the influence of the pressure on the phase transition temperature[12], and the significant lattice constant variation between AF and FM phases[13].

Over the last several years the co-called three-dimensional (3D) topological insulators are the subject of the intense research investigations. The most important of them Bi_2Se_3, Bi_2Te_3, Sb_2Te_3, and their alloys, are semiconductors with a narrow band gap of the order of 100-200 meV, and exhibit peculiar electronic properties related to the time reversal symmetry (T-symmetry) $\Theta H(\mathbf{k})\Theta^{-1}=H(-\mathbf{k})$ in the electronic structure Hamiltonian which includes spin-orbit

[11] L. Plucinski, Y. Zhao, B. Sinkovic, and E. Vescovo, "MgO/Fe interface: A study of the electonic structure", 2007 NSLS Activity Report, Science Highlights PDF, 34 (2007). Article was displayed on the main NSLS web page, and published in the electronic form. It is accessible under the link: http://www.bnl.gov/ps/nsls/newsroom/publications/activityreport/2007_NSLS_Activity_Report_Highlights.pdf

[12] N. I. Kulikov, E. T. Kulatov, L. I. Vinokurova, and M. Pardavi-Horvath, J. Phys. F: Met. Phys. 12, L91 (1992).

[13] L. Zsoldos, Phys. Status Solidi 20, K25 (1967), R. O. Cherifi et al. *Electric-field control of magnetic order above room temperature*, Nature Materials (2014), doi:10.1038/nmat3870.

coupling. In short, the band gap of topological insulators results from the band inversion related to the spin-orbit interaction[14], which leads to 2 dimensional *topological surface states* which appear either on the surface of the 3D topological insulator, which is an interface to the vacuum, or at the interface to the crystal which does not exhibit band inversion. The existence of these states can be predicted by means of topological theories, employing the topological invariant Z_2 used to describe the *quantum Hall effect*[15]. Three-dimensional topological insulators are characterized by the four Z_2 invariants, for which one uses the nomenclature (ν_0; ν_1 ν_2 ν_3). In the surface Brillouin zone there exist four $\Gamma_{1,2,3,4}$ points which are time-reversal invariant, and where the surface states, as long as they exist, must undergo Kramers degeneracy. Surface states related to the $\Gamma_{1,2,3,4}$ points are topologically protected as long as they cross the Fermi level odd number of times along the line which connects Γ_n and Γ_m. My research concerned only the so-called strong 3D topological insulators and their [0001] surfaces, for which the surface state in the form of the Dirac cone[16] exists at a single $\bar{\Gamma}$ point which is the surface Brillouin zone center.

My research program on three-dimensional topological insulators focuses on thin films of Bi_2Te_3 and Sb_2Te_3 evaporated using MBE under ultra-high vacuum on crystalline Si(111) substrates. Methodology of the growth of these layers has been described in the publication [33], and the main growth parameters are the substrate temperature, evaporation rate, and the relative evaporation rates of different evaporated elements. After growth samples are carried under the ambient conditions, without special protection, into the vacuum chamber of one of the experimental stations [30, 31], where they are cleaned under the ultra-high vacuum with their surface crystallization measured by the low energy electron diffraction (LEED), and the chemical analysis of the surface is performed using the Auger spectroscopy. Subsequently, on optimally prepared surfaces one carries angle-resolved or spin- and angle-resolved photoemission measurements.

Optimization of the surface preparation of Bi_2Te_3 has been described in the article [H4], where surfaces were cleaned by repeated sputtering with 500eV Ar+ ions and annealing up to 250ºC. Layers of the initial thickness of 20 nm were in this way etched away until the spectral lines related to the silicon substrate have appeared in the Auger spectra. Angle-resolved photoemission measurements on samples cooled with liquid nitrogen (down to around 90K) have shown, that clear Dirac cone band dispersions, characteristic to three-dimensional topological insulators, are formed in such prepared surfaces, and that in a modified form they exist also in very thin layers. Simultaneously, the lack of the clear quantum well effects in the ultrathin layers indicates that the sputter-anneal cleaning process does not lead to obtaining a flat and ideally atomically ordered surface, however, subsequent scanning tunneling microscopy (STM) measurements demonstrated that a large part of such prepared surface exhibits a local crystalline ordering on the atomic level.

