

INTERNATIONAL WORKSHOP ON BISMUTH-CONTAINING SEMICONDUCTORS: THEORY, SIMULATION AND EXPERIMENT PROGRAMME AND ABSTRACT BOOKLET

## 18 - 20 July 2011 University of Surrey, Guildford, UK







AT Advanced Technology Institute

IOP Institute of Physics Semiconductor Physics Group

#### Foreword

Welcome to the 2<sup>nd</sup> International Workshop on Bismuth-containing Semiconductors: Theory, Simulation and Experiment. This workshop follows on from the highly successful meeting held at the University of Michigan, Ann Arbor in 2010 and continues to develop as a forum to discuss research in bismuth containing alloys. The programme this year illustrates the increasing breadth of research in this field with representation from Europe, Asia, Africa and North America. We are very pleased to have a number of excellent invited speakers covering theory, growth and applications of bismuth-containing semiconductors.

The workshop would not have been possible without support and we are very grateful to acknowledge sponsorship from the Engineering and Physical Sciences Research Council (EPSRC), the University of Surrey's Institute of Advanced Studies and the Institute of Physics Semiconductor Physics group.

We are delighted to welcome you to Guildford and hope that you have an enjoyable and productive time in both the technical and social elements of the programme.

On behalf of the organising committees,

Stephen Sweeney Workshop Chair

#### Local Organising Committee

Stephen Sweeney Mirela Dumic Konstanze Hild Nadir Hossain Daren Lock Igor Marko

#### **International Programme Committee**

Shane Johnson, Arizona State University, USA Stephan Koch, Philipps-Universität, Marburg, Germany Joanna Mirecki Millunchick, Univ. of Michigan, Ann Arbor, USA Patricia Mooney, Simon Fraser University, Burnaby, Canada Stephen Sweeney, University of Surrey, Guildford, UK Tom Tiedje, University of Victoria, Victoria, Canada

## 2<sup>nd</sup> International Workshop on Bismuth-containing semiconductors: Theory, Simulation and Experiment

18<sup>th</sup>-20<sup>th</sup> July 2011, Guildford, Surrey, UK

Technical Programme Overview		
Monday	9:30-10:50	Theory of Bismuth alloys (I)
Monday	11:20-13:00	MBE growth of Bismuth alloys
Monday	14:00-15:20	Optical properties
Monday	15:50-17:30	Electrical and optical properties
Tuesday	9:30-10:50	Structural properties and analysis
Tuesday	11:20-13:00	Devices
Tuesday	14:00-15:20	MOVPE growth of Bismuth alloys
Tuesday	15:50-17:10	Novel alloys
Wednesday	9:30-10:50	Theory of Bismuth alloys (II)
Wednesday	11:20-12:40	Optoelectronic properties and applications

All locations are shown on the maps at the back of the programme.

