0_Programme Apropos 17	1
P0_List of posters	5
P1-1_Algirdas Jasinskas	6
P1-2_Jonas Gradauskas	7
P1-3_Karolis Stašys	8
P1-4_Linas Ardaravičius	9
P1-5_Roman Balagula	10
P2-1_Agnė Zdaniauskienė	11
P2-2_Karolina Maleckaite	
P2-3_Rokas Gegevičius	13
P2-4_Rokas Jasiunas	14
P2-5_Rugilė Lukaševičiūtė	15
P2-6_Šarūnas Jankauskas	16
P2-7_Vaidas Pudžaitis	17
P3-1_Andrius Kamarauskas	18
P3-2_Ieva Matulaitiene	19
P3-3_Ivan Yahniuk	20
P3-4_Juozas Vyšniauskas	21
P3-5_Liang Qi	22
P3-6_P.Mackonis	23
P3-6_Paulius Mackonis	24



Apropos 17

Phys Tech

Advanced Properties and Processes in Optoelectronic Materials and Systems 30 September – 1 October, 2020

Sattelite Event

Lithuania-Poland Workshop on Physics and Technology

CONFERENCE PROGRAMME

Center for Physical Sciences and Technology (FTMC), Vilnius, Lithuania Venue: FTMC at Sunrise Valley, Saulėtekio Ave. 3, Vilnius, Lithuania

30 September		
8:00-9:00		REGISTRATION
9:00-9:15		CONFERENCE OPENING CEREMONY Gintaras Valušis Director of Center for Physical Sciences and Technology Chair of Apropos 17 conference
9:15-10:35		Section 1: Semiconductor nanostructures and advanced photonics systems Chair Prof. <i>Carlito Jr.Salonga Ponseca</i>
9:15-9:45	Inv 1	Linas Minkevičius (Center for Physical Sciences and Technology, Vilnius, Lithuania) Review of innovative diffractive elements for Terahertz imaging applications
9:45-10:15	Inv2	Ramūnas Aleksiejūnas (Vilnius University, Lithuania) Impact of alloy disorder induced localization on hole diffusion in highly excited c-plane and m-plane InGaN quantum wells
10:15-10:35	01	<u>Janusz Sadowski (University of Warsaw, Institute of Physics, Warsaw,</u> <i>Poland, Linnaeus University, Sweden</i>) MoTe2 transition metal dichalcogenide grown by molecular beam epitaxy – polytypes, structural and electrical properties
10:35-11:00		Coffee break
11:00-13:00		Section 2: Nano and Biophotonics Chair Dr. <i>Kaibo Zheng</i>
11:00-11:30	Inv3	Šarūnas Meškinis (Kaunas University of Technology, Lithuania) Direct synthesis of the graphene on Si(100) substrate for solar cell applications

11:30-12:00	Inv4	Dovydas Banevičius (Vilnius University, Lithuania) Naphthyridine-based deep-blue TADF OLEDs with low efficiency roll-off
12:00-12:20	02	Rusnė Ivaškevičiūtė-Povilauskienė (Center for Physical Sciences and Technology, Vilnius, Lithuania) All-optical modulation of graphene layers
12:20-12:40	03	Lena Golubewa (Center for Physical Sciences and Technology, Vilnius, Lithuania) Raman spectroscopic investigation of multi-walled carbon nanotubes mediated neutrophil activation
12:40-13:00	04	Adil Rehman (Institute of High Pressure Physics, Warsaw, Poland) Modulation of electrical and noise characteristics of carbon nanotubes based devices
13:00-14:00		Lunch
14:00-15:50		<i>Special session:</i> Ultrafast THz techniques Chair Dr. <i>Ignas Grigelionis</i>
14:00-14:30	Inv5	Carlito S. Ponseca, Jr. (<i>Linköping University, Sweden</i>) - Ultrafast transient spectroscopy of organic and hybrid solar cells
14:30-14:50	05	<u>Kaibo Zheng (Lund University, Sweden, Technical University of Denmark,</u> Danmark) Ultrafast spectroscopy of Quantum dot solar cells
14:50-15:10	06	Ričardas Norkus (Center for Physical Sciences and Technology, Vilnius, Lithuania) Terahertz emission from a bulk GaSe crystal excited by above-bandgap photons
15:10-15:30	07	Daniil Pashnev (Center for Physical Sciences and Technology, Vilnius, Lithuania) Investigation of two-dimensional plasma resonances in grating-gated AlGaN/GaN heterostructures by terahertz time domain spectroscopy
15:30-15:50	08	Marek Maciaszek (University of Warsaw, Poland) On the origin of the 4.1 eV luminescence in hexagonal boron nitride
15:50-16:15		Coffee break
16:15-18:20		Section 1: Semiconductor nanostructures and advanced photonics systems Chair Prof. <i>Šarūnas Meškinis</i>
16:15-16:45	Inv6	Tadas Malinauskas (Vilnius University, Lithuania) Remote epitaxy of GaN via Graphene
16:45-17:05	09	Ivan Yahniuk (Institute of High Pressure Physics, Warsaw, Poland) Temperature-& Pressure-induced transitions in HgTe QWs
17:05-17:20	010	Roman M. Balagula (Center for Physical Sciences and Technology, Vilnius, Lithuania) Annealing-induced reduction of strain in GaAs/GaNAs core-shell nanowires
17:20-17:40	011	Andrea Zelioli (University of Modena, Italia) GaInAs/GaAs Quantum Structures For Near Infrared Vertical-External-Cavity Surface-Emitting Lasers
17:40-18:00	012	<u>Simona Pūkienė</u> (Center for Physical Sciences and Technology, Vilnius, Lithuania) A3-B5 QW structures for IR range optoelectronic devices
18:00-19:30		Poster session (18 posters) Coffee and Snaps

1 October			
9:00-11:00	PL LT Phys Tech	Satellite Event: Lithuanian Polish Workshop Chair Prof. Janusz Sadowski	
9:00-9:10		WORKSHOP OPENING CEREMONY Ambassador Urszula Doroszewska, Embassy of Poland Jerzy Łusakowski (Chair from Poland)	
9:10-9:35	Inv7	Nerija Žurauskienė (Center for Physical Sciences and Technology, Vilnius, Lithuania) Magnetoresistance Relaxation Phenomena in Nanostructured Lanthanum Manganite Films	
9:35-10:00	Inv8	Wojciech Pacuski (<i>University of Warsaw, Poland</i>) Narrow excitonic lines and large-scale homogeneity of transition metal dichalcogenides grown by MBE on hBN	
10:00-10:20	013	Maksym Dub (Institute of High Pressure Physics, Warsaw, Poland) Graphene gate GaN/AlGaN field effects transistors for THz detection	
10:20-10:40	014	Maria Szoła (Institute of High Pressure Physics, Warsaw, Poland) THz magnetospectroscopy of HgCdTe bulk crystals with different Cd content	
10:40-11:00	015	Paweł Komorowski (Warsaw University of Technology, Poland) Machin learning enhanced design of diffractive optical elements	
11:00-11:25		Coffee break	
11:25-13:05		Section 3: Ultrafast and THz phenomena Chair Dr. <i>Linas Minkevičius</i>	
11:25-11:55	Inv9	Alvydas Lisauskas (Vilnius University and Institute of High Pressure Physics, Warsaw, Poland) THz detectors and sources fabricated with CMOS technologies	
11:55-12:25	Inv10	Guillaume Ducournau (Université Lille, France) THz communications and advanced RF characterization enabled by THz photonics	
12:25-12:45	O16	Dmytro B. But (Institute of High Pressure Physics, Warsaw, Poland) Antenna Characterization of Monolithically Integrated Detectors for 0.62 THz	
12:45-13:05	017	Domas Jokubauskis (Center for Physical Sciences and Technology, Vilnius, Lithuania) Phase contrast sub THz imaging and applications	
13:05-14:00		Lunch	
14:00-15:50		Section 3: Ultrafast and THz phenomena Chair Prof. <i>Alvydas Lisauskas</i>	
14:00-15:50 14:00-14:30	Inv11	Section 3: Ultrafast and THz phenomena Chair Prof. Alvydas LisauskasVincas Tamošiūnas (Center for Physical Sciences and Technology, Vilnius, Vilnius University, Lithuania) Reflectance spectra of selective emitter solar cells in terahertz and sub-terahertz ranges	

14:50-15:10	019	<u>Ieva Žičkienė</u> (<i>Center for Physical Sciences and Technology, Vilnius, Lithuania</i>) Terahertz radiation induced by surface ballistic photogalvanic effect in GaAs LIPSS structures
15:10-15:30	020	Pavlo Sai (Institute of High Pressure Physics, Warsaw, Warsaw University of Technology, Poland) AlGaN/GaN dual grating gate structures investigated in high magnetic field
15:30-15:50	021	<u>Vladislovas Čižas</u> (Center for Physical Sciences and Technology, Vilnius, Lithuania) Fractional frequencies in microwave response of GaAs/AlGaAs superlattices
15:50-16:15		Coffee break
16:15-17:35		Section 4: Organics for Optoelectronics Chair Dr. Prof. <i>Nerija Žurauskienė</i>
16:15-16:35	022	Yuri Svirko (University of Eastern Finland, Joensuu, Finland) Light- induced currents and THz emission from graphene
16:35-16:55	023	Ernesta Poceviciute (Center for Physical Sciences and Technology, Vilnius, Lithuania) Studies of Receptor and Its Ligand Interaction Using FRET and TIRF Microscopy
16:55-17:15	024	Edvinas Navakauskas (Center for Physical Sciences and Technology, Vilnius, Lithuania) Structure determination of HEWL protein aggregates at liquid interfaces
17:15-17:35	025	<u>Wanessa Melo (Center for Physical Sciences and Technology, Vilnius,</u> Lithuania) Antimicrobial photodynamic therapy: an alternative to overcome the biofilm resistance
17:40		Closing Remarks

List of posters

P1-1 Algirdas Jasinskas Optically pumped semiconductor lasers based on InGaAs/GaAs and GaAsBi/GaAs quantum wells

P1-2 Jonas Gradauskas Three components of photovoltage simultaneously induced across GaAs pn junction

P1-3 Karolis Stašys Bismide-based Intersubband devices for Mid-Infrared Applications

P1-4 Linas Ardaravičius Determination of electron drift velocity from hot-electron effect in ZnO epilayers and AlGaN/GaN heterostructures

P1-5 Roman Balagula Optical properties of GeSi/Si quantum dots in mid- and far-IR range

P2-1 Agnė Zdaniauskienė In-situ SHINERS analysis of SAM from thiols with imidazole ring and intrachain amide groups

P2-2 Karolina Maleckaitė Polarity sensors based on thiophene-substituted BODIPY molecular rotors

P2-3 Rokas Gegevičius Energy Barriers in MAPbI3 Perovskite Films

P2-4 Rokas Jasiunas Benefits of MAPbI3 perovskite doping by Sr2+

P2-5 Rugilė Lukaševičiūtė Activity measurements of GMC superfamily flavoenzymes using Amplex Red assay

P2-6 Šarūnas Jankauskas Structural defect behavior of thermally annealed graphene, directly synthesized on Si(100) substrate using MW-PECVD

P2-7 Vaidas Pudžaitis In-situ probing of SAM and tBLM layer formation on nanostructured gold by ATR-SEIRAS

P3-1 Andrius Kamarauskas Impact of thin low specific conductivity layer on Fano resonance amplitude in an array of split ring resonators

P3-2 leva Matulaitienė Black silicon based substrates for surface enhanced Raman spectroscopy

P3-3 Ivan Yahniuk Terahertz detection and noise properties of (Cd1-xZnx)3As2

P3-4 Juozas Vyšniauskas Enhanced sensitivity AlGaN/GaN HEMT terahertz detector without ungated regions

P3-5 Liang Qi Performance of Titanium-based Microbolometers for Monitoring of Spatial Beam Profile in Terahertz Time-Domain Systems

P3-6 Paulius Mackonis Laser system for pumping THz and coherent X-ray sources of secondary radiation



<u>Algirdas Jasinskas</u>, Simona Pūkienė, Lukas Jočionis, Bronislovas Čechavičius, Ada Gajauskaitė and Renata Butkutė *Center for Physical Sciences and Technology, Saulėtekio av. 3, LT-10257*

Vilnius, Lithuania

Motivation

Low cost, reliable and compact electrically injected laser diodes have become irreplaceable in fields such as laser pumping, communications, medicine and more [1]. However, for some applications it is more convenient to have laser irradiation come out vertically from the device, rather than from its edge as in the case of laser diodes. More complex vertical cavity lasers exhibit this feature. Additionally, as in the case of vertical external cavity surface emitting lasers (VECSELS) – optical pumping allows achieving much greater output powers and beam quality while still maintaining wavelength versatility [2]. Essentially, these lasers combine advantages of both semiconductor and solid-state lasers, therefore they are very attractive and in great demand.

