SUMMARY OF PROFESSIONAL ACCOMPLISHMENTS

Modeling of selected optical properties of III-V semiconductor heterostructures

Dr. Eng. Marta Gładysiewicz-Kudrawiec
5 September 2016

Contents

1. Personal data

Names:	Marta Aleksandra Gładysiewicz-Kudrawiec (Marta Gładysiewicz in articles)
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Birth date:	28 June 1975
Birth place:	Wrocław, Poland
Citizenship:	Polish
Marital status:	Married; Kids: Jan, Małgorzata, Andrzej;

2. Education, scientific degree, employment, scientific interships, and teaching activity

Scientific degree:

PhD:	Institute of Physics, Wroclaw University of Technology, 27 November 2003; PhD thesis: „*Rola anizotropii i mechanizmów oddziaływania w układach nadprzewodzących”* (defense with honors);
MSc Eng.:	Wydział Podstawowych Problemów Techniki, Politechnika Wrocławska, May 1999; MSc thesis: *„Własności termodynamiczne układów nadprzewodzących BCS typu s dla modelowych postaci gęstości stanów”* (with honors);

Employment and positions:

- XI 2015 – up to now: Adjunct at the Department of Experimental Physics, Faculty of Fundamental Problems of Technology, Wroclaw University of Science and Technology;
- X 2007 – X 2015: Adjunct at the Institute of Physics, Wroclaw University of Science and Technology;
- I 2004 – IX 2007: Assistant at the Institute of Physics, Wroclaw University of Science and Technology;
- X 1999 – XII 2003: PhD studies at the Institute of Physics, Wroclaw University of Science and Technology;
- X 1994 – VI 1999: MSc studies (solid state physics) at the Faculty of Fundamental Problems of Technology, Wroclaw University of Science and Technology;

Scientific interships:

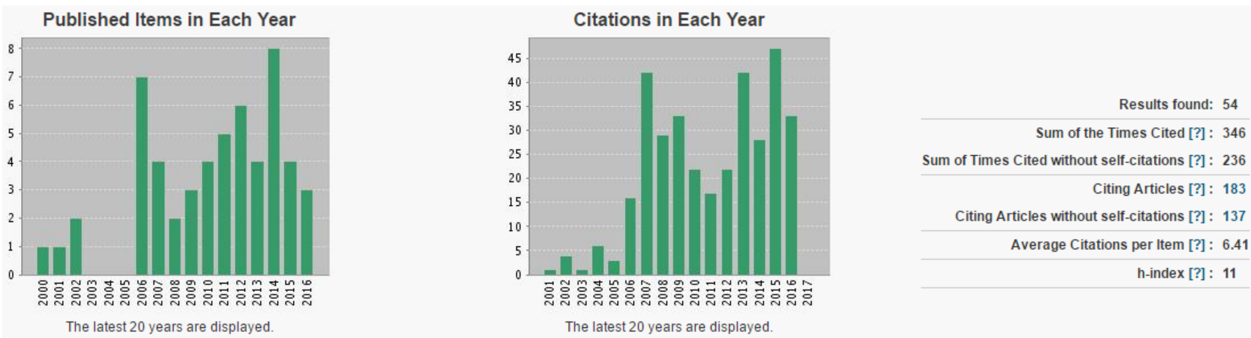
- VIII 2014 – Department of Physics and Computer Science, Wilfrid Laurier University, Waterloo, Canada;
- VII-IX 2013 – Laurence Berkeley National Laboratory, USA;
- VII-IX 2012 – Laurence Berkeley National Laboratory, USA;
- IX-XII 2010 – Department of Physics and Computer Science, Wilfrid Laurier University, Waterloo, Canada

Teaching activity:

- Physics: lectures, classes, and laboratories;
- Specialist courses: Delphi for physicists (lectures and laboratories); Programming in Object Pascal; Elements of object programming; Introduction to quantum mechanics; Computer physics for engineers; Programming in Fortran; Numerical methods; Elements of programming: Programming in c – first level; Procedural programming: Programming in c - second level; Design of materials and structures (laboratory);
- Supervising of Eng. and MSc. diplomas: 2 Eng. diplomas and 2 MSc. diplomas;
- Dissemination of science within the Dolnośląski Festiwal Nauki;
- Assistance in organization and conducting the competition: Międzyszkolny Konkurs Fizyczny we Wrocławiu;

3. Analysis of scientific achievements

According to *ISI Web of Science* the base record of the candidate on 20 September 2016 includes 54 articles where 50 was published after PhD degree. Within the 50 articles published after PhD degree 17 articles are the conference papers and 33 articles are papers published in regular journals such as *Journal of Applied Physics* (11), *Applied Physics Letters* (9), *IEEE Journal of Quantum Electronics* (2), *Journal of Physics D* (2), *Physical Review B* (1), *Physical Review Applied* (1), *Journal of Physics: Condensed Matter* (1), *Applied Physics A* (1), *Thin Solid Films* (1), *Solid State Communications* (1), *Physica Status Solidi (a)* (1). A detailed analysis of the base record of the candidate is presented below.



Total impact factor: ~85
Number of citations (without self-citations): 236
Index Hirsha: 11

4. List of oral presentations at international conferences and seminars

After PhD degree I presented results of my researches at 17 international conferences and workshops as posters (15) and oral presentations (9 including two invited talks). Moreover I presented results of my researches at proper scientific seminars. Titles and places of my selected oral presentations are listed below.