	Sunday 17 <sup>th</sup> July	
19:00 onwards	Workshop get-together: Boatman pub, River Wey, Guildford	
	Monday 18 <sup>th</sup> July: morning session	
08:30 onwards	<b>Registration:</b> The venue for the whole workshop (including the lunches) will be the Continuing Education Centre (CEC), level 2, Senate House	
09:15	Welcome	
	Theory of Bismuth alloys (I)	
9:30 (invited)	Theoretical Investigation of Band Structure of Bi Containing Isovalent III-V Alloys and the Validity of the Band Anticrossing Model Su-Huai Wei, A. Janotti, S. B. Zhang, H. X. Deng, J. Li, H. Peng, S. S. Li, JB. Xia, National Renewable Energy Laboratory, Theoretical Materials Science Group, Golden, USA	
10:10	Band anticrossing in dilute bismide alloys: Tight-binding and k.p analysis Christopher Broderick, Muhammad Usman, A. Lindsay, E. P. O'Reilly Photonics Theory Group, Tyndall National Institute and Physics Dept., University College Cork, Dyke Parade, Cork, Ireland	
10:30	Strong carrier-phonon coupling in Ga(AsBi) single quantum wells Alexej Chernikov <sup>1</sup> , Verena Bornwasser <sup>1</sup> , Martin Koch <sup>1</sup> , Stephan W. Koch <sup>1</sup> , Sangam Chatterjee <sup>1</sup> , Xianfeng Lu <sup>2</sup> , Shane R. Johnson <sup>2</sup> , Dan A.Beaton <sup>3</sup> , and Thomas Tiedje <sup>4</sup> <sup>1</sup> Philipps Universität Marburg, Department of Physics, Marburg, Germany, <sup>2</sup> Center for Photonics Innovation and School of Electrical, Computer, and Energy Engineering, Arizona State University, Engineering Research Center, Tempe, AZ, USA <sup>3</sup> Department of Physics and Astronomy, University of British Columbia, Vancouver, British Columbia, Canada <sup>4</sup> Department of Electrical and Computer Engineering, University of Victoria, Victoria, British Columbia, Canada	
10:50-11:20	Tea/Coffee break	
	MBE growth of Bismuth alloys	
11:20 (invited)	<b>Developments in molecular beam epitaxy growth of GaAsBi/GaAs(100)</b> Faebian Bastiman and J.P.R. David The University of Sheffield, Electronic and Electrical Engineering, Sheffield, UK	
12:00	High Bismuth Content GaAsBi Growth on GaAs, GaSb and InAs Substrates R.B. Lewis <sup>1,2</sup> , S.R. Johnson <sup>3</sup> , M. Masnadi-Shirazi <sup>2,4</sup> , N.A. Riordan <sup>3</sup> and T. Tiedje <sup>2</sup> <sup>1</sup> Dept. of Physics and Astronomy, University of British Columbia, Vancouver, Canada <sup>2</sup> Dept. of Electrical and Computer Engineering, University of Victoria, Victoria, Canada <sup>3</sup> Center for Photonics Innovation and School of Electrical, Computer, and Energy Engineering, Arizona State University, Tempe, Arizona, USA <sup>4</sup> Dept. of Electrical and Computer Engineering, University of British Columbia, Vancouver, Canada	
12:20	<b>Molecular Beam Epitaxy Growth of InSb<sub>x</sub>Bi<sub>1-x</sub></b> Yuxin Song and Shumin Wang Chalmers University of Technology, Microtechnology and Nanoscience, Gothenburg, Sweden	
12:40	Molecular Beam Epitaxy of GaN <sub>1-x</sub> Bi <sub>x</sub> with high Bi content Sergei Novikov <sup>1</sup> , A. J. Kent <sup>1</sup> , C. T. Foxon <sup>1</sup> , K. M. Yu <sup>2</sup> , A. X. Levander <sup>2,3</sup> , A. Tseng <sup>2,3</sup> , Z. Liliental-Weber <sup>2</sup> , O. D. Dubon <sup>2,3</sup> , J. Wu <sup>2,3</sup> , J. Denlinger <sup>4</sup> , F. Luckert <sup>5</sup> , P. R. Edwards <sup>5</sup> , R. W. Martin <sup>5</sup> and W. Walukiewicz <sup>2</sup> <sup>1</sup> School of Physics and Astronomy, University of Nottingham, Nottingham, UK <sup>2</sup> Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA, USA <sup>3</sup> Department of Materials Science & Engineering, University of California, Berkeley, CA, USA <sup>4</sup> Advanced Light Source, Lawrence Berkeley National Laboratory, 1 Cyclotron Road, Berkeley, CA, USA	
13:00-14:00	Lunch	