The goal of this work was to produce and characterize NIR region $(1-1.2 \ \mu m)$ optically pumped lasers based on two different gain materials – GaAsBi and InGaAs. The working principle of a VECSEL is shown in Fig. 1. Semiconductor chip with quantum well gain section is mounted on a heatsink and pumped by a diode laser. The resonator cavity is formed by using an external mirror.

Diode pump laser





TECHNOLOGIJOS MOKSLŲ

FIZINIŲ IR

VGA0432 – 1060 nm

CENTRAS

InGaAs VECSELs

Very similar laser structures were grown by changing QW material from GaAsBi to InGaAs. While using this compound, PL intensity increased by around 3 orders of magnitude and the results were much more reproducible than in the case of bismides.

VGA0422 – 1033 nm





Sample preparation and characterization

Resonant Periodic Gain (RPG) design (Fig. 2) was used in which a standing electromagnetic wave is formed at lasing wavelength which stimulates quantum well emission. QWs were placed in groups of 2-4 to reduce the overall thickness of the structure and improve thermal properties. Molecular Beam Epitaxy (MBE) equipment was used for growth of the samples. 28.5 period GaAs/AlAs DBR was grown on GaAs substrate, followed by the gain region (QWs and spacers), window layer and capping layer. Photoluminescence (PL), Reflectance and Atomic Force Microscopy (AFM) measurements were performed to characterize the grown lasers.



Fig. 3. Reflectance (black curve) and room temperature PL (blue curve) measurements of InGaAs MQW VECSELS. The central wavelengths of these lasers are 1033 and 1060 nm.

Surface quality

AFM measurements have shown dislocations going across all the surface of InGaAs QW samples (VGA0456) due to strain relaxation. While this roughness is very low and gets smoothened as the next VECSEL layers are deposited (VGA0432) this definitely shows, that strain relaxation would be a major issue when trying to reach longer wavelengths with this material.





Fig. 2. RPG design of one of the grown VECSEL structures. Purple line represents refractive index profile and green curve – electromagnetic field intensity.

GaAsBi VECSELs

Lasers based on GaAsBi QWs have shown PL in longer wavelengths than InGaAs QWs, however, due to technological challenges associated with GaAsBi MBE growth, it was often difficult to control Bi incorporation precisely and match the QW emission peak with resonant cavity wavelength (sample VGA0385).



Fig. 9. AFM images and average surface roughness (R_q) of different samples: top left – InGaAs MQW, top right – InGaAs VECSEL, bottom – GaAsBi MQW.

GaAsBi MQW samples, on the other hand, have shown worse overall surface quality (due to extreme growth conditions) which also gets improved as the top VECSEL layers are grown. As expected, no signs of similar dislocations were observed due to more rapid bandgap reduction of bismides.

Fig. 3. Reflectance (black curve) and room temperature PL (blue curve) measurements of GaAsBi MQW VECSELS. The central wavelengths of these lasers are 1193 and 1164 nm.

After many growth runs, sample VGA0390 exhibited PL peak at around 1164 nm well matched with the reflectivity dip of cavity resonance.

Conclusions

The grown VECSEL structures are yet to be measured in an optical pumping setup, but the primary characterization revealed high potential of these samples. Reflectivity dip at the center of Bragg mirror indicated standing electromagnetic wave which matched with desired lasing wavelength well and the emission wavelength of the QWs was matched with the resonant wavelength.

Structures based on InGaAs/GaAs quantum wells exhibited much higher intensities and were found to be much more reliable, however, bismide based structures have the potential to reach longer wavelengths while still using GaAs technological platform.

References

[1] D. Patil; Semiconductor laser diode: technology and applications, Intech (2012) pp. 217-219.[2] M. Guina et al., Journal of Physics D: Applied Physics 50 (2017).



VILNIUS GEDIMINAS TECHNICAL UNIVERSITY

CENTER

AND TECHNOLOGY

Three components of photovoltage simultaneously induced across GaAs p-n junction

Jonas Gradauskas^{1,2}, Steponas Ašmontas¹, Algirdas Sužiedėlis¹, Aldis Šilėnas¹, Aurimas Čerškus^{1,2}, Viktoras Vaičikauskas¹, Edmundas Širmulis¹, Ovidijus Žalys¹, Oleksandr Masalskyi²

jonas@pfi.lt

¹Center for Physical Sciences and Technology, Vilnius, Lithuania ²Vilnius Gediminas Technical University, Vilnius, Lithuania



INTRODUCTION

According to the Shockley-Queisser theory, only photons having energy close to a semiconductor hv forbidden energy gap E are effectively for electrical used generation. Lower power energy photons are assumed not absorbed at all, while as residual the extra energy higher energy photons is of reckoned in only through the process of carrier thermalization.



There again, hot carriers can be generated by the infrared radiation ("not absorbed at all") as well as by the photons supplying the mentioned extra residual energy. And the intraband light absorption has been demonstrated to rise a hot carrier photoemf across a semiconductor p-n junction illuminated with a CO₂ laser (hv=1.17 meV) radiation [1,2]. The photoemf had polarity opposite to that of the classical carrier generation-induced emf. We present experimental evidence of direct hot carrier influence on the net photovoltage formation across a semiconductor p-n junction. As an object of investigation, GaAs (E₂=1.42 eV) p-n junction was illuminated with 25 ns-long laser pulses of 1.06 μ m wavelength (hv=1.17 eV).Such experimental assortment allowed to investigate simultaneous rise of the hot carrier photovoltage and the classical photovoltage resulting from carrier generation due to two-photon absorption [3,4].

RESULTS. BOTH PHOTOVOLTAGES vs INTENSITY



Dependence of hot carrier photovoltage U_{hc} (red dots) and generation-induced photovoltage U_G (blue dots) across GaAs p-n junction on laser intensity at zero bias (solid dots) and -5 V of reverse bias voltage (open dots)

The reverse bias voltage acts against the hot carrier

RESULTS. THREE PHOTOVOLTAGE PULSES



Experimental traces of photovoltage across GaAs p-n junction at different excitation levels. No bias voltage is applied.

Simultaneous rise of hot carrier U_{hc} (reddish area) and carrier generation-induced U_{G} (bluish area) photovoltages is obvious. Thermalization-caused component U_{τ} (green area) can be seen following the U_{hc} in the case of low excitation level/

photovoltage formation.





Forward bias

Schematic description of hot carrier (red arrows) and generation-induced (blue arrows) photocurrents as forward and reverse bias voltage is applied. Hollow arrows stand for flows of holes

CONCLUSIONS

general, photoresponse in a p-n junction consists of three simultaneous components induced by:

- electron-hole pair generation,
- ✓ hot carriers.
- ✓ lattice heating after thermalisation.
- Hot carrier photovoltage across a p-n junction
 - \checkmark is evidenced experimentally,
 - rises prior to the thermalization,
 - \checkmark opposes the classical generation-induced photovoltage.

Solution Forward bias voltage increases the input of the hot carrier photovoltage.



RESULTS. PHOTORESTONSE



(How does the classical photovoltage bias a p-n junction?) > Hot carrier photovoltage may be the reason of still unattainable Schockley-Queisser limit.

ACKNOWLEDGMENT

This work was in part supported by the Research Council of Lithuania (grant No. 01.2.2-LMT-K-718-01-0050).

REFERENCES

1.S. Ašmontas, J. Gradauskas, D. Seliuta, E. Širmulis. Photoelectric properties of nonuniform semiconductor under infrared laser radiation. Proc. SPIE4423, 18-27 (2001). 2.F. Encinas-Sanz, J.M. Guerra. Laser-induced hot carrier photovoltaic effects in semiconductor junctions. Progress in Quantum Electronics 27, 267 (2003). 3.S. Ašmontas, J. Gradauskas, A. Sužiedėlis, A. Šilėnas, E. Širmulis, V. Švedas, V. Vaičikauskas, and O. Žalys, Appl. Phys. Lett. 113, 071103 (2018). S. Ašmontas, A. Šilėnas, Gradauskas, Sužiedėlis, Α. 4.J. V. Vaičikauskas, A. Čerškus, O. Žalys, O. Masalskyi.Unfolding hot carrier photovoltage across a p-n junction. Journal of Appl. Phys. impact in (in press)

Bismide-based Intersubband devices for Mid-Infrared Applications

<u>Karolis Stašys</u>¹, Ričardas Norkus¹, Sandra Stanionytė¹ and Jan Devenson¹ ¹Center for Physical Sciences and Technology, Sauletekio av. 3, LT-10257, Vilnius, Lithuania. Email: <u>karolis.stasys@ftmc.lt</u>



FIZINIŲ IR TECHNOLOGIJOS MOKSLŲ CENTRAS

Abstract:

Intersubband devices such as Quantum cascade lasers (QCLs) are considered now as standard light sources for many chemical sensing applications in the mid-infrared above 4 µm. Performances of diode lasers rapidly degrade below 3 µm due to fundamental limitations such as increasing influence of nonradiative Auger recombination. But this obstacle can be resolved by using bismides materials such as InAsBi/Al(As)Sb and InGaAsBi/AlAsSb in QCL superlattices structure [1,2]. In this work the MBE growth technique for the epitaxy of InAsBi/Al(As)Sb and InGaAs/AlAsSb quantum wells has been developed. Bismuth containing superlattices exhibited excellent interface contrast and crystalline quality. Obtained growth conditions can be considered as suitable for the growth of Bismide-based intersubband devices.

Main goal and challenges:

The main goal is the development of molecular beam epitaxy (MBE) procedure for the growth of InAsBi/Al(As)Sb and InGaAsBi/AlAsSb superlattices, which will be suitable for integration as active quantum wells into InAs/Al(As)Sb and InGaAs/AlAsSb injectors in Quantum Cascade Laser structures. There are two steps for each material system associated with the growth of such structures: 1) epitaxy of low temperature grown bismuth containing superlattices and 2) integration of low temperature grown bismide superlattices into high temperature grown superlattices – 4 stages in overall.

The challenge is that the main difference between these two material systems is that despite compositional similarity these two material systems are dedicated for the growth on different substrates – InAsBi/Al(As)Sb on InAs substrates, while InGaAsBi/AlAsSb on InP substrates. InAs/Al(As)Sb can be considered as lattice matched system while InGaAsBi/AlAsSb is strain balanced and more complicated for the growth. Advantage of the InAs-based system is that it has larger conduction band offset, thus, better carrier confinement, slightly lower electron effective mass, and also entire laser structure can be grown in the same process as no overgrowth is needed. InP based system mainly takes an advantage of better InP thermal conductivity. [3]

MBE growth of InGaAsBi/AlAsSb on (100) InP substrates:

As a first step, in order to find appropriate growth conditions for In_{0.7}Ga_{0.3}As_{1-x}Bi_x layers a set of samples have been grown on InP substrates at different growth temperatures varying As/Ga and As/Bi flux ratios. All samples were grown using solid source Veeco GEN Xplor molecular beam epitaxy (MBE) system, equipped with SUMMO group III element sources, Veeco As and Sb valved cracker sources and conventional Dual Filament bismuth source. The substrate temperature was controlled by a thermocouple (TC) and kSA BandIT broadband pyrometry module. The kSA 400 Reflection High-Energy Electron Diffraction (RHEED) system was used for in-situ surface characterisation. Each substrate prior to be loaded into the growth chamber has been outgassed at 200 °C in the load lock and later at 300 °C in the buffer chamber. The thicknesses of InGaAs buffer layers in samples varied from 100 nm to 270 nm depending on observation of RHEED pattern quality to decide if buffer layers is sufficiently smooth. All the samples were grown at temperatures, which are commonly used for the growth of ternary bismide alloys: 280 °C, 300 °C, and 320 °C. To ensure that only temperature will have an influence, the Bi/InGa ratio was kept the same. All grown samples had smooth surface and exhibited decent incorporation of bismuth. X-Ray measurement results are shown in Figure 1.