In the two subsequent articles on topological insulators [H5-H6] I have focused on the spin polarization in angle-resolved photoemission from the thin films of Bi_2Te_3 and Sb_2Te_3. An interpretation of the spin-polarized photoemission results in case where the emission of the polarized electrons is related to the strong spin-orbit coupling (SOC) presents an exceptional challenge. In the multielectron system with SOC, spin is not strictly a quantum number, and this causes each state to be polarized, with a certain weight, in both directions of the spin quantization axis. As a consequence, in case of the system with SOC, the direction and

[14] Therefore this band gap is in general smaller than the energy related to the band splitting due to the spin-orbit interaction.

[15] C. L. Kane and E. J. Mele, Phys. Rev. Lett. 95, 146802 (2005).

[16] According to the described theory the Dirac point in such Dirac cone undergoes Kramers degeneration.

magnitude of the spin polarization vector P measured in the *ensemble* of the emitted photoelectrons, which can in principle be precisely measured by a spin-polarimeter, are not directly related to the quantum-mechanical initial state of the electrons inside the crystal, due to the so-called *optical spin orientation* process[17]. In case of ferromagnets such as Fe, Co, or Ni effects due to SOC can be in many cases neglected because they lead to small energy corrections (in order of 20 meV or less for most of the bands) and the majority of bands is nearly 100% spin polarized, which means that the interpretation of the results using the spin quantum numbers m_s is approximately valid.[18] However, in case of spin-polarized electronic states such as topological surface states, which are intrinsically related to the strong spin-orbit coupling, more detailed analysis is mandatory, which takes into account relativistic effects in the band structure and the details of the photoemission process, related to the energy and polarization of the excitation radiation and to the geometry of the experimental setup.

In the articles [H5-H6] I presented a comparison between the polarization in the ensemble of emitted electrons and the ground state band structure calculations for the surfaces of Bi_2Te_3 and Sb_2Te_3. These investigations have shown that both the calculated and the measured polarization for the Bi_2Te_3 surface reaches around 50%. Due to the effects related to the photoemission process, mentioned on the previous paragraph, a direct comparison of experimental results for the ensemble of the photoemitted electrons with the calculations for the ground state, is not possible. However, the fact that experimental results show spin polarization of about 50 percent (i.e. much below 100%) indicates that the initial state of the topological surface state is not 100% spin polarized, in contrast to the early analytical calculations which didn't take into account crystal lattice potential. The collaboration between the institutes PGI-6 and PGI-9 of the Forschungszentrum Jülich on the optimization of the properties of topological insulator thin films is also documented among the "Selected Research Reports" published in the JARA-FIT Annual Report 2012[19].

Although the process of the *optical spin orientation* is known since the 1980s, publications which took into account this phenomenon in the interpretation of the experimental results from the topological insulators have appeared only at the end of the year 2012. The have demonstrated that the photoemission process can not only change the magnitude of the measured spin polarization but also its sign[20].

Invited article [H7] was a chance to present a review of my most important results in the field of spin-polarized photoemission. The contents included a short perspective on the history of the field, a viewpoint on the current scientific challenges, description of experimental techniques, and description of several recent experimental studies. In the Outlook of this review we have also pointed out that in the near future it might be possible to perform bulk-sensitive hard x-ray photoemission experiments (see Section 5b2)) with spin sensitivity. This would allow adding a new dimension in investigations of the bulk spin-electronic structure, since large part of the spectral weight in the hard x-ray photoemission is related to the electronic wave functions inside

[17] Look e.g. Tamura et al. "New Polarization Effect in Photoemission from Nonmagnetic Surfaces", Phys. Rev. Lett. 59, 934 (1987).

[18] Figure 4 in [H7] shows nearly 100% spin polarization in the ensemble of electrons emitted from a clean Fe(001) surface. However, at certain k-points and binding energies predicted energy corrections due to SOC can be as high as 150-200 meV, see e.g. M. N. Khan et al. J. Phys. Condens. Matter 20, 155208 (2008).

[19] G. Mussler, J. Kampmeier, J. Krumrain, S. Borisova, L. Plucinski, M. Luysberg, D. Grützmacher, "Molecular-Beam Epitaxy of Topological Insulator Bi_2Te_3 Thin Films", JARA-FIT Annual Report 35 (2012).

[20] See e.g. Ch. Jozwiak et al., Nature Physics 9, 293 (2013) oraz J. Sanchez-Barriga et al., Phys. Rev. X 4, 011046 (2014).

the bulk, which are not influenced by the inversion symmetry breaking at the surface and the gradient of the electric field near the surface.