	Monday 18 <sup>th</sup> July: afternoon session	
	Optical properties	
14:00 (invited)	Luminescence Dynamics in Ga(AsBi) Sebastian Imhof <sup>1</sup> , Christian Wagner <sup>1</sup> , Angela Thränhardt <sup>1</sup> , Alexej Chernikov <sup>2</sup> , Martin Koch <sup>2</sup> , Niko S. Köster <sup>2</sup> , Sangam Chatterjee <sup>2</sup> , Stephan W. Koch <sup>2</sup> , Oleg Rubel <sup>3</sup> , Xianfeng Lu <sup>4</sup> , Shane R. Johnson <sup>4</sup> , Daniel A. Beaton <sup>5</sup> , Tom Tiedje <sup>6</sup> <sup>1</sup> Technische Universität Chemnitz, Chemnitz, Germany, <sup>2</sup> Fachbereich Physik, Philipps-Universität Marburg, Marburg, Germany, <sup>3</sup> Thunder Bay Regional Research Institute, Thunder Bay and Department of Physics, Lakehead University, Thunder Bay, Ontario, Canada, <sup>4</sup> Department of Electrical Engineering, Arizona State University, Tempe, Arizona, USA, <sup>5</sup> Department of Physics and Astronomy, University of British Columbia, Vancouver, British Columbia, Canada,	
14:40	Photoluminescence Characterization of GaAsBi Quantum Wells Grown on GaAs Chaturvedi Gogineni <sup>1</sup> , N. A. Riordan <sup>1</sup> , X. Lu <sup>1,3</sup> , D. Ding <sup>1</sup> , YH. Zhang <sup>1</sup> , T. Tiedje <sup>2</sup> and S. R. Johnson <sup>1</sup> <sup>1</sup> Center for Photonics Innovation and School of Electrical, Computer, and Energy Engineering, Arizona State University, Engineering Research Center, Tempe, AZ, USA <sup>2</sup> Department of Electrical and Computer Engineering, University of Victoria, Victoria, BC, Canada <sup>3</sup> Varian Semiconductor Equipment Associates, Gloucester, MA, USA	
15:00	Resonance of bandgap and Spin orbit Splitting in GaAsBi / GaAs Alloys Zahida Batool <sup>1</sup> , Konstanze Hild <sup>1</sup> , T.J.C. Hosea <sup>2</sup> , A.R. Mohmad <sup>3</sup> , X. Lu <sup>4</sup> , T. Tiedje <sup>4</sup> , A. Krotkus <sup>5</sup> , V. Pačebutas <sup>5</sup> , R. Butkutė <sup>5</sup> and S.J. Sweeney <sup>1</sup> <sup>1</sup> Advanced Technology Insitute, University of Surrey, Guildford, GU27XH, UK <sup>2</sup> Ibnu Sina Institute for Fundamental Science Studies, Universiti Teknologi Malaysia, Johor Bahru, Johor 81310, Malaysia <sup>3</sup> Department of Electronic and Electrical Engineering, University of Sheffield, S1 3DJ, UK <sup>4</sup> Department of Electrical and Computer Engineering, University of Victoria, BC, V8W 3P6, Canada <sup>5</sup> Center for Physical Sciences and Technology, Optoelectronics, A. Gostauto 11, Vilnius 1180, Lithuania	
15:20-15:50	Tea/Coffee break	
	Electrical and optical properties	
15:50	Mechanism of enhanced photoluminescence in GaAs <sub>1-x</sub> Bi <sub>x</sub> alloys Abdul Rahman Mohmad <sup>1</sup> , F. Bastiman <sup>1</sup> , J. S. Ng <sup>1</sup> , J. P. R. David <sup>1</sup> , S.J.Sweeney <sup>2</sup> <sup>1</sup> University of Sheffield, Department of Electronic and Electrical Engineering, Sheffield, UK <sup>2</sup> Advanced Technology Institute, University of Surrey, Guildford, UK	
16:10	<b>Optical Characterization of GaAsBi Films using Spectroscopic Ellipsometry</b> Nathaniel Riordan <sup>1</sup> , S. R. Johnson <sup>1</sup> , R. B. Lewis <sup>2,5</sup> , M. Masnadi-Shirazi <sup>3,5</sup> , C. Gogineni <sup>1</sup> , X. Lu <sup>1,2</sup> , C. Xu <sup>4</sup> , J. Menendez <sup>4</sup> , and T. Tiedje <sup>5</sup> <sup>1</sup> Center for Photonics Innovation and School of Electrical, Computer, Arizona State University, Tempe, AZ, USA <sup>2</sup> Department of Physics and Astronomy, University of British Columbia, Vancouver, BC, Canada <sup>3</sup> Department of Electrical and Computer Engineering, University, Tempe, Arizona, USA <sup>5</sup> Department of Electrical and Computer Engineering, University of Victoria, Victoria, BC, Canada	
16:30	<b>Compositional evolution of Bi-induced acceptor states in GaAsBi alloys</b> Giorgio Pettinari <sup>1</sup> , H. Engelkamp <sup>2</sup> , P.C.M. Christianen <sup>2</sup> , J.C. Maan <sup>2</sup> , A. Polimeni <sup>3</sup> , M. Capizzi <sup>3</sup> <sup>1</sup> The University of Nottingham, School of Physics and Astronomy, University Park, Nottingham, UK, <sup>2</sup> High Field Magnet Laboratory, Radboud University Nijmegen. <sup>3</sup> CNISM-Dipartimento di Fisica, Sapienza Universit`a di Roma, Roma, Italy	
16:50	Photoinduced carriers type determination in GaBiAs epitaxial layers by contactless surface photovoltage spectroscopy Piotr Sitarek <sup>1</sup> , Robert Kudrawiec <sup>1</sup> , Jan Misiewicz <sup>1</sup> , Jaroslaw Serafinczuk <sup>2</sup> , S. V. Novikov <sup>3</sup> , M. Henini <sup>3</sup> <sup>1</sup> Institute of Physics, Wroclaw University of Technology, Wroclaw, Poland, <sup>2</sup> Faculty of Microsystem Electronics and Photonics, Wroclaw University of Technology, Wroclaw, Poland <sup>3</sup> School of Physics and Astronomy, University of Nottingham, NG7 2RD Nottingham, United Kingdom	
17:10-17:30	Effect of Bi alloying on the transport properties of the dilute bismide alloy, GaAsBi R.N. Kini <sup>1</sup> , A. J. Ptak <sup>2</sup> , B. Fluegel <sup>2</sup> , R. France <sup>2</sup> , R. C. Reedy <sup>2</sup> , and A. Mascarenhas <sup>2</sup> <sup>1</sup> Indian Institute of Science Education and Research Thiruvananthapuram, Thiruvananthapuram, Kerala, India <sup>2</sup> National Renewable Energy Laboratory, 1617 Cole Boulevard, Golden, Colorado 80401, USA	
18:30	BBQ on campus (by the lake)	