Samples grown at lower temperature have higher amount of incorporated bismuth. However, samples grown at temperatures 280 °C (5.3% Bi) and 300 °C (5.1% Bi) have difference of only 0.2% while the amount of incorporated bismuth in sample grown at 280 °C dropped to 4.2%. Moreover, it seems that the layer grown at 300 °C has better crystalline quality, as it has sharper main peak and visible fringes around bismide corresponding peak. Therefore, the temperature of 300 °C was stated to be the optimal temperature for the growth of InGaAsBi layers.



Fig. 1. Measured high resolution X-Ray diffraction curves of InGaAsBi samples grown at different temperatures



Fig. 2. XRD (004) rocking curves measured on three InAsBi samples VIA001, VIA003, and VIA012.

MBE growth of InAsBi/AlAsSb on (100) InAs substrates:

In difference with InGaAsBi/AlAsSb material system, the InAs/Al(As)Sb system is considered as nearly lattice matched to the substrate. Hence easier calibration and adjustment procedures are needed. On the other hand, this material system quite close in composition to the first one. Hence, in similarity, initial bismide growth conditions were found in the same way. The optimal growth temperature of InAsBi material has been determined by the As cap desorption temperature, which occurs at nearly 300 °C. Each substrate prior to be loaded into the growth chamber has been outgassed at 200 °C in the load lock and later at 300 °C in the buffer chamber. The native oxide removal was performed at 525 – 530 °C temperature according to the pyrometer readings and under ~1×105 Torr beam equivalent pressure (BEP) As₂ flux. After that the substrate temperature was decreased to 500 – 515 °C for InAs buffer layer growth. RHEED oscillation measurements were performed to estimate the growth rate of InAs and III/V ratios prior to the growth of InAsBi layers. InAsBi layers in all samples were grown at 320 °C temperature according to the thermocouple readings. Thicknesses of below presented grown InAsBi layers in samples VIA001, VIA003, VIA012 are respectively 390 nm, 400 nm, and 500 nm. All the samples were grown at the 0.5 monolayer/s growth rate. The bismuth content in InAsBi layers was determined from the X-ray diffraction (XRD) (004) rocking curves. XRD traces obtained on all three InAsBi samples are presented in Figure 5. Flattened top of InAsBi peak of VIA012 suggests the possible layer relaxation due to higher bismuth concentration. To prove that (115) Reciprocal Space Maps (RSM) of two InAsBi samples with the largest 20 shifts from the substrate were registered and are presented in Figure 6. Two strong peaks can be clearly distinguished on these maps: the upper peak can be associated with the InP substrate, the lower one with the InAsBi layer, red lines on the maps correspond to fully strained and fully relaxed states and the blue line shows different relaxation states with the same Bi content. It can be seen from this figure that InAsBi layer with lower Bi content (Fig. 6a) grown on InAs substrate is strained, whereas InAsBi layers with higher Bi content have a relaxation level of 40%. The composition of all InAsBi layers and other parameters are given in Table 1.



Sample	Bi concentration, %	Bi concentration, % Relaxation, %	
VIA012	2.7	0%	390
VIA001	3.6	0%	400
VIA003	4.55	40%	480

Table 1. Main parameters of the investigated samples.

Fig. 3. Reciprocal Space Maps (RSM) of two InAsBi samples: VIA003 (a) and VIA012 (b). The red lines on the maps correspond to fully strained and fully relaxed lattice states and the blue line indicates the states with the same Bi content and different relaxation levels.

Conclusions:

The MBE growth technique for the epitaxy of InAsBi/Al(As)Sb and InGaAs/AlAsSb quantum wells has been developed. Bismuth containing superlattices exhibited excellent interface contrast and crystalline quality. Obtained growth conditions can be considered as suitable for the growth of Bismide-based intersubband devices. Measured intervalley scattering confirmed that incorporation of Bi into the quantum well can reduce carrier escape to lateral valley.

Using developed growth technique and optimized growth conditions the InAsBi/AlAsSb intersubband emission structure has been grown. The electroluminescence spectrum has been obtained from fabricated EL structure. Emission wavelength peak in vicinity of 3.3 µm has been recorded. This confirmed that there is no degradation in performance associated with insertion of Bi and further design modifications are possible to exploit advantage of Bi in quantum wells for development of short wavelength intersubband devices.





Fig. 4. EL emission spectrum obtained from InAsBi/Al(As)Sb sample.

Sources:

[1] R Butkute, A Geižutis, V Pačebutas. B Čechavičius, V Bukauskas, V Kondrotas, P Ludewig, K Volz, A Krotkus; Electronics Letters. 50. 1155–1157. 10.1049/el.2014.1741, 2014
 [2] K. Alberi, J. Wu, W. Walukiewicz, K. M. Yu, O. D. Dubon, S. P. Watkins, C. X. Wang, X. Liu, Y.- J. Cho, and J. Furdyna.;. Phys. Rev. B, 75:045203, 2007
 [3] J. Devenson. InAs/AISb SHORT WAVELENGTH QUANTUM CASCADE LASERS. Dissertation, 2010.



APROPOS 17, Vilnius, Lithuania 2020/09/30

Drift velocity, gate length, and cut-off frequency in FET Effective carrier saturation velocity in a field-effect transisto



AlGaN/GaN HEMT: A. Veriatchikh et al., WOCSDICE (2003) & ISCS (2003) DOI: 10.1109/ISCSPC.2003.1354444 v_e = 1.1x10¹ cm/s; Zn0 FET: S. Sasa et al., Phys. Stat. Sol. A 208, 449 (2011); f_T = 1.75 GHz

Maximum electron drift velocity in ZnO

The highest experimental electron velocity value is close to the peak value obtained by Monte Carlo simulation [1]. Highest experimental room temperature electron drift velocity in nominally undoped ZnO at 320 kV/cm; v_{elonax} = $2.740.3 \times 10^7$ cm/s [2]. Electrical pulses of few nanoseconds (3 ns) in duration were used. Experimental results up to moderate electric fields are in good agreement with theoretical calculations by spherical harmonics expansion (SHE) method.



density

 J. D. Albrecht, P. P. Ruden, S. Limpijumnong, W. R. Lambrecht, and K. F. Brennan, J. Appl. Phys 86, 6864 (1999).
 L. Ardaravičius, O. Kiprijanović, M. Ramonas, E. Šermukšnis, J. Liberis, A. Šimuković, A. Matulionis, Md. B. Ullah, K. Ding, V. Avrutin, Ü. Özgür, and H. Morkoç, J. Appl. Phys. 126, 185703 (2019). Electron density $n_0 = \sigma_0/e\mu_0 = 1.9 \times 10^{17} \text{ cm}^3$ (circles);1×10¹⁷ cm³ (solid lines [1]).

Differential mobility, conductivity, and effective defect



Calculated differential mobility ratio at low (2 kV/cm) and moderate (100 kV/cm) electric fields, $\mu_0 / \mu(100)$, versus the total charged defect density N_{eff} is compared with the ratio of conductivities, $\sigma_0 / \sigma(E_m)$, obtained from the experiment [4]:



Drift velocity in AlGaN/AIN/GaN and ZnO

For higher low-field electron mobility (1880 cm²/(Vs)) AIN-spacer containing structure electron drift velocity saturates and attains the value of 1.6×10^7 at 9.6×10^{-10} electron billion drift velocity values in epitaxial ZnO and 2DEG GaN channel are similar.



Determination of electron drift velocity from hot-electron effect in ZnO epilayers and AlGaN/AlN/GaN heterostructures

Oleg Kiprijanovič and Linas Ardaravičius

Email:linas.ardaravicius@ftmc.lt

Zinc oxide (ZnO) is a semiconductor with a direct and relatively wide bandgap. High electron drift velocity saturation (3.2×10^7 cm/s) was attained from Monte Carlo calculations (1) and recent experimental findings of the drift velocity (-2.7×10^7 cm/s at 320 kV/cm) and electric fields (430 kV/cm) were reported for nominally undoped ZnO epilayers at room temperature [2]. These results are promising to field-effect transistors (FETs) for high-frequency and high-power operations. The dependence of electron drift velocity on the electron density was deduced at room temperature for doped ZnO [3]. The electron low-field mobility in ZnO is mainly determined by scattering on charged defects. There is an experimental evidence that double charged oxygen vacancies act as shallow donors and charged scattering centres. The goal of this work is to examine the electron scattering by charged defects through the study of hot-electron flector in nominally undoped ZnO epilayers at room temperature -Notage dependence is measured up to high electric fields, and the experimental evidence that double charged oxygen vacancies act as shallow donors and charged scattering centres. The goal of this work is to examine the electron scattering by charged defects through the study of hot-electron flectorn flects in nominally undoped ZnO epilayers at room temperature -Notage dependence is measured up to high electric fields, and the experimental results are fitted with the solution of the Boltzmann kinetic equation [4]. The results are used for the estimation of electron density, drift velocity and low-field mobility. The electron scattering by the double-charged oxygen vacancies and other charged defects is discussed. charged defects is discussed

Na georetics is used as a consisting candidate for future high-electron-mobility transistors (HEMTs) used in microwave high-power applications, GaN-based heterostructure two-dimensional electron gas (2DEG) channels have attracted much interest [5]. The insertion of a thin AIN spacer layer prevents electron penetration into adjacent AIGaN layer and simultaneously improves the sheet charge density and mobility compared with the conventional AIGaN/GaN heterostructure having equivalent AIGaN parameters. Our goal is to extract the key transport parameter – the charge density labeling that the conventional AIGaN/GaN heterostructure having equivalent AIGaN parameters. Our goal is to extract the key transport parameter – the charge density labeling that the conventional AIGaN/GaN heterostructure having equivalent AIGaN parameters. Our goal is to extract the key transport parameter – the charge density and mobility compared with the conventional AIGaN/GaN heterostructure having equivalent AIGaN parameters.

[3] L. Ardaravičius, O. Kiprijanovič, J. Liberis, M. Ramonas, E. Šermukšnis, A. Matulionis, M. Toporkov, V. Avrutin, U. Özgur, and H. Morkoç, Mater. Res. Express 4, 066301 (2017). [5] A.S.A. Fletcher and D. Nirmal, Superlattices and Microstructures 109, 519-537 (2017).