- *Electronic band structure and material gain of III-V-Bi quantum wells grown on GaAs, InP and GaSb substrates*, 8th International Conference on Low Dimensional Structures and Devices, Mayan Riviera, Mexico, August 28 - September 2, 2016 (oral).
- *Material gain in dilute nitrides materials using 8-band and 10-band models*, Energy Materials Nanotechnology - Summer 2015, Cancun-Mexico, 15-19 June 2015 (invited).
- *Electronic band structure and material gain of Ga(In)BiAs/GaAs quantum wells grown on GaAs calculated with 14-band and 8-band kp model*, Workshop of bismuth-contacting semiconductors, Madison-Wisconsin, 19-22 July 2015 (oral).
- *Theoretical calculations of electronic band structure and material gain of III-V-Bi quantum wells grown on GaAs, InP, and GaSb substrates*, Compound Semiconductor Week, Santa Barbara – USA, June 28-July 2 2015 (oral).

- *Influence of AlN layer on electric field distribution in GaN(cap)/AlGaN/GaN transistor heterostructures*, International Workshop on Nitrides 2014, Wrocław-Poland, 24-29 August 2014 (invited).
- *Distribution of built-in electric field in AlGaN/GaN transistor heterostructures: The role of surface states*, 10^{th} International Conference on Nitrde Semiconductors, Washington-USA, 25-30 August 2013 (oral).
- *The influence of inhomogeneities on broadening of fundamental transition in polar and nonpolar InGaN quantum wells dedicated for green emitters*, Spring Meeting of the European-Materials-Research-Society, Nicea-France, 09-13 Maj 2011 (oral).
- *Hydrostatic pressure tuning of emission wavelength and optical gain in GaInNAs/GaAs quantum wells*, V workshop on physics and technology of semiconductor lasers, Kraków-Poland, 17-20 November 2013 (oral).
- *Electronic band structure and optical gain of dilute nitrides quantum wells*, Seminar at the Department of Physics and Computer Science, Wilfrid Laurier University, Waterloo 19 August 2014 (oral).

5. Participation in scientific projects

- *Struktura pasmowa, wzmocnienie optyczne oraz inne parametry nowoczesnych laserów półprzewodnikowych*, grant SONATA BIS from NCN for years 2014-2019 (1 455 700 PLN) – principal investigator.
- *Inżynieria pasm w związkach Ge(Si)Sn i ich niskowymiarowych heterostrukturach przeznaczonych do zastosowań laserowych*, grant OPUS 5 from NCN for years 2014-2016 (690 160 PLN) – principal investigator.
- *Położenie poziomu Fermiego na powierzchni GaN oraz rozkład pól elektrycznych w heterostrukturach AlGaN/GaN osadzanych na podłożach GaN o różnej orientacji krystalograficznej*, grant OPUS from NCN for years 2012-2015 (599 200 PLN) – investigator.
- *Pomiary i obliczenia wzmocnienia optycznego w wybranych półprzewodnikowych strukturach laserowych*, grant from MNiSzW (39 konkurs) for years 2010-2012 (198 000 PLN) – principal investigator.
- *Nowe materiały z grupy III-V-N przeznaczone na lasery, wzmacniacze oraz inne przyrządy półprzewodnikowe: Własności fizyczne- charakteryzacja optyczna*, grant from MNiSzW for support COST action for years 2009-2012 (625 400 PLN) – investigator.
- *Wpływ stanów powierzchniowych oraz głębokich poziomów defektowych na położenie poziomu Fermiego w wybranych materiałach i strukturach półprzewodnikowych grupy III-V*, grant from MNiSzW (35 call) for years 2008-2010 (198 000 PLN) – investigator.
- *Kwantowe nanostruktury półprzewodnikowe do zastosowań w biologii i medycynie (NANOBIOM)*, project from European Union within the Innowacyjna Gospodarka program, realized in years 2007-2014 – investigator.

6. Scientific achievements for “habilitacja” degree

After defense of PhD thesis (27 November 2003) on the theory of superconductivity (thesis entitled *Własności termodynamiczne układów nadprzewodzących typu BCS dla modelowych postaci gęstości stanów* performed under supervision of prof. Ryszard Gonczark) I was continuing work in this subject for two years. Within this subject after PhD defense I published two articles and one monography entitled *Scenariusz Van Hoof* published by Oficyna Wydawnicza Politechniki Wrocławskiej 2004. At the same time I started theoretical calculations for semiconductor heterostructures. My work in the field of semiconductors was focused on issues which were investigated experimentally at the OSN laboratory supervised by prof. Jan Misiewicz. Such collaboration takes place up to now. I focus my research around theoretical problems which are very close to such semiconductor devices as lasers or transistors and recently solar cells. My investigations concern materials which are studied at the OSN laboratory and thereby they can be confronted/compared with experimental results. Such situation takes place in the case of studies of electric field distribution in AlGaN/GaN heterostructurs and studies of inhomogeneitis in polar QWs. In the case of calculations of the material gain, measurements related to this issue has been developed within the grant from MNiSzW entitled *Pomiary i obliczenia wzmocnienia optycznego w wybranych półprzewodnikowych strukturach laserowych*, where I was the principal investigator. Currently such measurements and other optical measurement for laser structures are carried out within the Sonata Bis grant from NCN (*Struktura pasmowa, wzmocnienie optyczne oraz inne parametry nowoczesnych laserów półprzewodnikowych*), where I am the principal investigator. In this case I also expect a confrontation of my theoretical predictions with experimental data. Such a possibility is present for InGaN/GaN investigated in collaboration with prof. Czesław Skierbiszewski from the Institute of High Pressure Physics Polish Academy of Science.