5. Other scientific achievements.

5a). Achievements before the PhD defense

In 1998 during the fifth year of study at the "Technical Physics and Applied Mathematics" department at the Warsaw University of Technology I started the work under the supervision of Dr. Jacek Krzywinski, who was then working at the Institute of Physics, Polish Academy of Sciences (PAN) in Warsaw[21]. This collaboration allowed me to move to Hamburg, where I worked for several months at a modern linear accelerator then known as "Tesla Test Facility – Free Electron Laser" (TTF-FEL) at the large research laboratory Deutsches Elektronen-Synchrotron (DESY). Currently TTF-FEL is a part of the "Flash" facility at DESY.

Work under the supervision of Dr. Krzywinski resulted in two publications on interaction of short pulses of the vacuum ultraviolet (VUV) radiation with the hydrogen atom, motivated by the parameters of the radiation produced by the TTF-FEL [1, 3]. In these papers we have described, among other things, a stabilization of the hydrogen atom ionization cross section with respect to the radiation intensity. I continued working at the TTF-FEL throughout my PhD student appointment at DESY, and the result of this commitment is documented in subsequent publications related to, often groundbreaking, achievements in the undulator-produced Self-Amplified-Spontaneous-Emission (SASE) at the TTF-FEL [2, 5, 6, 9, 10].

In 1999 I commenced my PhD student appointment in the group of Prof. Robert L. Johnson from the Hamburg University. During this graduate appointment I was based permanently at the HASYLAB (Hamburg Synchrotron Laboratory) laboratory in DESY, and I was responsible for the experimental station F2.2 "Winkelemi" which was utilizing the radiation produced by the dipole bending magnet in the DORIS II storage ring, and designed to perform angle-resolved photoemission with photons of energies between 5 and 40 eV.

The subject of my PhD thesis was the valence band electronic structure of GaN and ZnSe, which are wide band gap semiconductors. Results related directly to the thesis were published in the three first-author articles in renowned journals [8, 12, 13] and in one subsequent article related to the impact of multi-electron (quasiparticle) interactions on photoemission results in semiconductors [S1]. On the course of my PhD student appointment I performed and published also other measurements and calculations, both self-reliantly [11] and in collaboration with the group of Prof. Wiesendanger from the Hamburg University [7].

During my PhD student appointment I established a close collaboration with Prof. B. A. Orlowski and Prof. B. J. Kowalski from the Institute of Physics, Polish Academy of Sciences in Warsaw, which concerned photoemission characterization of the single crystal gallium nitride (GaN) samples produced at the Institute of High Pressure Physics "Unipress" in Warsaw by the group of Dr. I. Grzegory and Prof. S. Porowski. Correspondingly, measurements on epitaxial layers of zinc selenide (ZnSe) were performed in collaboration with the group of Prof. E. Umbach and Prof. L. Molenkamp from the Würzburg University, who have supervised a large molecular beam epitaxy (MBE) facility able to produce thin films of ultimate quality. During that time I

[21] Currently Dr. Krzywinski works at SLAC, California, USA.

visited several times both Institute of Physics in Warsaw and the Würzburg University to discuss the research strategies and to present my results at the seminars.

Also at this time, owing to the collaboration with Dr. Andrzej Fleszar (Würzburg University) and with Thomas Strasser (then a PhD student at the University of Kiel) I learned the foundations of the electronic band structure calculations using the density functional theory (DFT) approach.

5b). Summary of the scientific achievements after obtaining doctoral degree, which are not the part of the habilitation achievement

5b1). Postdoctoral appointment in the group of Prof. Kevin E. Smith

Upon completing the doctoral degree I have decided for a postdoctoral stays in the leading synchrotron laboratories in the USA. During part of this time I have worked in the group of Prof. Kevin Smith from the Boston University. There I continued the research on nitride semiconductors which resulted in subsequent publications related to that subject [15, 16, 18] with a highlight of this series of papers being an influential article on the two-dimensional electron gas (2DEG) on the surface of the narrow band gap nitride InN [20], which exhibits properties that can be controlled by the method of the surface preparation, and which shows non-parabolic band dispersions near the Fermi level. This work was appreciated by the experts with an invitation to publish a report in *2007 NSLS Activity Report*.[22] Since the beginning of my postdoctoral appointment I was responsible for supporting the research activities of PhD and undergraduate students. At the time of my appointment in the group of Prof. Smith I was responsible for supporting the younger members of the group, in particular during their measurements at the synchrotron laboratory.