Intentionally undoped ZnO samples

The investigated epitaxial ZnO layers were grown in Virginia Commonwealth university (USA) by (PA-MBE) on highly-resistive Galv prepared by MCCVD on c-plane sapphire. ZnO epilayer width w = 300 µm and thickness d = 350-375 nm. The transmission line measurement (TLM) patterns were processed with evaporated TJAu (25 nm/30 nm) stacks acting as ohmic contacts. The contact resistance (R_c = 23±100) was estimated at low electric fields from the dependence of the sample resistance on the interelectrode distance (L = 1.7-15.8 µm). The channel resistance, the length and the cross section area were used to estimate the low-field conductivity. Electron mobility in the channel was estimated from Hall effect and magnetoresistance measurement data. More overen-rich conditions as well as lower substrate temperature during the growth f.340° C) groue.

lower el	ectron density.	iporat	
	Sample		#1153(#1161)
	Epilayer conductivity σ_0		4.7(5.5) S/cm
	Magnetoresistance electron mobility		188(146) cm²/(Vs)
	Electron drift mobility μ_0		195(178) cm ² /(Vs)
	Electron density n ₀		1.5(1.9)x10 ¹⁷ cm ⁻⁹
	Hall electron mobility		53(50) cm ² /(Vs)
	Oxygen vacancy density		1.6(1.9)x10 ¹⁷ cm ⁻³
	Other charged defect density		1.7(2.0)x10 ¹⁷ cm ⁻³
∏i/Au	Ti/Au		
	Zn0 (350-375 nm)		$\sigma(E_{\perp})$
	GaN (2.5 μm)	n($(E_m) = \frac{O(E_m)}{e\mu(E_m)} = n_0 = \frac{1}{e^{2m}}$
	c-sapphire		
<10 ⁶	ZnO -		Experimental current d electric field (<i>j</i> -E) results for can be approximated with line E < 50 kV/cm; A solid lin
105	3 ns ▲ #1161 [4]		dashed dotted lines stand t
	• #1153 [2]		Ohm's law. 50 kV/cm $\leq E = E \leq 250$ l
(10 [°] -	· · · · · · · · · · · · · · · · · · ·		Dashed and dotted lines
<10 ⁵			lower slope illustrates the s
			Ohm's law
(10 ⁵ -	ا المعر		$G(E_m)$ - differential conduction E_m can be found from the slow

0 50 100 150 200 250 300 350 Electric field (kV/cm

AIGaN/AIN/GaN 2DEG channel

The heterostructures were grown in Virginia Commonwealth university (USA) by MOCVD on c-sapphire substrates. The 2DEG channel formed in the top-most portion of 3.2 µm-thick GaN layer. Transmission-line measurement (TLM) patterns with meas etching were fabricated with the electrode dimensions of 300x80 µm² and the gaps from 3 to 27 µm. The magnetoresistance measurements were performed on the TLM structures. The contact resistance R, was evaluated from the TLM length-dependent resistance measurements; the values were found to be much lower compared to the resistance of the 6.9 µm length channel. The Hall mobility and the TLM-evaluated resistance value were also utilized simultaneously for estimation of the sheet 2DEG density.

 $\sigma(E_m) = \frac{dj}{dE}(E_m)$

Sample	#4338			
Channel conductivity σ_0	1.6 mS	Ti/Au		Ti/Au
Magnetoresistance electron mobility	1700 cm ² /(Vs)		Al _{0.18} Ga _{0.82} N (20 nm) AIN (1 nm)	
Hall sheet electron density	8.6x10 ¹² cm ⁻²		GaN (3.2 µm)	
TLM sheet electron density	5.2x10 ¹² cm ⁻²			
Hall electron mobility	1880 cm ² /(Vs)		c-sapphire	

Experimental setup for measurements of subnanosecond pulsed current-voltage (I-U) dependence



1 - high-voltage attenuator, 2 - wide-band switch, 3 - sample holder, 4 - sample under test, 5 - reference resistor, 6 - tunable wide-band attenuator. L. Ardaravičius, O. Kiprijanovič, J. Liberis, A. Matulionis, E. Šermukšnis, R. A. Ferreyra, V. Avrutin, Ü. Özgür, and H. Morkoç, Semicond. Sci. Technol. **30**, 105016 (2015).

Transient current and electric field measurements



The transmitted current (a) and electric field (b) waveforms for the ZnO sample #1161 The highest current of 0.8 A corresponds to 320 kV/cm peak field at 26 dB attenuation The current deduced during the rise edge nearly coinc ides with that available from the falling edge. The coincider nce suggests that neither the sample temperature nor the

[4] L. Ardaravičius, O. Kiprijanović, M. Ramonas, E. Šermukšnis, A. Šimuković, and A. Matulionis, Lithuanian J. Phys. 60, 48-56 (2020).

Drift velocity in ZnO and Zn cell temperature

The highest experimental value for the electron drift velocity of $\sim 2.9 \times 10^7$ cm/s ($\sim 2.7 \times 10^7$ cm/s) is found at 320 kV/cm in the sample #1153 (#1161) with the electron density of 1.5×10^{17} cm⁻³ (1.9×10^{17} cm⁻³). A correlation with the growth conditions is resolved: a slightly higher drift velocity is estimated for the sample #1153 with a lower density of oxygen vacancies. This wafer has been grown at lower Zn cell temperature (340 °C). The highest drift velocity value is close to that obtained from Monte Carlo calculations [11] Monte Carlo calculations [1].



circles(triangles); 1x10¹⁷ cm⁻³ (solid line [1]).

Acknowledgments

Authors are thankful to Dr. E. Šermukšnis and Prof. A. Matulionis from Center for Physical Sciences and Technology, Lithuania, for discussion and Prof. H. Morkoç group at Virginia Commonwealth University (USA) for ZnO and nitride samples.

electron density change with time and electric field.

Optical properties of GeSi/Si quantum dots in mid- and far-IR range

Roman M. Balagula¹, Anton N. Sofronov², Hayk A. Sarkisyan³, and Dmitry A. Firsov²

¹ Center for Physical Sciences and Technology, Vilnius, Lithuania ²Peter the Great St. Petersburg Polytechnic University, St. Petersburg, Russia ³Russian-Armenian University, Yerevan, Armenia

1. Samples: high-density array of Ge/Si quantum dots

2. Mid-IR optical absorption



L_{eff} – is different for doped and undoped samples! Doped structure – $L_{eff} = 15 \text{ nm}$ – distance between δ -layers. Undoped structure – L_{eff} = 500 μ m – bipolar diffusion length.

Apropos 17

Materials and Systems

29 September –

01 October, 2020

Advanced Properties and Processes in Optoelectronic

3. Far-IR optical absorption 2 holes/QD 20% Optical transmission 4 holes/QD 6 holes/QD Nothing happens with the increase of the average number of holes in QDs 10 20 30 40

Photon energy, meV

50

60

Energy of transitions to low excited levels does not depend on the number of holes in QDs

For multiparticle states this effect is observed in parabolic potential: In magnetic field W. Kohn Phys. Rev. 123, 1242 (1961) In "parabolic" QDs - P.A. Maksym, T. Chakraborty Phys. Rev. Lett. 65,108 (1990), F.M. Peeters Phys. Rev. B 42, 1486(R) (1990)



5. Where is a parabolic potential in "rectangular-band-profile" QD?

Adiabatic separation of hole motion in xy-plane and along z-axis: $\rho_0 >> h$

According to D.B. Hayrapetyan, E.M. Kazaryan, and H.A. Sarkisyan. Physica E, 75, 353 (2016)

$$\hat{H}_{0}\Psi + U_{\text{conf}}\Psi = \mathcal{E}\Psi \qquad \Psi(\rho, \varphi, z) = f(\vec{\rho})\chi(z(\rho))$$
$$\Delta E_{v} \gg \hbar\omega:$$

At fixed ρ the hole is confined along z in 1D infinite well of width $z_2 - z_1 = a(\rho)$ $a(\rho) = \sqrt{R^2 - \rho^2} - (R - h)$ $\chi_n(z(\rho)) = \sqrt{\frac{2}{a(\rho)}} \sin\left(\frac{\pi n}{a(\rho)}z\right)$ $\mathcal{E}_n^{(z)} = \frac{\pi^2 \hbar^2 n^2}{2m(a(\rho))^2} \equiv U_n^{\text{eff}}(\rho)$

if $\rho << \rho_0$: Hole confinement potential in xy– plane

 $U_{n}^{\text{eff}}(\rho) = \frac{\pi^{2}\hbar^{2}n^{2}}{2mh^{2}} + \frac{m\Omega_{n}^{2}}{2}\rho^{2}$

 $\Omega_n^2 = \frac{\pi^2 \hbar^2 n^2}{m^2 h^3 R}$

$$\hat{H}(1,2,\ldots,N) = \sum_{j=1}^{N} \hat{H}_{0}^{j} + \sum_{j=1}^{N} U_{\text{conf}}(\vec{r_{j}}) + V(\vec{r_{1}},\ldots,\vec{r_{N}})$$

Adiabatic separation: $\Psi(\vec{r_1}, \dots, \vec{r_N}) = f(\vec{\rho_1}, \dots, \vec{\rho_N})\chi_{n_1,\dots,n_N}(z_1(\rho_1), \dots, z_N(\rho_N))$

$$n_1 = \dots = n_N = 1$$

$$V = \frac{1}{2} \sum_{\substack{i,j=1\\i\neq j}}^N \frac{e^2}{\varepsilon |\vec{\rho_i} - \vec{\rho_j}|} \qquad \hat{H}^{2\mathrm{D}} = \frac{1}{2m} \sum_{j=1}^N \left(\hat{P}_{xj}^2 + \hat{P}_{yj}^2 \right) + \frac{m\Omega_2}{2} \sum_{j=1}^N \rho_j^2 + \frac{1}{2} \sum_{\substack{i,j=1\\i\neq j}}^N \frac{e^2}{\varepsilon |\vec{\rho_i} - \vec{\rho_j}|}$$

Changing variables from ρ_i to CM motion and relative motion of the particles:

$$\vec{R}_{\rm CM} = \frac{1}{\sqrt{N}} \sum_{j=1}^{N} \vec{\rho}_j \qquad \qquad \hat{H}^{\rm 2D} = \hat{H}^{\rm 2D}_{\rm CM} + \hat{H}^{\rm 2D}_{\rm Rel} = -\frac{\hbar^2}{2M} \frac{d^2}{dR^2_{\rm CM}} + \frac{M\Omega^2}{2} R^2_{\rm CM} + \hat{H}^{\rm 2D}_{\rm Rel}$$

The EM wave perturbation operator in dipole approximation

 $\Delta \hat{H} = e \vec{E}(t) \sum \vec{\rho_j} = \sqrt{N} e \vec{E}(t) \vec{R}_{\rm CM}$ depends on only CM coordinate.

Single-particle-like optical transitions in many-particle system are observed.

```
Optical absorption at the lowest intelevel resonance does not depend
  on the Coulomb interaction and number of holes inside the QD.
                                             \pi\hbar^2
```

Transition energy
$$\hbar\Omega = \frac{\pi n}{m\sqrt{h^3R}}$$

For the largest QDs in ensemble $h \approx 2.95$ nm, $\rho_0 \approx 9$ nm, and $\hbar\Omega \approx 31$ meV

7. Far-IR optical absorption at higher temperatures

i-Si

i-Si

Ge

i-Si

i-Si



8. Mid-IR photoinduced absorption dynamics



Conclusions

- 1. Equilibrium and photoinduced absorption in GeSi QDs related to intersubband hole transitions are investigated.
- 2. The effect of thermal depopulation of the GeSi/Si quantum dots at temperatures below 300 K is observed in photoinduced absorption of undoped samples when the bipolar diffusion of charge carriers is not restricted.

Redistribution of the holes over the smaller ODs in ensemble depends on the nominal doping

> From temperature dependences of characteristic times we find $\Delta E = 25$ meV and $\delta E = 70$ meV

e-mail:roman.balagula@ftmc.lt

2. Equilibrium absorption depends on doping differently in mid-IR and FIR optical regions.

3. Kohn's theorem applicability to such structures was experimentally shown.

- There is a certain energy range where the motion of the holes in Ge/Si quantum dots is equivalent to the motion of 2D particles in parabolic potential.
- The analytical size-quantization theory developed for holes in Ge/Si QDs on the basis of the adiabatic approximation gives good agreement with the experimental energy of the lower intraband resonance.
- The resonance frequency does not depend on the interaction between holes and is of a single-particle character.
- The conditions for generalized Kohn's theorem are satisfied due to the specific geometric shape of the QDs.

4. The existence of potential barrier for holes at the heterointerface and its influence on optical properties was experimentally proven.

5. First investigation of photoinduced absorption dynamics in QD structures was performed. Two stage behavior of absorption relaxation is qualitatively explained.

In-situ SHINERS analysis of SAM from thiols with imidazole ring and intrachain amide groups

Agnė Zdaniauskienė¹, Tatjana Charkova¹, Rita Sadzevičienė¹, Gediminas Niaura¹

¹Department of Organic Chemistry, Center for Physical Sciences and Technology, Saulétekio Ave. 3, LT-10257 Vilnius, Lithuania Email: agne.zdaniauskiene@ftmc.lt

The self-assembled monolayers (SAMs) constructed by the adsorbtion of thiols on noble metals are widely used to analyze the interaction of functional groups with adsorbates, study electron transfer processes and develop bioelectronic devices [1].