My scientific achievement for “habilitacja” degree is a series of 15 articles on the analysis of selected properties of III-V heterostructures. After my PhD defense I have published over 45 scientific articles (11 in *Journal of Applied Physics* and 9 in *Applied Physics Letters*) in the field of semiconductor physics. For “habilitacja” degree I have selected 15 articles where I am the first author and where my contribution is dominating and the contribution of other authors is subsidiary and will not be used for their scientific promotion. In my scientific achievement I have focus on three scientific issues i.e., the material gain in quantum wells (6 articles), the distribution of built-in electric field in AlGaN/GaN heterostructures (5 articles), and inhomogeneities in polar quantum wells (4 articles).

6.1 List of scientific articles for “habilitacja” degree

<u>Material gain in quantum wells</u>

[H1] **M. Gladysiewicz**, R. Kudrawiec, J. M. Miloszewski, P. Weetman, J. Misiewicz, and M. S. Wartak, *Band structure and the material gain of GaInNAs/GaAs quantum wells modeled within 10-band and 8-band kp model*, J. Appl. Phys. 113, 063514 (2013). IF=2.28

My contribution to [H1] consists in the proposition of the model, theoretical calculations, and writing the manuscript. My percentage contribution to [H1] I evaluate to be 70%.

[H2] **M. Gładysiewicz**, R. Kudrawiec, and M. S. Wartak, *Theoretical studies of optical gain tuning by hydrostatic pressure in GaInNAs/GaAs quantum wells*, J. Appl. Phys. 115, 033515 (2014). IF=2.28

[H3] **M. Gladysiewicz**, R. Kudrawiec, and M. S. Wartak, *Material Gain in $Ga_{0.66}In_{0.34}N_yAs_{1-y}$, $GaN_yAs_{0.69-y}Sb_{0.31}$, and $GaN_yP_{0.46}Sb_{0.54-y}$ Quantum Wells Grown on GaAs Substrates: Comparative Theoretical Studies*, IEEE Journal of Quantum Electronics 50, 996 (2014). IF=1.89

[H4] **M. Gładysiewicz**, R. Kudrawiec, and M. Wartak, *Electronic Band Structure and Material Gain of Dilute Nitride Quantum Wells Grown on InP Substrate*, IEEE Journal of Quantum Electronics 51 (2015). IF=1.89

[H5] **M. Gladysiewicz**, R. Kudrawiec, and M. S. Wartak, *8-band and 14-band kp modeling of electronic band structure and material gain in Ga(In)AsBi quantum wells grown on GaAs and InP substrates*, J. Appl. Phys. 118, 055702 (2015). IF=2.28

[H6] **M. Gladysiewicz**, R. Kudrawiec, and M. S. Wartak, *Electronic band structure and material gain of III-V-Bi quantum wells grown on GaSb substrate and dedicated for mid infrared spectral range*, J. Appl. Phys. 119, 075701 (2016). IF=2.28

My contribution to [H2-H6] consists in the proposition of the material system to study, theoretical calculations, and writing manuscripts. My percentage contribution to [H2-H6] I evaluate to be 80% for each of the article.

Distribution of electric field in AlGaN/GaN heterostructures

[H7] **M. Gladysiewicz**, R. Kudrawiec, J. Misiewicz, G. Cywinski, M. Siekacz, P. Wolny, and C. Skierbiszewski, *The surface boundary conditions in GaN/AlGaN/GaN transistor heterostructures*, App. Phys. Lett. 98 231902 (2011). IF=3.57

[H8] **M. Gladysiewicz**, , L. Janicki, J. Misiewicz, M. Sobanska, K. Klosek, Z.R. Zytkiewicz, and R. Kudrawiec, *Engineering of electric field distribution in GaN(cap)/AlGaN/GaN heterostructures: Theoretical and experimental studies*, J. Phys. D (2016). IF=2.72

[H9] **M. Gladysiewicz**, R. Kudrawiec, J. Misiewicz, K. Klosek, M. Sobanska, J. Borysiuk, and Z. R. Zytkiewicz, *Influence of AlN layer on electric field distribution in GaN/AlGaN/GaN transistor heterostructures*, J. Appl. Phys. 114, 163527 (2013). IF=2.28

[H10] **M. Gladysiewicz**, L. Janicki, M. Siekacz, G. Cywinski, C. Skierbiszewski, and R. Kudrawiec, *Theoretical and experimental studies of electric field distribution in N-polar GaN/AlGaN/GaN heterostructures*, Appl. Phys. Lett. 107, 262107 (2015). IF=3.57

My contribution to [H7-H11] consists in the interpretation of experimental results, theoretical calculations, and writing manuscripts. My percentage contribution to [H7-H11] I evaluate to be 60% for each of the article.