5b2). Appointment in the group of Prof. Charles Fadley

My research on magnetic properties of solids described in the “Scientific Achievement” is conducted using variety of spectroscopic techniques, however, photoemission measurements performed at photon energies below 200 eV are surface sensitive, which impedes detailed investigations of the bulk electronic structure. Surface sensitivity is useful in numerous studies, however, for example in case of Heusler alloys or dilute magnetic semiconductors (DMS) surface sensitivity becomes a major obstacle, because usually for these materials surface and bulk properties are significantly different. A reliable method to increase the bulk sensitivity is the use of high energy excitation photons in the photoemission experiment, which results in high energies of electrons emitted from the Fermi level region. In case of such measurements one uses acronyms HAXPES (hard x-ray photoelectron spectroscopy) or HARPES (hard x-ray ARPES), when additionally angular dependence of the photoelectrons is measured. In case of kinetic energies of the order of 2-6 keV the mean free path of the electrons in solids reaches 50-100 Å, which is an order of magnitude higher than in case of conventional photoemission measurements.

[22] L. Colakerol, T.D. Veal, H.-K. Jeong, L. Plucinski, A. DeMasi, T. Learmonth, P.-A. Glans, S. Wang, Y. Zhang, L.F.J. Piper, P.H. Jefferson, A. Fedorov, T.-C. Chen, T. D. Moustakas, C.F. McConville, and K.E. Smith, “Unveiling Electronic Properties Near a Semiconductor Surface” 2007 NSLS Activity Report, 17 (2007). This report has also been displayed on the main NSLS web page as a “Science Highlight”.

In 2006, fascinated by the new capabilities of the hard x-ray photoemission I joined the group of Prof. Charles Fadley at the Lawrence Berkeley National Laboratory in California. My appointment in this group has fructified in number of pioneering publications related to the HARPES technique. The essence of the HARPES technique is in the possibility to map band dispersions in bulk crystals, that is the measurement of the energy eigenvalues E_{bin} with respect to the position in reciprocal **k**-space vector in the bulk Brilouin zone. Traditionally the energy resolution of such measurement is limited to $\Delta E > 100 – 200$ meV due to the lack of the intense radiation sources for energies above 1-2 keV. This limitation is, however, not fundamental, and it will be discarded in the future as the new radiation sources are being developed (e.g. synchrotron radiation sources of the newest generation). Nevertheless, for high energies of incident photons and emitted electrons the resolution of the HARPES measurement is limited also in the space of the reciprocal lattice vector **k** due to the vibrations of the crystal lattice and the large **G** vector of the reciprocal lattice, which is necessary for the photoemission process to take place. In the pioneering work [26], using the measurement of the band dispersions in tungsten for photon energy 870 eV and temperatures between 300K and 780K I demonstrated, using the Debye-Waller model, that tungsten electronic bands should be observed in photoemission measurement up to photon energies of about 6 keV in case of cryogenic cooling down to 4K, and that the cryogenic cooling opens up the opportunity to map band dispersions in a number of other materials for slightly lower photon energies up to about 3 keV. These predictions have been confirmed in subsequent ground-breaking publications in which I am a co-author [35, 39], where the experimentally measured dispersion of bulk bands for tungsten at 6 keV and for gallium arsenide at 3.2 keV has been presented.

The feasibility to perform HARPES measurements using the standard MgKα x-ray tube has been demonstrated in the publication [32], and the extension of the theoretical interpretation by taking into account phonon-related effects has been presented in the publication [44]. I have also participated in the development of the standing wave photoemission technique, which allows attaining an information on electronic structure of buried interfaces using the soft x-ray radiation [25, 37]. Moreover, we have recently extended this method by including the ARPES mapping to characterize the properties of the interface between $SrTiO_3$ and $La_{0.7}Sr_{0.3}MnO_3$ [43].

Out of the articles mentioned above, the publication [39] deserves a special attention, since it concerns the bulk electronic structure of the most important dilute magnetic semiconductor $Ga_{1-x}Mn_xAs$ and its subject is thematically related to the publications [H1-H7]. In this work we have presented an analysis of the HARPES spectra for photon energy of 3.2 keV, which have shown that manganese energy levels in $Ga_{1-x}Mn_xAs$ lie approx. 400 meV below the Fermi level, but the spectral changes take place all over the valence band, which allowed to provide a more precise interpretation of the origin of magnetism in this compound.

Ground-breaking publications [35, 39] have also been appreciated by experts by announcements in joined reports of Forschungszentrum Jülich and RWTH Aachen (JARA-FIT Annual Report) in the section of selected research reports, and press releases in the main Forschungszentrum Jülich web page[23].