Introduction of amide functionality in the hydrocarbon chain of adsorbing molecules considerably increases the stability of the formed SAMs due to the formation of hydrogen bonds between the adjacent molecular chains in the monolayer [2]. A terminal histidine (His) ring group containing monolayers provide a possibility to study various interactions of the ring with solution components. The unique structure of His makes it play multiple roles in the molecular interactions - it is an important ligand for metal coordination in peptides and proteins [3].

Shell-isolated nanoparticle-enhanced Raman spectroscopy (SHINERS) method employs the ultrathin shell to isolate the metal nanospheres from the probed object and thus prevents a potentially disturbing interaction. Meanwhile, the very short metal–molecule separation can still result in a significant nanoparticle-enhanced Raman signal [4].

The present work focused on *in situ* SHINERS study of SAM formed from N-(2-(1H-imidazol-4-yl)ethyl)-6-mercaptohexanamide (IMHA) at smooth Au surface in aqueous solutions.

SHINERS method employing synthesized spherical Ag nanoparticles with 85 ± 5 nm core size and SiO₂ shell of 3 nm thickness allowed to obtain significantly enhanced SHINERS spectrum of IMHA compared to the Raman spectrum (Fig. 1). Bands from all parts (terminal imidazole ring, hydrocarbon chain, and sulfur group) of IMHA are clearly visible.

Therefore, it was shown that SHINERS is a perspective technique allowing the collection of molecular level information from smooth Au surface for a better understanding of molecular structures and functions.



Fig. 1 Raman spectrum of IMHA adsorbed on smooth Au surface (a) and SHINERS spectrum from smooth Au surface with adsorbed IMHA (b).

REFERENCES

J. C. Love, L. A. Estroff, J. K. Kriebel, R. G. Nuzzo, G. M. Whitesides; *Chem. Rev.* **105** (2005) pp. 1103–1170.
 M. Kim, J. N. Hohman, A. C. Serino, P. S. Weiss; *J. Phys. Chem. C* **114** (2010) pp. 19744–19751.
 S. M. Liao, Q. S. Du, J. Z. Meng, Z. W. Pang, R. B. Huang; *Chem. Cent. J.* **7** (2013).
 J.R. Anema, J.F. Li, Z.L. Yang, Ren B, Z.Q. Tian; *Annu. Rev. Anal. Chem.* **4** (2011) pp. 129–150.

Polarity sensors based on thiophene-substituted **BODIPY molecular rotors**



Vilnius University

Karolina Maleckaitė¹, Jelena Dodonova², Sigitas Tumkevičius², Aurimas Vyšniauskas¹

BODIPY

karolina.maleckaite@ftmc.lt

Background

• Easy way to image viscosity is provided by viscosity-sensitive fluorophores - molecular **rotors.** [1]

• **BODIPY based** molecular rotors are very of their promising because easy functionalization, high molar extinction coefficients, monoexponential fluorescence lifetime and photostability. [2]

 A recent research has showed that attached thiophene moieties to the BODIPY core can **rotate** and this suggests that these derivatives could be sensitive to viscosity. [3]

• In this work two thiophene-substituted





Orientation polarisability

Lippert's equation was used to rank pure solvents by their polarity.

 $\Delta f = \frac{\varepsilon - 1}{2\varepsilon + 1} - \frac{n^2 - 1}{2n^2 + 1}$ $n^2 - 1$

Here ε is a relative permittivity and n is the refractive index of a pure solvent.

Polarity impact

 Increasing orientation polarization of the solvent (Δf) decreases fluorescence's lifetime intensity, and **yield** for quantum both studied molecules.

Sensor



BODIPY molecular rotors with (BDP-N) and without (**BDP-T**) -NO₂ group are investigated.



Thiophene impact 0.2 Absorbance: ---BODIPY Tol thiophene • Attaching Norm. FL intensity, a.u. **BDP-T Tol** BODIPY moieties to BDP-N Tol C0 increases the conjugated sorban Fluorescence: **BODIPY Tol** system. **BDP-T Tol BDP-N Tol** Ab • Longer, more biocompatible wavelengths are achieved as well as a Stokes shift in larger 0.0 contrast to BODIPY. 400 500 600 700 Wavelength, nm

Viscosity impact

 Fluorescence spectroscopy show measurements negligible distinction between lifetimes when solvent viscosity is increased.

• BDP-T **BDP-N** and derivatives cannot be used as microviscosity sensors.



evaluation (a relative change of FL lifetime, when Δf changes by 0.1) shows that **BDP-N** is more sensitive to polarity than BDP-T (31% and 22%, respectively).

• BDP-T and BDP-N can be used as polarity sensors.



Conclusions

0.1

0.2

BDP-T

BDP-N

0

0.0

Adding thiophene moieties in 2- and 6- BODIPY positions increases

Temperature impact

• BDP-T **BDP-N** and dissolved in cyclohexane and **BDP-T** in chloroform showed decreasing FL lifetime with increasing temperature.

• Reverse dependence is for **BDP-N** in seen chloroform.

 The studied derivatives are not temperature sensors.



molecule's conjugation, redshifts fluorescent spectra and enables to achieve large Stokes shift. Furthermore, a transformation of viscosity sensor to polarity sensor is achieved.

- Fluorescence decays of **BDP-T** and **BDP-N** are monoexponential, which simplifies data analysis and reduces photon counts required for measurements.
- It is possible to create a polarity probe based on these molecules, especially **BDP-N**, which is more sensitive to solvent polarity than **BDP-T**.

References

[1] M. K. Kuimova, Phys. Chem. Chem. Phys. vol 14, no 37, p. 12671, 2012. [2] S. Toliautas et al., Chem. Eur. J., vol. 25, 44, p. 10342-10349, 2019. [3] Y. Chen et al., J. Org. Chem. vol. 77, 5, p. 2192-2206, 2012.

¹ Center for Physical Sciences and Technology, Saulėtekio av. 3, Vilnius, Lithuania

² Institute of Chemistry, Faculty of Chemistry and Geosciences, Vilnius University, Naugarduko str. 24, Vilnius, Lithuania

Energy Barriers in MAPbI₃ Perovskite Films FOR PHYSICAL SCIENCES

Rokas Gegevičius, Rokas Jasiūnas, Marius Franckevičius, Vidmantas Gulbinas

Molecular Compound Physics Department, Centre for Physical Sciences and Technology, Saulėtekio Ave. 3, LT-10257 Vilnius, Lithuania.

- In this work, **Transient Photocurrent**, **Time-Delayed Collection Field** and **Transient Fluorescence** techniques are combined to address charge carrier trapping processes during their lateral motion in prototypical methylammonium lead iodide perovskite (MAPbI₃) films formed on interdigitated electrodes.
- Carrier mobility decreases on hundreds of ns timescale, and its rate depends on the motion character—it is faster when charge carriers drift in the electric field and slower when the motion is caused by diffusion only. This difference becomes particularly evident at low temperatures. Based on the time-delayed collection field data and carrier motion modelling results, it is demonstrated that the rapid mobility decay at low temperatures is mainly caused by the energy barriers, most likely formed at crystallite boundaries.
- Suggested concept of the potential barriers moves beyond the conventional understanding of carrier mobility, diffusion, and recombination processes in hybrid perovskites.



CENTER

AND TECHNOLOGY



3.8eV





Figure 1. a) Top view scanning electron microscope (SEM) images of MAPbI₃ and b) The cross-sectional SEM image demonstrates lateral configurations of the perovskite films deposited on IDE.









Figure 3. Transient photocurrent kinetics a) at different excitation intensities and b) at constant excitation intensity of 15 nJ cm⁻²

Figure 4. a) Photocurrent kinetics at different temperatures measured at 2 V applied voltage and 15 nJcm⁻² excitation intensity, b) photocurrent kinetics at 100 K at different applied voltages.





Figure 5. Photocurrent kinetics at different temperatures obtained by modified TDCF measurements under 15 nJ cm⁻² excitation intensity.







Benefits of MAPbl₃ perovskite doping by Sr²⁺

<u>Rokas Jasiūnas¹</u>, Rokas Gegevičius¹, Marius Franckevičius¹, Nga Phung², Antonio Abate² and Vidmantas Gulbinas¹

¹Department of Molecular Compound Physics, Center for Physical Sciences and Technology, Saulėtekio Avenue 3, LT-10257 Vilnius, Lithuania.

² Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Kekuléstr. 5, Berlin D-12489, Germany.

rokas.jasiunas@ftmc.lt



Introduction

Hybrid perovskite materials have witnessed immense development in a range of optoelectronic devices, such as bright tunable LEDs, fast and sensitive photodetectors, and especially efficient solar cells. Chemical doping of perovskites with foreign atoms is a promising way to tailor material properties towards improving performance and stability of solar cells.

In this work [1], we discuss the efficiency increase in perovskite solar cells based on MAPbI₃ active layer, doped with 0.1 to 5 % of Sr^{2+} agent. A small amount <1 % of Sr^{2+} added to the perovskite improves open-circuit voltage by ~100 mV and consequently enhances the power conversion efficiency from 16.8 % to 17.8 %.

By employing transient photoluminescence, transient photocurrent and time-delayed collection field measurements we show that doping of $MAPbI_3$ by low content of Sr^{2+} additives (≤ 0.4 %) reduces the electron trapping efficiency. Whereas the reduced trapped electron density suppress nonradiative Shockley-Read-Hall recombination, which positively impacts open circuit voltage of perovskite solar cells.



Fig. 1 Energy surface in MAPbl₃ film with and without small amount of Sr²⁺ doping



Transient Photoluminescence

Figure 2 shows the transient PL dynamics of the investigated MAPbl₃ films. The decay kinetics were fitted with multiexponential decay functions, and the relaxation times obtained from the approximations are provided in **Table 1**.

Sr ²⁺ content in MAPbl ₃	A1	τ1 [ns]	A2	τ2 [ns]	A3	τ3 [ns]
0%	0.84	20.2	0.22	37.6	-	-
0.1%	0.67	20.9	0.36	64.2	-	-
0.2%	0.65	26.9	0.35	93.5	-	-
0.4%	0.7	27.8	0.31	125.6	-	-
1.0%	0.59	1.4	0.55	27.8	0.20	128.9
5.0%	1.00	2.32	0.35	15.4	0.03	63.8



II. Transient Photocurrent

Figure 3 a) Photocurrent kinetics of pristine MAPbl₃ at indicated applied voltages and b) normalized photocurrent kinetics in samples with different Sr²⁺ concentrations at 1.0 V applied voltage. The insert in (b) shows integrated photocurrent kinetics (not normalized).

III. Time Delayed Collection Field





IV. CONCLUSIONS

Figure 5 summarizes results in a simple representative model (note that the SEM image does not correspond to the actual Sr²⁺ concentration sample but is used as a base for the schematic). Here, the green arrow shows the direction of an electric field.

Figure 4. Dependencies of extracted charge value on delay time between the optical excitation pulse and electrical extraction pulse, obtained in different samples with 0 V generation and 1 V extraction voltages. The extracted charge was normalized to the extracted charge at zero delay time.

In Figure 5a, the carrier dynamic is shown in a neat MAPbl₃ film. After the generation of charge carriers, holes are easily extracted (red arrow), whereas electrons swiftly fall (solid blue arrow) into a trap state (glowing yellow circle), from which they are slowly extracted by the electric field (dotted blue line).

The trap density decreases significantly in the presence of a low amount of Sr^{2+} additives (Figure 5b), which, despite resulting in increased V_{OC} , also enhances bimolecular recombination, as shown in the figure.

Higher Sr²⁺ concentration (Figure 5c), leads to the formation of deep trap states (glowing red circles). Electrons generated in the vicinity of such trap states fall into them and contribute to the slow photocurrent component.

References:

[1] Jasiūnas, R.; Gegevičius, R.; Franckevičius, M.; Phung, N.; Abate, A.; Gulbinas, V. Suppression of Electron Trapping in MAPbI3 Perovskite by Sr2b Doping. Phys. Status Solidi RRL 2020, 5.