[H11] **M. Gladysiewicz** and R. Kudrawiec, *Quantum Confinement in Thin GaN Cap Layers Deposited on AlGaN/GaN Heterostructures: The Issue of Polar Surface Quantum Well*, Jap. J. Appl. Phys. 52, 08JL05 (2013). IF=1.13

My contribution to [H12] consists in the proposition of the model, theoretical calculations, and writing the manuscript. My percentage contribution to [H1] I evaluate to be 90%.

Inhomogeneities in polar quantum wells

[H12] **M. Gładysiewicz**, R. Kudrawiec, J. Misiewicz, G. Cywiński, M. Siekacz, C. Skierbiszewski, *Broadening of intersubband and interband transitions in InGaN/AlInN multi-quantum wells*, J. Phys. D: Appl. Phys. 43 195101 (2010). IF=2.72

My contribution to [H13] consists in the interpretation of experimental results, theoretical calculations, and writing the manuscript. My percentage contribution to [H13] I evaluate to be 60%.

[H13] **M. Gładysiewicz** and R. Kudrawiec, *Random approach to determine the broadening of intersubband and interband transitions in (In)GaN/Al(In)N quantum wells*, Journal of Physics: Condensed Matter 22 485801 (2010). IF=2.35

My contribution to [H14] consists in the proposition of the model, theoretical calculations, and writing the manuscript. My percentage contribution to [H1] I evaluate to be 90%.

[H14] **M. Gladysiewicz** and R. Kudrawiec, *Theoretical studies of the influence of structural inhomogeneities on the radiative recombination time in polar InGaN quantum wells*, Phys. Status Solidi (a) 209, 752 (2012). IF=1.61

My contribution to [H15] consists in the proposition of the model, theoretical calculations, and writing the manuscript. My percentage contribution to [H15] I evaluate to be 90%.

[H15] **M. Gladysiewicz**, R. Kudrawiec, M. Syperek, J. Misiewicz, M. Siekacz, G. Cywinski, A. Khachapuridze, T. Suski, C. Skierbiszewski, *Influence of quantum well inhomogeneities on absorption, spontaneous emission, photoluminescence decay time, and lasing in polar InGaN quantum wells emitting in the blue-green spectral region*, Applied Physics A: Materials Science and Processing 115, 1015 (2014). [IF=1.70].

My contribution to [H15] consists in the proposition of the model for interpretation of experimental data, theoretical calculations, and writing the manuscript. My percentage contribution to [H15] I evaluate to be 50%.

Coauthors' statements on their individual contribution to joint papers are given in separate attachments entitled „Oświadczenia współautorów".

6.2 Resume of articles on material gain calculations in selected III-V quantum wells

Quantum wells (QWs) are the active region in novel semiconductor lasers. Material (optical) gain is the fundamental feature of the QW, which determines the utility of a given QW in laser applications. It concerns both the spectral position of thegain peak and its intensity. Therefore the material gain calculations are very important part of design and optimization of novel semiconductor heterostructures dedicated for laser applications. I have performed such calculations for QWs containing dilute nitrides and dilute bismides alloys. I have selected this material system because of its unusual electronic band structure, which was a challenge for theoretical calculations, as well as the lack of scientific articles on material gain calculations for this materials system excluding GaInNAs/GaAs QWs.[1] I have proposed and analyzed the proper model [H1, H2, H5] and solved the material problem consists the selection of proper contents of QWs for laser structures deposited on GaAs [H3, H5], InP [H4, H5], and GaSb [H6] substrate. The most important aspects of [H1-H6] are presented below.

Nitrogen in dilute nitrides is an unusual component since its incorporation into III-V host leads to reduction of the energy gap and the lattice constant. The simultaneous reduction of the energy gap and the lattice constant is the most important feature of dilute nitrides since such correlation is not observed for other III-V alloys. This feature is very important for semiconductor devices since the lattice constant is this factor which limits tuning the energy gap and band gap discontinues at QW interfaces. The small amount of nitrogen in III-V host allows to avoid problems with too large band gap and/or too large strains. Incorporation of a few percent of nitrogen to III-V QWs deposited on GaAs or InP substrates allows to obtain a QW with emission which cover very broad spectral range as shown in [H3, H4].

The key issue in material gain calculations for QWs containing dilute nitrides is the correct calculations of dispersion of electron subbands in the QW. The characteristic feature of dilute nitrides is its unusual electronic band structure in the conduction band, i.e. the non-parabolic dispersion of conduction band.[2] The band anticrossing (BAC) model[3] can be applied to describe the electronic band structure in the conduction band. This model assumes that nitrogen atoms create a resonant level which interacts with the conduction band of III-V host. Due to this interaction two non-parabolic bands appear in the conduction band instead of the nitrogen resonant level and the conduction band of the III-V host. For regular III-V semiconductors the 8-band ***kp*** model can be applied to describe the electronic band structure near the center of the Brillouin zone. In the case of dilute nitrides a natural development of the ***kp*** model is 10-band ***kp*** model, which takes into account the interaction of III-V host bands with the nitrogen resonant level. Such a model has been described and compared with the 8-band model in [H1] for GaInNAs/GaAs QW, which is the most explored dilute nitride QWs. In [H2] it has been shown that the 10-band ***kp*** model is necessary to explain experimental results on the decrease of the material gain intensity in GaInNAs/GaAs QW with the increase in the hydrostatic pressure[4] In this case the 8-band model is not able to reproduce the experimental data since the effect of gain decrease with the increase in the hydrostatic pressure is due to the interaction between the nitrogen level and the conduction band. This interaction is not