	Tuesday 19 <sup>th</sup> July: morning session
	Structural properties and analysis
09:30	Atomic Structure of Bi-induced GaAs (001) Surfaces Adam Duzik, John C. Thomas, Anton van der Ven, Joanna M. Millunchick University of Michigan, Materials Science and Engineering, Ann Arbor, USA
09:50	Structural Characteristics of Bi-containing III/V semiconductors Peter Ludewig <sup>1</sup> , R. Fritz <sup>1</sup> , A. Beyer <sup>1</sup> , S. Chatterjee <sup>1</sup> , K. Volz <sup>1</sup> , X. Lu <sup>2</sup> , R. Lewis <sup>2</sup> , T. Tiedje <sup>3</sup> , R. Butkutė <sup>4</sup> , A. Krotkus <sup>4</sup> <sup>1</sup> Department of Physics and Material Sciences Center, Philipps-University Marburg, Germany <sup>2</sup> Department of Physics and Astronomy, University of British Columbia, Canada <sup>3</sup> Electrical and Computer Engineering, University of Victoria, Victoria, Canada <sup>4</sup> Semiconductor Physics Institute of Center for Physical Sciences and Technology, Vilnius, Lithuania
10:10	Transmission Electron Microscopy characterization of InAs(Bi)/GaAs QDs David L. Sales <sup>1</sup> , D. F. Reyes <sup>1</sup> , M. Roldan <sup>1</sup> , S. I. Molina <sup>1</sup> and D. Gonzalez <sup>1</sup> , F. Bastiman <sup>2</sup> , C. Hunter <sup>2</sup> <sup>1</sup> Materials Science and Metallurgy and Inorganic Chemistry, Facultad de Ciencias, Universidad de Cadiz, Puerto Real, Cadiz, Spain <sup>2</sup> The University of Sheffield, Electronic and Electrical Engineering, Sheffield, UK
	Mechanisms of Droplet Formation during Ga(In)AsBi Molecular
10:30	Beam Epitaxy Growth Gülin Vardar, M. V. Warren, M. Kang, S. Jeon, R. S. Goldman(a) The University of Michigan, Materials Science and Engineering, Ann Arbor, USA (a)also: Physics, University of Michigan, Ann Arbor, MI 48109-2136, USA
10:50-11:20	Tea/Coffee break
	Devices
11:20 (invited)	The Prospects for use of Highly Mismatched Alloys in Long-Wavelength Infrared Detectors Stefan Svensson <sup>1</sup> , W. L. Sarney <sup>1</sup> , H. Hier <sup>1</sup> , G. Belenky <sup>2</sup> <sup>1</sup> US Army Research Lab, Adelphi, USA, <sup>2</sup> Department of Electrical and Computer Engineering, State University of New York at Stony Brook, Stony Brook, NY, USA
12:00	Novel GalnAsSbBi Materials for Mid-Infrared Type-I Quantum Well Lasers Dongsheng Fan <sup>1</sup> , Shui-Qing Yu <sup>1</sup> , Zhiming M. Wang <sup>2</sup> and S.R. Johnson <sup>3</sup> <sup>1</sup> Department of Electrical Engineering, University of Arkansas, 3217 Bell Engineering, Fayetteville, Arkansas, USA, <sup>2</sup> Institute of Nanoscale Science and Engineering, University of Arkansas, Fayetteville, Arkansas, USA <sup>3</sup> Center for Photonics Innovation and School of Electrical, Computer, and Energy Engineering, Arizona State University, Tempe, AZ, USA
12:20	Spectral and Thermal Properties of GaAs <sub>1-x</sub> Bi <sub>x</sub> LEDs N. Hossain <sup>1</sup> , I. P. Marko <sup>1</sup> , K. Hild <sup>1</sup> , S. R. Jin <sup>1</sup> , R. B. Lewis <sup>2</sup> , D. A. Beaton <sup>2</sup> , X. Lu <sup>2*</sup> , T. Tiedje <sup>2</sup> and S. J. Sweeney <sup>1</sup> <sup>1</sup> Advanced Technology Institute, University of Surrey, Guildford, Surrey, UK. <sup>2</sup> Department of Electrical and Computer Engineering, University of Victoria,, Victoria, B.C., Canada. <sup>*</sup> now with Varian Semiconductor Equipment Associates, Gloucester, MA, USA
12:40	Lasing in GaAsBi with low temperature dependence of oscillation wavelength Masihiro Yoshimoto, Yoriko Tominaga and Kunishige Oe Kyoto Institute of Technology, Dept. of Electronics, Matsugasaki, Sakyo, Kyoto, Japan
13:00-14:00	Lunch