P2-5

Activity measurements of GMC superfamily flavoenzymes using Amplex Red assay

Rugilė Lukaševičiūtė¹ and Renata Karpicz¹

¹Department of Molecular Compound Physics, Center for Physical Sciences and Technology, Lithuania rugile.lukaseviciute@ftmc.lt

Usage of biosensing systems containing enzymes is the promising and accurate method for detection of various compounds concentration in biological samples. Some of the most important properties describing enzyme are selectivity and enzymatic activity. In order to create and improve biosensor it is necessary to understand the properties of immobilized enzyme related to the influence of the surrounding environment.

The glucose-methanol-choline (GMC) superfamily is large family of oxidoreductases typically containing FAD-binding domain. Some members include oxidases like glucose oxidase (GOx), pyranose oxidase (POx), cholesterol oxidase (ChOx) and alcohol oxidase (AIOx). Electron donor substrates for GMC oxidoreductases range from various sugars and alcohols to cholesterol [1]. Amplex Red (10-acetyl-3,7-dihydroxyphenoxamine) is colorless and nonfluorescent reagent that is widely used as a probe to detect H_2O_2 in various biological samples [2]. In reactions catalysed by GOx, POx, ChOx and AIOx hydrogen peroxide is formed which then reacts with Amplex Red in the presence of horseradish peroxidase (HRP) and forms colored, highly fluorescent compound resorufin. Resorufin has exitation and emission maximum of 571 nm and because of high exitation coefficient enzyme activity can be determined fluorometrically or spectrophotometrically.

The purpose of this research was to evaluate activity of GOx, POx, ChOx and AlOx enzymes in different acidic values using Amplex Red reagent and determine optimal pH values for every enzyme. Our results show that Amplex Red assay can be used in measuring H_2O_2 released after enzymatic reaction. With decreasing acidity of the medium enzyme's activity increases. The amount of formed resorufin during enzymatic reactions increases respectively by reducing pH. At optimal medium acidity formed resorufin amount is largest whitch shows that enzyme's activity there is the highest.

REFERENCES

L. Sutzl, G. Floey, E. J. Gillam, M. Boden, D. Haltrich "The GMC superfamily of oxidoreductases revised: analysis and evaluation of fungal GMC oxidoreductases," Biotechnology for Biofuels, 12, article 118, 2019.
 Baozhong Zhao, Fiona A. Summers, Ronald P. Mason "Photooxidation of Amplex red to resorufin: Implications of exposing the Amplex red assay to light," Free Radical Biology and Medicine, 53 1080-1087, 2012.

Structural defect behavior of thermally annealed graphene, directly synthesized on Si(100) substrate using MW-PECVD

<u>Šarūnas Jankauskas</u>¹, Rimantas Gudaitis¹, Andrius Vasiliauskas¹ and Šarūnas Meškinis¹

¹ Institute of Materials Science of Kaunas University of Technology, K. Baršausko Str. 59, LT-51423, Kaunas, Lithuania Email: sarunas.jankauskas@ktu.lt

Graphene, material with exceptional physical properties, when synthesized using exfoliation, lacks certain qualities when grown directly on semiconducting surfaces. Although, microwave plasma enhanced chemical vapor deposition (MW-PECVD) can increase production rates of graphene, this form of synthesis introduces fair amount of defects [1]. To tackle this issue thermal annealing is rather straight forward method, which usually increases the overall quality of graphene by reducing the number of defects and other structural deformations, however there are other predominant effects, such as doping and strain, which could damage the sample [2]. Graphitic structure examination is usually based on Raman spectroscopy measurements which helps to determine both structure quality and thickness (graphene case).

In this work, four graphene samples were grown on Si(100) substrates, using MW-PECVD system (IPLAS Innovative Plasma Systems GmbH). Samples were thermally annealed using different temperatures (200-800°C) and environments (Ar, N2, vacuum) in order to thoroughly evaluate the changes of graphitic structures. All annealing's were performed for 30 min. The characterization of graphene samples was carried out using Raman spectrometer (Renishaw inVia, 532 nm, 4.5 mW) by analyzing changes in D, 2D and G bands. After annealing in Ar environment at temperatures, lower than 800°C, I_{2D}/I_G ratio changed from 1.04 to 0.47 and I_D/I_G ratio changed from 1.3 to 1.45, suggesting appearance of additional deformations. At higher temperatures (800°C, Ar) the graphitic structure collapses due to difference in thermal expansion coefficients between the graphene sheets and the substrate. Annealing in N₂ environment, I_{2D}/I_G changed from 1.6 to 0.62 and I_D/I_G from 1.56 to 2.02 hinting a huge increase in defective sites and strain development. After investigating changes in Raman spectrum after annealing in vacuum we have found out that I_{2D}/I_G changed from 0.61 to 0.23 and I_D/I_G from 1.53 to 1.71, showing that the dominant effect is rather defect formation than reduction, however values indicate a large number of layers, which could lead to inconclusive estimations.

In conclusion, we can see that our graphene structures are imperfect, which is true for such materials synthesized using MW-PECVD, however we believe that defect reduction could be achieved when samples exhibit more prominent graphene characteristics.

REFERENCES

[1] S. Zheng et al.; *RSC Advances* 7 (2017) pp. 33185-33193.
[2] M. Alyobi et al.; *Crystals* 7 (2017) pp. 349.

In-situ probing of SAM and tBLM layer formation on nanostructured gold by ATR-SEIRAS

Vaidas Pudžaitis¹, Martynas Talaikis², Gediminas Niaura¹

¹Department of Organic chemistry, Center for Physical Sciences and Technology, Sauletekio ave. 3, LT-10257 Vilnius, Lithuania. ²Institute of Biochemistry, Life Sciences Center, Vilnius University, Saulėtekio av. 7, LT-10257 Vilnius, Lithuania

INTRODUCTION

Attenuated total reflection surface-enhanced infrared reflection absorption spectroscopy (ATR-SEIRAS) is a powerful tool for in-situ analysis of molecular phenomena at the nanostructured metal surface. Various processes can be monitored in the water environment and under electrode potential control. Even more, a good signal-to-noise ratio provides the possibility to track the formation process of the self-assembled monolayers (SAMs). We demonstrate the use of ATR-SEIRAS for probing a two-step process of tethered bilayer lipid membrane (tBLM) formation. The tBLMs are living-cell membrane mimicking constructions which are used for biosensing applications, and as a platform for fundamental studies of biological membranes.

EXPERIMENT

During the first step (Fig. 1A), SAM layer is formed from lipid-like WC14 [20-tetradecyloxy-3,6,9,12,15,18,22-heptaoxahexatricontane-1-thiol] compound mix with β-mercaptoethanol (BME) on the nanostructured gold surface (Picture 1) [1]. Surface was prepared by electroless plating procedure on 0.25 µm polished silicon with 7.5 mM NaAuCl₄ solution containing Na₂SO₃, Na₂S₂O₃, NH₄Cl and NH₄F salts at room temperature [2].



Picture 1. AFM image of 0.25 µm polished Si prism surface (left) covered with gold by electroless plating (right).

SAM formation was monitored on FT-IR spectrometer equipped with MCT detector (Bruker, Vertex 80v) and VeeMaxTM ATR accessory (PIKE technologies) at 4 cm⁻¹ resolution (~11 s/spectrum). EtOH solution on gold was used as a reference spectrum. Data representing 1mM WC14:BME (3:7 ratio respectively) SAM formation are shown in figure 1C. By observing C-H stretching peaks of WC14 (Fig. 1D), it can be confirmed – initial SAM formation is complete in ~2-3 min time. On a second step (Fig. 1B), ethanol was exchanged with water, which lead to WC14 methyl and ethyl peak shifts of 2 cm-1 towards lower energy (data not shown). This step was used as a reference for further FTIR observations. The tBLM was deposited from multilamellar vesicles (MVCs) prepared from 1,2-dioleoylsn-glycero-3-phosphocholine (DOPC) and cholesterol (CHOL) by pipetting 100 µl [3]. DOPC tBLM formation in ~15-20 min can be observed by plotting C-H stretch peak intensities against time (Fig. 1F). Additionally, water exchange from SAM's surface can be seen occurring concurrently (Fig. 1E).



CONCLUSIONS

We demonstrate, that ATR-SEIRAS can provide complementary and in some cases unique molecular level information to already widely used methods. We show, that WC14 based SAM absorbs to the nanostructured gold surface in 2-3 min., while the DOPC based tBLM is formed in 20 min., pushing ethanol and water molecules (for SAM and tBLM respectively) away from the surface at a similar rate. Additionally, we see phase exchange (EtOH to H₂O) effect on C-H stretch vibrations, that confirms tighter SAM ordering.

REFERENCES

[1] R. Butvidyte et all; Langmuir 29 (2013) pp. 8645-8656.

[2] H. Miyake, S. Ye, M. Osawa; Electrochemistry Communications 4 (2002) pp. 973-977

[3] T. Ragaliauskas, M. Mickevicius, B. Rakovska, T. Penkauskas, D. J. Vanderah, F. Heinrich, G. Valincius; Biochimica et Biophysica Acta 1859 (2017) pp. 669-678.

Impact of thin low specific conductivity layer on Fano resonance amplitude in an array of split ring resonators

A. Kamarauskas, G. Šlekas, D. Seliuta, and Ž. Kancleris

¹Center for Physical Sciences and Technology, Vilnius, Lithuania. Email: andrius.kamarauskas@ftmc.lt

The electromagnetic manifestation of Fano resonance was discovered in metasurface (MS) by Fedotov et al. [1] and later was widely investigated by many other researchers. Usually, it occurs in MS made from asymmetric split-ring resonators, but it was also observed in mirror-symmetric MS made from usual split-rings [2]. In this case, Fano resonance arises due to the interaction of 3rd order plasmonic mode and lattice mode.

Calculated dependences of transmittance at the maximum amplitude of the Fano resonance on specific conductivity of the layer situated on the front and back sides of the MS are shown in Fig. 2. It is seen that the difference in the transmitted signal through the MS is observed depending on the layer position when the conductivity of the layer is as low as 0.01 S/cm. On the



Fig. 1 The array of split-ring resonators with conductive layer on a top. The electric field is perpendicular to resonators' gap.



Fig. 2 The transmittance at the maximum amplitude of the Fano resonance versus specific conductivity of the layer. Resonance frequency at front side configuration is 222.9 GHz, at back side - 224.4 GHz.

one hand, the decrease of the transmittance on the conductivity is larger when the layer is placed on the resonator plane. On the other hand, the dynamic range is wider in the back side configuration. High sensitivity of the Fano resonance amplitude in the proposed structure to the low-to-mid conductivity planar sheet could be useful in sensing applications or modulation of electromagnetic waves.

REFERENCES

[1] V. Fedotov et al., Phys. Rev. Lett. 99, (2007) 147401.

[2] D. Seliuta et al., Optics Letters 44, (2019) pp. 759-762.

Black silicon based substrates for surface enhanced Raman spectroscopy

leva Matulaitienė¹, Lena Golubewa¹, Renata Karpicz¹, Algirdas Selskis¹ and Polina Kuzhir^{2,3}



 ¹ Center for Physical Sciences and Technology, Sauletekio Ave. 3, LT-10257 Vilnius, Lithuania.
 ² Institute for Nuclear Problems of BSU, Bobruiskaya 11, 220030 Minsk, Belarus.
 ³ Institute of Photonics, University of Eastern Finland, Yliopistokatu 2, FI-80100 Joensuu, Finland. Email: ieva.matulaitiene@ftmc.lt.

The evolution of new technologies brought to humankind not only comfortable environment, but also new treats. The major treat is environmental pollution that leads to various diseases and requires new processes, diagnostic systems. Surface enhanced Raman spectroscopy (SERS) is one of the most sensitive techniques of vibrational spectroscopy that gives information about the material in molecular level. Nowadays there are plenty techniques for SERS substrates fabrication, that must meet three conditions: certain metal surface (Au, Ag, Cu), the surface is rough and sample must be near or adsorbed at the surface [1]. In this study, we represent black silicon based substrates (bSi) for SERS application.





Fig. 3. (a) top-view SEM image of bSi/Au showing horizontally (perpendicular to the wavevector k⁻¹) oriented bi-spheres and dumbbell-like particles; (b) side-view SEM image of bSi/Au showing vertically (along the wavevector k⁻¹) oriented bi-spheres and dumbbell-like particles; (c) elementary nanostructures selected for numerical simulation of the E-field enhancement.