[1] M. Kondow, K. Uomi, A. Niwa, T. Kikatani, S. Watahiki, and Y. Yazawa, Jpn. J. Appl. Phys., Part 1 35, 1273 (1996), oraz referencje w pracy [H1].
[2] M. Henini, *Dilute Nitride Semiconductors* (Elsevier Ltd, Oxford, 2005).
[3] W. Shan, W. Walukiewicz, J.W. Ager, III, E.E. Haller, J.F. Geisz, D.J. Friedman, J.M. Olson, and S.R. Kurtz, Phys. Rev. Lett. 82, 1221 (1999).
[4] A. Bercha, F. Dybala, K. Komorowska, P. Adamiec, R. Bohdan, W. Trzeciakowski, J.A. Gupta, P.J. Barrios, G. Pakulski, A. Delage, and Z.R. Wasilewski, Proceeding SPIE 5722, 565 (2005).

included in the 8-band ***kp*** model. For GaInNAs this issue is discussed in [H1]. In case of such materials as GaNAsSb or GaNPSb the knowledge of BAC parameters is more problematic and therefore the application of 8-band ***kp*** model to calculate the electronic band structure and the material gain is recommended. In this case the band gap for quaternary alloys can be calculated with the interpolation of energy gap proposed in [5] and [6]. Such approach has been applied in [H3, H4] to calculate the material gain in III-V-N QWs deposited on GaAs [H3] and InP [H4] substrate. In the case of QWs deposited on GaAs substrate it has been shown that GaNAsSb/GaAs and GaNPAs/GaAs QWs have strong material gain and its spectral position is observed at longer wavelengths if it is compared with the material gain of GaInNAs/GaAs QW with the same nitrogen concentration and built-in compressive strain. It means that these QWs are very promising gain medium for lasers operating in telecommunication windows at 1.55μm [H3]. For QWs deposited on InP substrate three active regions (i.e. GaInNAs, GaNAsSb and GaNPSb QWs with different barriers lattice matched to InP) have been analyzed and QWs with the positive material gain have been identified. In this case it has been observed that the studied QWs are able to cover the spectral range of ~2.0-3.5μm [H4].

For dilute bismides the BAC model can be applied to describe the electronic band structure similarly as for dilute nitrides. The difference is that Bi atoms create the resonant level in the valence band and this level interacts with the valence band. Since Bi atoms are described by three levels (each level is twice degenerated) the 14-band ***kp*** model can be applied instead of the 8-band ***kp*** model to describe the electronic band structure near the center of the Brillouin zone and calculate the material gain for QWs containing dilute bismides. As shown in [7] the incorporation of Bi atoms into III-V host also changes the conduction band. A model including the interaction of Bi levels with the valence band and Bi-related changes in the conduction band has been proposed in [H5] and applied to calculate the material gain in GaInAsBi QWs deposited on GaAs and InP substrate. In this wok it has been shown that GaInAsBi/GaAs QWs have a good material gain which can be tuned from ~1.3μm to ~1.5μm by changing Bi concentration from 3% to 5%. For GaInAsBi QWs deposited on InP substrates the increase in Bi concentration from 0 to 5% at the same compressive strain in the QW (i.e., ε=2%) shifts the gain peak from ~2μm to ~4μm [H5].

In the case of dilute nitrides and bismides the well-known problem is the deterioration of the optical quality of these materials with the increase in nitrogen or bismuth concentration. This issue is discussed in proper papers [H1, H3-H5]. However in the case of GaSb with a few percentage of Bi atoms the situation is different since the Sb and Bi atoms are similar and hence III-Sb-Bi alloys are similar to other regular III-V alloys and therefore the 8-band ***kp*** model is appropriate to describe the electronic band structure near the center of the Brillouin zone in such alloys.

For GaSb-based lasers the well-known problem is the shallow QW in the valence band. Incorporation of As atoms into GaInSb/GaSb QW leads to a redshift of QW emission due to the bandgap reduction of GaInAsSb as well a reduction of built-in strain in the QW region. However above some As concentration GaInAsSb/GaSb QW starts to be type II that is very unfavorable for laser applications. Therefore very recommended solution is the incorporation of a component in GaIn(As)Sb/GaSb QW, which is able to enhance the quantum confinement in the valence band. As shown in [H6] Bi atoms are such component. To calculate the electronic band structure and the material gain for GaSb-based QWs containing dilute bismides I applied 8-band ***kp*** model. Bi-

[5] R. Kudrawiec, J. Appl. Phys. 101, 023522 (2007).
[6] R. Kudrawiec, J. Appl. Phys. 101, 116101 (2007).
[7] R. Kudrawiec, J. Kopaczek, M. P. Polak, P. Scharoch, M. Gladysiewicz, J. Misiewicz, R. D. Richards, F. Bastiman, and J. P. R David, J. Appl. Phys. 116, 233508 (2014).

related changes in the conduction band have been modeled after [8]. For quaternary and quinary III-V-Bi alloys I have proposed a proper interpolation [H6] and with this interpolation and 8-band ***kp*** model I have calculated the electronic band structure and the materials gain for GaSbBi/GaSb, GaInSbBi/GaSb and GaInAsSbBi/GaSb QWs. Various barriers lattice matched to GaSb have been considered for GaInAsSbBi QWs. On the basis of all these calculations it has been shown that the incorporation of Bi atoms in GaSb-based QWs is a very promising solution for pushing the QW emission to longer wavelengths at the preserving type I character of the QW [H6].