	Tuesday 19 <sup>th</sup> July: afternoon session	
	MOVPE growth of Bismuth alloys	
14:00 (invited)	Challenges and prospects of metastable III/V-materials grown by MOVPE Wolfgang Stolz and Kerstin Volz Philipps-University Marburg, Department of Physics & Materials Science Center, Marburg, Germany	
14:40 (invited)	Atmospheric-pressure metalorganic vapour phase epitaxy of GaAsBi alloy on different oriented GaAs substrates Hedi Fitouri, Imed Zaied, Zied Chine, Ahmed Rebey and Belgacem El Jani, Faculty of Sciences of Monastir, Department of Physics, Monastir, Tunisia	
15:20-15:50	Tea/Coffee break	
	Novel alloys	
15:50	Growth and Characterization of high quality InSbBi layers grown by Liquid Phase Epitaxy Tushar Dhabal Das, S. C. Das, and S. Dhar University of Calcutta, Dept. of Electronic Science, Kolkata, India	
16:10	<b>Optical characterization of GaBiAs/GaAs and InGaBiAs/InP epitaxial layers</b> Vaidas Pačebutas, R. Butkutė, J. Devenson, B. Čechavičius, L. Dapkus and A. Krotkus <i>Center for Physical Sciences and Technology, Optoelectronics, Vilnius, Lithuania</i>	
16:30	<b>Growth of dilute nitride (GaIn)(NAs) on InP by MOVPE</b> Peter Ludewig K. Werner, S. Reinhard, W. Stolz and K. Volz Philipps-University Marburg, Department of Physics & Materials Science Center, Marburg, Germany	
16:50-17:10	Bismide-nitride alloys — promising candidates for near- and mid-infrared photonics Shirong Jin and S.J. Sweeney Advanced Technology Institute, University of Surrey, Guildford, UK	
18:30	Coach to leave for Conference Dinner from piazza (bus stop).	