[23] Press releases were displayed in October 2012 and in August 2011. They are accessible under the links http://www.fz-juelich.de/SharedDocs/Pressemitteilungen/UK/DE/2012/12-10-14halbleiter-nature-materials.html and http://www.fz-juelich.de/SharedDocs/Pressemitteilungen/UK/DE/2011/11-08-18photoemissionsspektroskopie.html.

5b3). Development of instrumentation for photoemission measurements

In the age of technological progress the development of measurement techniques is of great importance, in particular in case of scientific research which focuses on new, previously undescribed phenomena. In 2006 I accepted the offer to work in Forschungszentrum Jülich (Germany) in the institute of the current name Peter-Grünberg-Institut-6 (PGI-6) lead by Prof. Claus M. Schneider, where I work up to this date. This group specializes in the experimental research on the electronic structure of solids, with the main emphasis on magnetism and on the modern instrumentation. Exceptional opportunities created at PGI-6 allowed me to build 2 large experimental photoemission facilities described in articles [30, 31], to participate in the construction of the most efficient commercially available spin polarimeter [S2], and in a number of fascinating research programs [27, 35, 38].

In the article [30] I have described an experimental facility which I put in operation at the synchrotron laboratory DELTA in Dortmund, and which is permanently based there to date. This system allows simultaneous measurement of the two dimensional E(k) ARPES spectra and the one-dimensional spin-polarized photoemission energy distribution curves. At the time of commencing the operation it was one of the first (if not the first) system where the spin detector has been coupled to the hemispherical analyzer allowing high angular resolution in spin-polarized ARPES measurements.

Article [31] concerns two ARPES systems, which allow measurements at a high energy resolution for low energy electrons by using the highly monochromatic photons of the low energy between 8.4 eV and 11.6 eV. One of the systems has been put in operation by me in FZ Jülich, and the second one under the supervision of Prof. S. Suga at the Osaka University in Japan.

Article [S2] concerns building the spin detector of the newest generation, which allows to perform photoemission studies with spin resolution at data acquisition times by one or two orders of magnitude shorter than when using conventional Mott detectors.

Article [S3] concerns setting up the facility to perform time-resolved photoemission at the synchrotron laboratory DELTA in Dortmund, where ultrafast (below 100 femtoseconds) VUV photon pulses are produced by the modulation of the electron beam in the storage ring by means of the femtosecond laser pulse. Such process is called the “coherent harmonic generation” (CHG). The time of one full rotation in the DELTA storage ring is 384 ns (2.6 MHz), however, the modulation laser, which operates at a 795 nm wavelength operates efficiently only at 1 kHz. Therefore, even if only one electron bunch is present in the storage ring, CHG system produces only standard synchrotron pulses with FWHM of about 100 ps with the frequency of 2.6 MHz, and only one out of 2600 pulses is modulated by the laser, characterized by high brightness and has FWHM below 100 fs. The facility described in the article [30] is equipped with an electron detector which is capable of time resolution of below one nanosecond, which allows to separate CHG pulses from the conventional synchrotron pulses, which in turn is the basis of our future time-resolved photoemission measurements to be performed using stroboscopic techniques.

5b4). Future plans and research directions

I am currently extending the research on thin films of three-dimensional topological insulators. The research program focuses on measurements of superlattices which contain materials of *n*

and *p* characteristics (e.g. Bi_2Te_3 and Sb_2Te_3) [24] and on engineering and measurements of ternary compounds to control the position of the Fermi level within the fundamental band gap. Furthermore, I am focusing on the influence of the surface and bulk doping of topological insulators with magnetic atoms (e.g. chromium or iron).

I am pursuing the research on thin magnetic films. By using ultrathin epitaxial films of Fe(001) as a prototype single-domain ferromagnet I investigate the influence of the effects related to the spin-orbit coupling on the dispersions of the bulk and surface electronic band structures.

Moreover, I am continuing an intense scientific collaboration with the group of Prof. Fadley, which mainly concerns investigations of the electronic structure of interfaces using the HARPES technique. I also actively participate in a number of research projects within the PGI-6 institute, in particular in the program related to the ultrafast demagnetization measured by the laser-based stroboscopic techniques, and in microscopic measurements of the electronic structure using photoemission microscopy (PEEM).

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[24] In these compounds there exist an "intrinsic" *n*- and *p*-type doping, likely related to different natures of lattice defects, stoichiometry imbalance, or unintentional doping in the growth process of bulk crystals and thin films.