Summarizing above works, it is clear that they are a series of articles with a significant contribution in the field of modeling of the electronic band structure and material gain as well as in the field of searchers of novel QW materials for lasers operating in various spectral regions. It is the subject matter, which I began in collaboration with dr Marek Wartak during my scientific stay at the Department of Physics and Computer Science, Wilfrid Laurier University. I am continuing this subject matter and now I am focus on InGaN/GaN QWs and GeSn-based QWs. I have an original software developed by myself in Pascal for calculations of the electronic band structure and the material gain for III-V QWs in cubic structure and an original software developed by myself in c++ for calculations of the electronic band structure and the material gain for polar InGaN/GaN QWs. Together with my student we have developed a software for calculations of GeSn-based QWs and recent results on material gain calculations in this material system has been accepted to for publication in Scientific Reports.

6.3 Resume of articles on distribution of built-in electric field in AlGaN/GaN heterostructures

AlGaN/GaN heterostructures are the active region of novel high power transistors, which can operate at high temperatures. Nowdays very intensive researches on the optimization of AlGaN/GaN heterostructures are carried out in many laboratories in the Word and in Poland. At the laboratory for Optical Spectroscopy of Nanostructures (OSN) www.osn.if.pwr.wroc.pl at the Wroclaw University of Science and Technology researchers apply the photoreflectance and contactless electroreflectance spectrscopy to investigate semiconductor heterostructures. These methods allow to determine the built-in electric field in semiconductor layers but they do not give information about the electric field distribution in the whole semiconductor heterostructure. The goal of my studies was the interpretation of experimental results and theoretical analysis of the influence of surface boundary conditions (i.e., the Fermi level position on semiconductor surface), residual doping in (Al)GaN layers and their thickness on the distribution of electrif field and concentration of two dimensional electron gas in AlGaN/GaN heterostructures. In the fromework of these studies we published 11 papers and 5 of them I included to this profesional accomplishment.

In [H7] GaN(cap)/AlGaN/GaN(buffor) heterostructures of various thickness of AlGaN layer were studied and it has been observed that the built-in electric field in AlGaN layer strongly depends on the thickness of this layer. In order to explain this phenomenon, I have solved Schrödinger and Poisson equation in self-consistent manner for various Fermi level position on GaN surface. Comparing theoretical calculations with experimental data I was able to determine the Fermi level position for which theoretical predictions are able to reproduce experimental data. In this case I have observed that independently on the thickness of AlGaN layer the agreement between theoretical predictions and experimental data is observed for the same Fermi level position at GaN surface within the accuracy of the applied theoretical and experimental methods. It means that the Fermi level position at GaN surface can be treated as the surface boundary condition for the distribution of built-in electric field in GaN(cap)/AlGaN/GaN(buffer) heterostructures. This finding was not obvious in the context of previous studies of such heterostructures. For the investigated samples it has been determined that the Fermi level at GaN surface is located 0.55 eV below the conduction band that is different than the value which was used by other authors who without the access to experimental data assumed that the Fermi level is located at the middle of GaN energy gap i.e. 1.7 eV below the conduction band. It is worth to underline that the Fermi level determined in [H7] is consistent with the density of surface states determined theoretically from first principles[8] and later studies of Fermi level position on GaN surface by using contactless electroreflectance,[9] as well as studies of electric field distribution in GaN(cap)/AlGaN/GaN(buffor) heterostructures of different GaN(cap) thickness [H8] and GaN(cap)/AlGaN/GaN(buffor) heterostructures with a thin AlN layer [H9]. In [H8] besides the determination of the surface boundary condition in GaN(cap)/AlGaN/GaN(buffor) heterostructure (i.e., determination of the Fermi level on GaN surface) it has been shown that the distribution of electric field in such heterostructures results from discontinuities in total polarization at the interfaces and the distribution of free carriers, which accumulates at these interfaces. The change in the thickness of particular layers leads to changes in the distribution of free carriers an in consequence changes in the distribution of electric field [H8].

In order to improve the mobility of two-dimensional electron gas in AlGaN/GaN heterostructures, a thin AlN layer is very often incorporated into such heterostructure This layer reduces alloy scattering at the AlGaN/GaN interface. A lot of paper on the comparison of AlGaN/GaN heterostructures with and without the AlN layer can be found in the literature but any of them consider the influence of AlN layer on the distribution of built-in electric field in such heterostructures. My theoretical predictions clearly show that the thin AlN layer significantly influence the electric field distribution and such an effect has been observed experimentally in [H9]. Performing calculations of electric field distribution in AlGaN/AlN/GaN heterostructures with different thickness of AlN layer it has been shown that thickness of this layer influence the built-in electric field in AlGaN layer and the whole heterostructure. A good agreement between theoretical predictions and experimental data has been obtained in [H9].