	Wednesday 20 <sup>th</sup> July: morning session
	Theory of Bismuth alloys (II)
09:30 (invited)	Imposing changes in band and spin-orbit gaps in GaNBi alloys Mohamed Ferhat <sup>4</sup> , A. Belabbes <sup>1,4</sup> , A. Zaoui <sup>2</sup> , S. Laref <sup>3,1</sup> <sup>1</sup> Institut für Festköpertheorie und Theoretische Optik, Friedrich-Schiller-Universität, Jena, Germany. <sup>2</sup> LML, Ecole Polytechnique de Lille, Université des Sciences et de la Technologie de Lille, Cité Scientifique, Villeneuve D'Asq, France <sup>3</sup> Université de Lyon, Institut de Chimie de Lyon, Laboratoire de Chimie, Ecole Normale Supérieur de Lyon, Lyon, France <sup>4</sup> Département de Physique, Université des Sciences et de la Technologie d'Oran, Oran. Algeria
10:10	Electronic structure calculations for supercells containing dilute 'Bi' inside GaAs – an atomistic tight-binding approach Muhammad Usman, Chris Broderick, Andrew Lindsay and Eoin P. O'Reilly Tyndall National Institute, Photonic Theory Group, Lee Maltings, Cork, Ireland
10:30	<b>Energy broadening of the perturbed valence band states in GaAs<sub>1-x</sub>Bi<sub>x</sub></b> Nikolaos Vogiatzis and Judy M. Rorison University of Bristol, Electrical and Electronic Engineering, Woodland Rd., Merchant Venturers Building, Bristol, UK
10:50-11:20	Tea/Coffee break
	Optoelectronic properties and applications
11:20	Band gap, spin orbit splitting and radiative transitions of GaNAsBi layers matched on GaAs substrates Mohamed Mourad Habchi, Ahmed Rebey and Belgacem el Jani Faculty of Sciences of Monastir, Boulevard of environment, Monastir, Tunisia
11:40	Nonequilibrium carrier trapping and recombination in GaBiAs layers Arūnas Krotkus, R. Adomavičius, K.Bertulis and A. Koroliov Center for Physical Sciences and Technology, Optoelectronics, Vilnius, Lithuania
12:00	The effect of Bi on the growth and performance of Type II strained layer superlattices for IR photodetectors Wendy Sarney <sup>1</sup> , Stefan Svensson <sup>1</sup> , Harry Hier <sup>1</sup> , Ding Wang <sup>2</sup> , Dmitry Donetsky <sup>2</sup> and Gregory Belenky <sup>2</sup> <sup>1</sup> US Army Research Laboratory, Electro-optics & Photonics Division, RDRL-SEE-I,, Adelphi,, USA <sup>2</sup> Department of Electrical and Computer Engineering, State University of New York at Stony Brook, Stony Brook, NY, USA
12:20	Thermoelectric and Optoelectronic Properties of Dilute Bismuthide Materials on InP Substrates Joshua Zide, P. B. Dongmo, J. P. Petropoulos and YJ. Zhong University of Delaware, Materials Science and Engineering, Newark, USA
12:40	Closing session
13:00	Pick up packed lunch, optional Lab tour (ATI).
14:00	Optional excursion to Hampton Court Palace (leaving from piazza).