Fig. 4. E-filed enhancement maps at the irradiation wavelength of 790. (a) Si@Au (44nm@21nm), (b) Au bi-sphere (r = 25 nm, distance 47.5nm), (c) Au bi-sphere (r = 25 nm, distance 55 nm), (d) dumbbell-like structure (r_0 = 13.5 nm). Δ and ∇ are maximum and minimum values of the E-filed enhancement, respectively.

We perform a new bSi material possessing the unique properties allowing the use of the bSi sputtered with gold substrate as a highly sensitive stable SERS-active platform for detection of not only trace amounts of small organic molecules, but also living cells. The produced bSi surface due to its significant roughness, submicron regular cone structures evenly distributed over the entire surface, their high density allows to obtain the SERS-active surface with sufficiently good EF of about 108 and to create evenly distributed hot spots through the deposition of only 25÷50 nm gold layer instead of 100-400 nm traditionally used, significantly reducing production costs. Simulation results fully proved high E-field enhancement and revealed the major impact of LSPR in SERS properties of BS/Au substrates. Moreover, it was established that only vertical nanostructures alignment along bSi/Au cones provides appearance of the resonant absorption in NIR and significant E-field enhancement with EF of 10⁴-10⁸.

The BS/Au substrates may be easily fabricated in a large-scale using existing techniques, with the tune control of specific surface parameters, providing efficient enhancement, stability and reproducibility, and is a promising substrate for biosensor systems.

AcknowledgementsThis work was financially supported by joint project no. S-LB-19-4 from the Research Council of Lithuania Foundation, the Belarusian Republican Foundation for Fundamental Research (BRFFR) project F19LITG-003.

Fig.1. SEM images of bSi (a, b) and bSi/Au (c, d) substrates; (e) TEM image of the silicon cone covered by 25-50 nm thick gold layer.

The enhancement factor of the SERS-active bSi/Au substrate

I_{BSi/Au}

/N_{BSi/Au}

 I_{bulk}/N_{bulk}

where $I_{BSi/Au}$ ($N_{BSi/Au}$) and I_{bulk} (N_{bulk}) are Raman intensities (numbers of irradiated molecules) of 4-MBA monolayer on the

bSi/Au substrate and bulk 4-MBA on the SiO₂ substrate obtained at the same laser

and

accumulation, respectively.

time

 $\approx 2 \times 10^8$

EF =

power



Fig. 2. Raman spectra of 4-MBA monolayer on SiO_2/Au smooth substrate (a), of bulk 4-MBA (b), and SERS spectra of 4-MBA (c) and living rat glioma cell (d) on the bSi/Au substrate. Excitation wavelength is 785 nm.

Assignments of vibrational bands of 4-MBA in solid and adsorbed

Raman solid state (cm ⁻¹)	bSi/Au/ 4-MBA (cm ⁻¹)	Calculated Au ₁ - 4-MBA (cm ⁻¹)	Peak assignment
-	521	498	v(CS)
631	631	642	V _{6b}
-	693	-	γ(CH) out-of-plane
-	713	-	v _{4b} + γ(CCC) out-of-plane
806	-	766	V _{10a}
-	848	-	β(COO⁻)
909	-	-	β(SH)
-	1013	-	in-plane ring breathing, b ₂
1097	1077	1059	v ₁₂ (a ₁) in-plane aromatic ring breathing mode + v(CS), a ₁
-	1142	-	v_{15} (b ₂) δ (CH) deformation
1179	1180	1162	v_9 (a ₁) δ (CH) deformation
1290	-	-	V ₃
-	-	1326	v (COO ⁻) stretching mode
_	1418	_	v (COO ⁻) stretching mode
-	1480	-	v(CC) + γ(CH)
1598	1587	1585	v _{8a} (a ₁) totally symmetric aromatic ring vibration

Terahertz detection and noise properties of $(Cd_{1-x}Zn_x)_3As_2$

I. Yahnyuk¹, D. But¹, D. Yavorskiy¹, G. Grabecki², K. Grasza², W. Knap^{1,3} and S. Rumyantsev¹

¹ International Research Centre CENTERA, Institute of High Pressure Physics, Polish Academy of Sciences, 01-142 Warsaw, Poland
 ² Institute of Physics PAS, al. Lotników 32/46, PL 02-668 Warsaw, Poland

³ Laboratoire Charles Coulomb (L2C), UMR CNRS 5221, F-34095 Montpellier, France



Although Cd_3As_2 as a semiconductor material is known for almost a century, it has not found wide applications so far. The main reasons are difficulties in technology and doping. However, the large tunability of band gap from 0 eV for Cd_3As_2 to 1 eV for Zn_3As_2 makes it an ideal material for infrared and terahertz applications. Also interests in this material was renewed by the theoretical study showing the presence of a pair of symmetry protected threedimensional Dirac cones [2]. Indirect proof of this theoretical prediction is the extremely high electron mobility and the strong dependence of the electrons effective mass on their concentration. Extraordinary electronic properties and high mobility make it interesting for terahertz applications.

Evolution of the surface transport through topological phase transition. Zn doping-induced topological phase transition from a Dirac semimetal (DSM) to a trivial insulator in $(Cd_{1-x}Zn_x)_3As_2$ [1]



In this work, crystals of $(Cd_{0.4}Zn_{0.6})_3As_2$ were grown by were grown by horizontal Bridgman method [3]. The studied samples of bulk material were in a few millimeters in size with Hall bar geometry and indium contacts.



Reference:

Conclusions

[1] Shinichi Nishihaya, et.al, [Nat.Comm. 10, 2564 (2019)]
[2] Z. Wang, H. Weng, Q. Wu, X. Dai, and Z. Fang, Phys. Rev. B 2013, 88, 125427.
[3] G. Grabecki et al., Apparent metal-insulator transition in

[3] G. Grabecki et al., Apparent metal-insulator transition (Cd_{0.4}Zn_{0.6})₃As₂ (in preparation) □ The high frequency detection was studied at sub-terahertz frequencies of 100GHz and 140 GHz.

Relatively high amplitude of the response in a few millivolt ranges for an incident power of

approximately 35 mW.

□ The current dependence of the response had some signs of the bolometric mechanism.

Acknowledgements: The "Center for Terahertz Research and Applications (CENTERA)" project is carried out within the 'International Research Agendas' programme of the Foundation for Polish Science co-financed by the European Union under the European Regional Development Fund.



Enhanced sensitivity AIGaN/GaN HEMT terahertz detector without ungated regions

Juozas Vyšniauskas¹, Kęstutis Ikamas^{1,2} and Alvydas Lisauskas^{1,3}

¹ Institute of Applied Electrodynamics and Telecommunications, Vilnius University, Vilnius, Lithuania.

² Department of Defence Technologies, Military Academy of Lithuania, Vilnius, Lithuania. ³ CENTERA Labs, Institute of High Pressure Physics PAS, Warsaw, Poland. Email: juozas.vysniauskas@ff.vu.lt.

AlGaN/GaN HEMTs [1,2] and nMOS [3] transistors are reported as the most sensitive field effect transistor-based terahertz detectors. The advantage of HEMT is high electron mobility (up to $1500 \text{ cm}^2/\text{Vs}$) and the disadvantage is the presence of passive ungated regions which introduce additional series impedance contributing to the loss of high-frequency signal. The advantage of nMOS is the absence of ungated regions and the disadvantage is low electron mobility (about 250 cm²/Vs) due to high acceptor density (about 2e18 cm⁻³) in the channel.



Here, we propose the HEMT-based THz detector with 5 nm HfO_2 dielectric between the

Fig. 1 Current responsivity of the HEMT without and with ungated regions L_{UG} and gate length L_{G} .

gate electrode and the AlGaN layer, which allows to separate the gate from the source and drain terminals without involving ungated regions.

For numerical calculations of detector characteristics, we have employed two-dimensional hydrodynamic modeling performed with Synopsys TCAD Sentaurus program package comprising Poisson's equation, continuity equation, current density equation and energy balance equation for electrons and holes. It accounts for the formation of spontaneous and piezoelectric polarization charges in GaN and AlGaN layers, as well as the dependence of carrier mobility on doping density and carrier temperature.

The comparison of current responsivity of the HEMT with and without ungated regions and the gate length $L_G = 100$ nm is shown in Fig. 1. The results clearly indicate that the presence of ungated regions with the length $L_{UG} = 100$ nm reduces the maximum of the current responsivity at 1 THz by about 2 times. The minimum NEP at 1 THz is about 3 times lower in the HEMT without ungated regions.

REFERENCES

- [1] M. Bauer at al; IEEE Transactions on Terahertz Science and Technology 9, 430 (2019).
- [2] J. Sun at al; Applied Physics Letters 116, 161109 (2020).
- [3] K. Ikamas at al; IEEE Electron Device Letters 39, 1413 (2018).



Performance of Titanium-based Microbolometers for Monitoring of Spatial Beam Profile

in Terahertz Time-Domain Systems

Liang Qi¹, Linas Minkevičius¹, Andrzej Urbanowicz¹, Andrej Švigelj², Janez Trontelj², Domas Jokubauskis¹ and Gintaras Valušis¹

1 Center for Physical Sciences and Technology, Saulėtekio Ave. 3, LT-10257 Vilnius, Lithuania

2 Laboratory for Microelectronics, Faculty of Electrical Engineering, University of Ljubljana, Tržaška 25, 1000 Ljubljana, Slovenia

Email: liang.qi@ftmc.lt

Spatial mode profile and its control in terahertz (THz) imaging and spectroscopic systems is one of the most important constituents to enable high data quality. Moreover, convenience in use and abilities for precise optical alignment without additional optical components would be attractive advantage in practical implementation of the systems.

In this communication, convenient and easy-to-use both resonant and broadband antenna coupled ultrasensitive titaniumbased microbolometers are demonstrated for fine adjustment and control spatial mode profiles in THz time-domain systems. The



devices were found well-suited for implementation for medical imaging aims [1].

Three types of microbolometers [2] with the narrow band dipole antenna of 0.3 THz, 0.7 THz and a log-periodic broadband antenna [3] were explored. Femtosecond laser with a wavelength of 780nm, pulse duration of 90 fs and output power of 150mW at 80 MHz pulse repetition rate was used for optical excitation. The photoconductive antennas made from LT-GaAs offers a wide transmission spectrum from 0 to 5THz in the experiment.



Fig. 1. The scheme of THz titanium-based microbolometer with dipole antenna.



Fig. 3. The beam profile evolution of System 1 and System 2, separately recovered by three different detectors. (a) recorded by 0.3THz detector, (b) recorded by 0.7THz detector, (c) recorded by broadband detector.



Fig. 2. The schematic diagrams and parameters of TDS setups in System 1 and System 2, photos of three microbolometers. The angle θ is defined on the photo of 0.7THz detector.





Fig. 5. The spatial characteristic of System 1 without Lens1 along z- axis detected by 0.7 THz microbolometer.

Fig. 4. The evolution of beam profile, peak power and SNR with different polarization in System 1 and System 2.

CONCLUSIONS

Spatial mode profiles and polarization-resolved mode structures are recorded by titanium-based microbolometers in two THz timedomain systems. It is found that three microbolometers reproduce well the spatial mode profile of time-domain spectrometer. Polarization-sensitive mode control possibilities are also examined in details.

REFERENCES

[1] I. Kašalynas, R. Venckevičius, L. Minkevičius, A. Sešek, F. Wahaia, V. Tamošiūnas, B. Voisiat, D. Seliuta, G. Valušis, A. Švigelj, and J. Trontelj, Sensors 16, (2016) 432.

[2] J. Trontelj, G. Valušis, R. Venckevičius, I. Kašalynas, A. Sešek and A. Švigelj; Terahertz Emit. Receiv. Appl. V 9199(2014) pp. 91990K.
 [3] L. Minkevičius, L. Qi, A. Siemion, D. Jokubauskis, A. Sešek, A. Švigelj, J. Trontelj, D. Seliuta, I. Kašalynas and G. Valušis; Appl. Sci.10(2020) pp.3400.