For recent years GaN/AlGaN/GaN(buffor) heterostructures deposited on N-polar GaN surface (i.e., along the (000-1) direction) were intensively investigated. [10] In such heterostructures the two-dimensional electron gas is formed at the GaN/AlGaN interface instead of AlGaN/GaN interface as it takes place in heterostructures deposited on Ga-polar GaN surface (i.e., along the (0001) direction). An advance of such approach is the possibility of the total depletion of conduction channel as well as an effective elimination of the second conductivity channel though the buffer/substrate. While the concentration of two-dimensional electron gas at the AlGaN/GaN interface in heterostructurs deposited along the (0001) direction was determined by many authors a credible calculations of the two-dimensional electron concentration in GaN/AlGaN heterostructures deposited along the (000-1) direction do not exist mainly due to the lack of experimental data on the Fermi level position at the N-polar GaN surface. According to theoretical

[8] D. Segev, Ch.G. Van de Walle, J. Cryst. Growth 300, 199 (2007).
[9] R. Kudrawiec, M. Gladysiewicz, L. Janicki, J. Misiewicz, G. Cywinski, C. Cheze, P. Wolny, P. Prystawko, and C. Skierbiszewski, Appl. Phys. Lett. 100, 181603 (2012).
[10] M. H. Wong, S. Keller, N. S. Dasgupta, D. J. Denninghoff, S. Kolluri, D.F. Brown, J. Lu, N.A. Fichtenbaum, E. Ahmadi, U. Singisetti, A. Chini, S. Rajan, S. P DenBaars, J.S. Speck and U.K. Mishra, Semicond. Sci. Technol. 28, 074009 (2013)

calculations of surface density of states for such surface[11] it is expected that the Fermi level can be located 2.2 eV below the conduction band. However experimental studies of N-polar GaN surface do not confirm these predictions and recent studies of N-polar GaN/GaN:Si structures by using contactless electroreflectance spectroscopy shows that the Fermi level on N-polar GaN surface is located 0.3 eV below the conduction band.[12] Such state of the art motivated me to theoretical studies of the electric field distribution and two-dimensional electron gas concentration in N-polar GaN(channel)/AlGaN/GaN(buffer) heterostructures of various thicknesses of GaN(channel) and AlGaN layer. Results of these studies are reported in [H10]. In this work I have determined the range of thickness of GaN(channel) and AlGaN layer, for which the two-dimensional electron gas is formed at the GaN(channel)/AlGaN interface, moreover it has been determined how the concentration of two-dimensional electron gas depends on the Fermi level position on GaN surface. Obtained results allowed us to conclude that such heterostructure is very promising in sensors with the chemical gate since the concentration of two-dimensional electron gas in such heterostructure strongly depends on the Fermi level position on the surface of such heterostructure.

An additional issue, which has appeared during the analysis of built-in electric field in AlGaN/GaN hetrostructures, is the surface quantum well which is formed on the top of AlGaN/GaN hetrostructure if this heterostructure is capped by a thin GaN layer. A 2-3 nm thick GaN layer is a typical cap which protects AlGaN surface before oxidation and improves electric contacts to this hetrostructure. The effect of quantum confinement in thin GaN cap layer was reported for the first time in [13] and also was observed in [H7, H8]. However theoretical solution of such problem was not reported in the literature. In [H11] this problem has been detailed described and solved theoretically. It is a problem of a surface QW with the built-in electric field and different potential barriers. On one side it is AlGaN barrier and on the other side it is air (vacuum). It is worth noting that this problem is not symmetric for (0001) and (000-1) direction. Moreover for thin QWs it is important to consider fluctuations of QW width. Results present in [H11] take into account QW inhomogeneitis and compare surface QWs grown along (0001) and (000-1) direction on AlGaN layer.

Investigations of built-in electric field in AlGaN/GaN heterostructures are very intensively continued at the OSN laboratory at Wroclaw University of Science and Technology. I am responsible for theoretical calculations of the electric field distribution and two-dimensional electron concentration in such heterostructures as well as a comparison of these calculations with experimental data. All programs to analyze the AlGaN/GaN heterostructures are written by myself in Pascal. These programs are still developed and improved. Currently we study very intensively N-polar GaN/AlGaN/GaN heterostructurs passivated by SiN. The aim of our studies is to calculate the electric field distribution and two-dimensional electron gas concentration in such heterostructures and determine the Fermi level position at the SiN/GaN interface.

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[11] D. Segev and Ch.G. Van de Walle, Europhys. Lett. 76, 305 (2006).

[12] R. Kudrawiec, L. Janicki, M. Gladysiewicz, J. Misiewicz, G. Cywinski, M. Boćkowski, G. Muzioł, C. Chèze, M. Sawicka and C. Skierbiszewski, Appl. Phys. Lett. 103, 052107 (2013).

[13] M. Motyka, M. Syperek, R. Kudrawiec, J. Misiewicz, M. Rudziński, P.R. Hageman, P.K. Larsen, Appl. Phys. Lett. 89, 231912 (2006).

6.4 Resume of articles on inhomogenities in polar quantum wells

Inhomogeneity of QW width and content can be a key issue in the interpretation of optical properties of polar QWs. For cubic GaAs/AlGaAs and InGaAs/GaAs QWs grown along (001) direction such a problem does not exist or can be neglected. In the case of GaN QWs grown along polar directions usually we deal with a very thin QWs since for light emitters we need to have a significant electron-hole overlap. For a comparison, a typical InGaAs/GaAs QW has 8nm width (~30 monolayers) while a typical InGaN/GaN QW dedicated for light emitters has the width <3nm (<14 monolayers). It suggest that the fluctuation of QW width by 1 monolayer is more important in InGaN/GaN QWs. Taking into account this fact that InGaN/GaN are grown along the polar direction it is interesting to know the role of polarization effects in broadening of the optical transitions and other phenomena. Such issues are studies in [H12-H15].

To explain the large broadening of interband and intersubband optical transitions in narrow QWs (width < 2nm) dedicated for light modulators an analytical approach has been proposed in [H12]. In this approach the dependence of energy of optical transition (interband and intersubband) on the QW width has been calculated and next it has been proposed that the inhomogeneous broadening of the optical transition is associated with the fluctuation of QW width. This broadening can be calculated by multiply the fluctuation of QW width by the width derivative of transition energy. If we know the broadening of optical transitions we can determine the fluctuation of QW width, which for studied QW samples equals 2 monolayers [H12]. This approach is very simply but it is difficult to apply in the case of a significant fluctuation of both the QW width and the content. A model of random QW has been proposed for such situations. In this model it is possible to consider simultaneously fluctuation of QW width and fluctuation of QW content.

The model of random QW assume that locally the QW can have different width and content but the scale of this fluctuation is larger than the scale of quantization in this material system. For GaN it can be assumed that it is above 10nm. It means that the optical answer for a sample corresponds to answers from thousands homogenous areas with the size > 10nm. To simulate such answer a thousand QW of different width and content is generated in a random manner. The nominal QW width and content are the mean value in the Gaussian distribution while the fluctuation of QW width and content are described by the standard deviation in the Gaussian distribution (unphysical numbers are eliminated). For such generated QW we calculate energies of optical transitions and their probabilities. Next, a proper histogram is built. In this histogram the energy is divided by equal parts and the probability of optical transitions in each part is counted. As shown in [H13] the model of random QW very well explains broadening of optical transitions observed in absorption-like experiments such as contactless electroreflectance and modulated transmission.

The model of random QW also simulates very well the broadening of photoluminescence (PL) spectra of InGaN/GaN QWs.[14] In the case of time resolved PL of InGaN/GaN QWs a spectral dispersion of PL decay time and a non-exponential PL decay are very often observed. Such features of time resolved PL are attributed to the effect of carrier localization. Since the effect of carrier localization is included in the model of random QW it is expected that the mentioned features of time-resolved PL spectra will be reproduced within the model of random QW [H14]. Time resolved PL spectra for an inhomogeneous polar InGaN/GaN QW are simulated in [H14]. In this work the phenomenon of non-radiative recombination and the process of exciton hopping are neglected but

[14] M. Gladysiewicz, R. Kudrawiec, J. Misiewicz, M. Siekacz, G. Cywinski, and C. Skierbiszewski, Phys. Status Solidi C 8, 2282 (2011).

despite these simplicities it is observed that the model of random QW reproduce spectral features observed experimentally. It is also shown that the built-in electric field enhances the dispersion of PL decay time and the non-exponential decay of PL.

The homogeneity of InGaN/GaN QW is the key issue in the production of the active part of lasers dedicated for green spectral range. This issue is analyzed in details in [H15]. In order to achieve emission at ~500nm from InGaN/GaN QW, the indium concentration has to be high (~25%). It leads to large strains (large piezoelectric polarization) and hence a large built-in electric field. As shown in [H15] and [15] the built-in electric field in inhomogeneous QWs causes an extra broadening of optical transitions and therefore such QW is not good gain medium for lasers. Screening of built-in electric field due to optical pumping significantly narrows broadening of emission peak and this issue can be investigated within the model of random QW [H15]. However it also blueshifts emission peak. Therefore a spectral shift is observed between the stimulated emission and the spontaneous emission obtained at low excitation conditions. As shown in [H15] this shift is correlated with the QW inhomogeneities since these inhomogeneities are responsible for this shift.

The issue of influence of QW inhomogeneities on optical properties of QWs is still explored. The proposed model of random QW is very powerful and works in other material systems as well. Therefore this model is developed and applied to other material systems (i.e., ZnO/ZnMgO and other QWs). I am working on including the non-radiative recombination and the process of exciton hoping in this model. This model is implemented in c++. The program allows very simply generation of results and their comparison for various parameters as well as visualization of these results as shown in [H13-H15].

7. Summary

My scientific achievement selected for “habilitacja” degree in physics can be summarized within three points:

i) Developing the model and determination of material parameters for calculations of the electronic band structure and the material gain for quantum wells containing dilute nitrides and dilute bismides [H1-H6].

ii) Founding boundary conditions for calculations of the electric field distribution in polar AlGaN/GaN transistor heterostructures and the interpretation of built-in electric fields obtained by studies of AlGaN/GaN heterostructures by contactless electroreflectance spectroscopy [H7-H11].

iii) Proposition and developing of the model of “random” quantum well used to explain optical properties (broadening of optical transitions and decay time of photoluminescence) observed for inhomogeneous InGaN/GaN quantum wells [H12-H15].

[15] M. Gladysiewicz and R. Kudrawiec, Phys. Status Solidi C 9, 830 (2012).