Laser system for pumping THz and coherent X-ray NATO sources of secondary radiation Science for Peace CENTER NATO and Security (SPS) FOR PHYSICAL SCIENCES OTAN Programme AND TECHNOLOGY HOSTITUNOP

Paulius Mackonis, Augustinas Petrulėnas, Vytenis Girdauskas and Aleksej Rodin

Solid State Laser Laboratory, Center for Physical Sciences and Technology, Savanoriu 231, LT-02300 Vilnius, Lithuania.

We demonstrate compact TW-class VIS-NIR wavelength range Noncollinear Optical Parametrical Chirped Pulse Amplifier (NOPCPA) with an almost lossless spectral bandwidth due to the formation of "M"-shaped picosecond pumping pulses after the SHG-conversion. Moreover, the reuse of depleted pulses after the first SHG cascade increases the overall efficiency.

Compact TW-class VIS – NIR wavelength range laser system

The progress of natural science as well as a paradigm shift in the economy became inconceivable without the implementation of superstrong electromagnetic fields. However, the commissioning of high-intensity lasers within ELI framework is more a form of budget redistribution than a solution, because the cumbersome and time-consuming laser architecture is doomed to downtime, while scientists and technologists remain on the



waiting list.

Ultrashort, high energy, tunable wavelength laser pulses are in demand for a wide range of applications in ultrafast and strong field physics. Of great interest is their use for driving secondary radiation sources, such as the generation of THz and attosecond X-ray pulses. In addition, filamentation of ultrahigh intensity laser pulses in air opens up unprecedented opportunities for remote gas sensing. Recent studies have shown that an increase in the wavelength of the driving laser radiation makes it possible to generate higher photon energy attosecond X-ray pulses [1], as well as improve the efficiency of THz generation [2]. Furthermore, filamentation in air also benefits from longer driving wavelength because the wavelength scaling of the critical power of self-focusing allows more energy to be contained in a single filament.

In this work we present a cost-effective laser system that provides a choice of output pulses: >20 mJ, 1.2 ps with M²<1.1 at 1030 nm [3] or >2 mJ, <20 fs with $M^2 \sim 1.2$ at 790 nm [4], as well as probe supercontinuum (SC) at 500 – 2400 nm [5]. A multi-octave SC in the range up to 2400 nm allows the use of a similar OPCPA architecture to develop a sub-TW laser in the 2 µm spectral range for the high order harmonics generation or remote sensing of gases by filamentation. However, to eliminate the need for expensive periodically poled nonlinear crystals, we are developing an alternative concept for broadband Transient Stimulated Raman Chirped Pulse Amplification (TSRCPA) [6].

PUMPING SOURCE Yb:YAG CPA and Pulse Compressor



Fig. 1 The output energy (black) and gain (red) of CPA versus the seed energy (left) and autocorrelation trace of amplified pulses after compression (right).



OPCPA SEED AND PUMP PULSES Supercontinuum and Second Harmonic Generation

Fig. 3 SHG Conversion efficiency in the first and second SHG cascades (left). Temporal profiles of the second harmonic pulse after the second SHG cascade (right).

 \checkmark Compressed pulses converted to the \checkmark Further frequency doubling of depleted second harmonics in LBO and BBO pulses in BBO provides "M"-shaped

crystals with 62% and 70% efficiency: pump pulses at 515 nm with 5 mJ output energy and ~2 ps pulsewidth.

Amplified pulses with a total gain of \sim 3.500, \checkmark Pulse compression up to \sim 1.2 ps. an output energy of up to 22 mJ.

✓ Excellent beam quality $M^2 < 1.1$.

- Stable single-filament supercontinnum spanning ~500 nm to ~2400 nm in YAG rod of 15 mm length.
- \checkmark SC shows an energy stability exceeding the pumping laser.
- overall ~85% efficiently.
- ✓ After the first SHG cascade: **12 mJ** output

 \checkmark Pulses energy stability better than 1 %. energy at 515nm and ~ **1.2 ps** pulsewidth. **IN PROGRESS: Transient Stimulated Raman OPCPA – VIS-NIR Chirped Pulse Amplification** compact femtosecond VIS – NIR – SWIR laser system KGd(WO₄)₂ Pumping source Intensity [a 0.1 Intensity [a.u.] Yb:YAG CPA-compressor 1030 nm, 1.2 ps, 20 mJ, 100 Hz 0.0 1100 1160 1120 1140 Wavelength [nm] Intensity [a.u.] CH SC generation Two-cascaded SHG 0.1 0.0 in YAG Gaussian & M-shaped 900 750 800 850 700 950 0.01 500 – 2400 nm pulses, 515 nm Wavelength [nm] -m 1472 1468 1476 1464 1480 -Autocorrelation trace Wavelength [nm] --- Gaussian fit Intensity [a.u.] ⁵⁰ 1.0 Autocorrelation trace **OPCPA-VIS-NIR** Sech² fits τ_{AC} = 28 fs **Chirped mirrors** Intensity [a.u.] in BBO $\tau = 20 \text{ fs}$ compressor 700 – 1000 nm τ_{AC} = 224 fs 0.5 τ = 145 fs Pulse **TSRCPA** in KGW, CH_4 , H_2 0.0 100 -100 0 compression 1100 – 1800 nm Delay [fs] 0.0 0.5 Fig. 5 Spectrum of amplified pulses after three OPCPA stage -0.5 0.0 -1.0 (top) and autocorrelation trace after comression (bottom). Delay [ps] **OPCPA – SWIR**

Fig. 4 Layout of a compact femtosecond VIS – NIR – SWIR laser system.

Conclutions & future work

- \checkmark The pump-to-signal efficiency of ~20% and the pulse energy of ~2.1 mJ after the third OPCPA stage was reached.
- ✓ Amplified spectrum corresponding to Fourier-limited pulsewidth of ~8.6 fs.
- \checkmark Pulse compression up to **20 fs**.
- ✓ Beam quality $M^2 < 1.25$.

Fig. 6 TSRCPA output spectra in KGd(WO₄)₂ (top) and CH₄ (middle). Autocorrelation trace of compressed pulse after TSRCPA in KGd(WO₄)₂ crystal (bottom).

1.0

✓ Frequency shift during amplification of chirped SC pulses in a stimulated Raman amplifier based on solids or gases.

 \checkmark Possible pulse compression.

Acknowledgment

- Two of the co-authors are grateful to Eksma Ltd for providing student scholarships.
 - This research was sponsored in part by the NATO SPS Programme under grant G5734.
 - The solutions developed during the project were implemented at Ekspla Ltd in technological and scientific lasers.
- Recycling of depleted pulses at fundamental wavelength after the first SHG stage improves the overall harmonics conversion efficiency up to 85%.
- The use of "M"-shaped pump pulses made it possible to maintain a wide spectral bandwidth of amplified pulses in OPCPA stages with a high gain, while Gaussian pump pulses provided efficient energy extraction at the last stage.
- Laser system was built with an output energy of 2.1 mJ at a repetition rate of 100 Hz with support of a spectral bandwidth corresponding to a transform-limited pulsewidth of 8.6 fs. Pulse compression up to 20 fs at 790 nm was demonstrated.
- Transient Stimulated Raman Chirped Pulse Amplification shows a potential as an alternative to OPCPA or a complimentary method for developing intense femtosecond laser pulse source with frequency conversion.

References

[1] M.C.Chen, P.Arpin, T.Popmintchev, M.Gerrity, B.Zhang, M.Seaberg, D.Popmintchev, M.M.Murnane and H.C.Kapteyn, "Bright, Coherent, Ultrafast Soft X-Ray Harmonics Spanning the Water Window from a Tabletop Light Source," Phys. Rev. Lett. 105, 173901 (2010). [2] M.Clerici, M.Peccianti, B.E.Schmidt, L.Caspani, M.Shalaby, M.Giguere, A.Lotti, A.Couairon, F.Legare, T.Ozaki, D.Faccio and R.Morandotti, "Wavelength Scaling of Terahertz Generation by Gas Ionization," Phys. Rev. Lett. 110, 253901 (2013). [3] P.Mackonis, A.Rodin, "Laser with 1.2 ps, 20 mJ pulses at 100 Hz based on CPA with a low doping level Yb:YAG rods for seeding and pumping of OPCPA," Opt. Express 28(2), 1261-1268 (2020). [4] P.Mackonis, A.Rodin, "OPCPA investigation with control over the temporal shape of 1.2 ps pump pulses," Opt. Express 28(8), 12020-12027 (2020). [5] P.Mackonis, A.Petrulenas, V.Girdauskas, and A.M.Rodin, "Stable 1100 - 2400 nm supercontinuum in YAG with picosecond pumping for simplified OPCPA," in 2019 Conference on Lasers and Electro-Optics Europe and European Quantum Electronics Conference, OSA Technical Digest. (Optical Society of America, 2019), paper ca_p_43.

[6] P.Mackonis, A.Rodin, A.Petrulenas, V.Girdauskas and A.Michailovas, "Two-stage transient stimulated Raman chirped pulse amplification in KGd(WO₄)₂ with compression to 145 fs," (to be published).

Laser system for pumping THz and coherent X-ray sources of secondary radiation

Paulius Mackonis, Augustinas Petrulenas, Vytenis Girdauskas, Aleksej Rodin

Solid State Laser laboratory, Center for Physical Sciences and Technology Savanoriu 231, LT-02300 Vilnius, Lithuania. Email: paulius.mackonis@ftmc.lt

The progress of natural science as well as a paradigm shift in the economy became inconceivable without the implementation of superstrong electromagnetic fields. However, the commissioning of high-intensity lasers within ELI framework is more a form of budget redistribution than a solution, because the cumbersome and time-consuming laser architecture is doomed to downtime, while scientists and technologists remain on the waiting list.

Fig. 1 Layout of high peak power laser system at FTMC.

On the contrary, a cost-effective laser system built on two 1.5 m^2 breadboards (Fig. 1) by the efforts of one graduate and 1-2 students provides a choice of output pulses: >20 mJ, 1 ps with M^2 <1.1 at 1030 nm [1] or >2 mJ, <20 fs with M^2 ~1.2 at 790 nm [2], as well as probe supercontinuum (SC) at 600 – 2500 nm [3]. Using more pump diodes or increasing their power allows to further scale the peak power over 1 TW. Laser is based on easily reproducible modules: fiber laser front-end, two-stage double-pass Yb:YAG chirped pulse amplifier (CPA), grating compressor, SC generation, two cascades of second harmonic generation (SHG), three stages of noncollinear optical parametric chirped pulse amplifier (OPCPA), and chirped mirrors compressor. Using the same pump source for OPCPA and SC provides inherent synchronization and greatly simplifies the scheme. The energy conversion efficiency was improved due to the reuse of pump pulses depleted in SHG [1], and the maintenance of a wide OPCPA bandwidth due to their temporal shaping [2]. The solutions developed during the project were implemented at Ekspla Ltd in technological and scientific lasers. The obtained ultrashort high-energy laser pulses are ideally suited for the generation of highly efficient THz [4] and coherent X-ray radiation.

The demonstration of a multi-octave SC in the range up to 2500 nm [3] allows the use of a similar OPCPA architecture to develop a sub-TW laser in the 2 µm spectral range for the high order harmonics generation or remote sensing of gases by filamentation. However, to eliminate the need for expensive periodically poled nonlinear crystals, we are developing an alternative concept for broadband Transient Stimulated Raman Chirped Pulse Amplification (TSRCPA).

Two of the co-authors are grateful to Eksma Ltd for providing student scholarships. This research was sponsored in part by the NATO SPS Programme under grant G5734.

REFERENCES

- [1] P. Mackonis, A.M. Rodin; Opt. Express 28 (2020) pp.1261–1268.
- [2] P. Mackonis, A.M. Rodin; Opt. Express 28 (2020) pp.12020–12027.
- [3] P. Mackonis, A. Petrulenas, V. Girdauskas, A.M. Rodin; CLEO/Europe-2019, CA-P.43 MON.
- [4] J.A.Fülöp, L. Pálfalvi, S. Klingebiel, G. Almási, F. Krausz, S. Karsch, J. Hebling; Opt. Lett 37 (2012) pp.557–559.