# ABSTRACTS

## Theoretical Investigation of Band Structure of Bi Containing Isovalent III-V Alloys and the Validity of the Band Anticrossing Model

Su-Huai Wei, A. Janotti, S. B. Zhang, H. X. Deng, J. Li, H. Peng, S. S. Li, J.-B. Xia,

National Renewable Energy Laboratory, Theoretical Materials Science Group, 1617 Cole Blvd, Golden, 80401, USA

Recent advances in optoelectronic device applications require design and growth of materials with specific structural and optical properties. For example, it is highly desirable to have a good quality material that is lattice matched to GaAs and has a band (~ 1 eV) for application in 1.3-µm solid-state lasers and high-efficiency multijunction solar cells. Using first-principles band structure and total energy method we have investigated the stability and band structure of GaAs<sub>1-x-v</sub>N<sub>x</sub>Bi<sub>v</sub> alloys. We find that (i) coalloying small-sized N and large-sized Bi in GaAs can significantly reduce the strain, thus stabilize the alloy against phase separation; (ii) due to the large size and relativistic effect, the alloystabilized zinc-blende GaBi has a very negative band gap, thus the alloy band gap is very sensitive to the concentration of Bi as well as N; (iii) relative to Ga As, GaAs<sub>1-x-v</sub>N<sub>x</sub>Bi<sub>y</sub> alloys have a high valenceband maximum, thus they can be doped more easily p-type; (iv) N and Bi substitution on As sites in GaAs introducing isovalent defect levels at impurity limit or defect bands when the alloy concentration increases. We show that at the impurity limit the N (Bi)-induced impurity level is above (below) the conduction (valence) band edge of GaAs. These trends reverse at high concentration, i.e., the conduction-band edge of  $GaAs_{1-x}N_x$  becomes an N-derived state and the valence-band edge of GaAs<sub>1-x</sub>Bi<sub>x</sub> becomes a Bi-derived state, as expected from their band characters. We argue that this band crossing phenomenon cannot be described by the popular band anticrossing (BAC) model but can be naturally explained by a simple band broadening picture.

#### Band anticrossing in dilute bismide alloys: Tight-binding and k.p analysis

Christopher Broderick, Muhammad Usman, A. Lindsay, E. P. O'Reilly Photonics Theory Group, Tyndall National Institute and Physics Dept., University College Cork, Dyke Parade, Cork, Ireland

We have developed an atomistic sp3s\* tight-binding (TB) Hamiltonian which allows accurate calculation of the electronic structure of GaBiP and GaBiAs. Supercell calculations allow us to trace the origin of the observed bowing of the band gap ( $E_g$ ) and spin-orbit splitting ( $E_{so}$ ) in these alloys to a band anticrossing (BAC) interaction between the host matrix valence band maximum (VBM) and Bi-related defect states lying in the valence band in GaAs [1].

We describe how we have used the TB Hamiltonian to explicitly identify the presence of both the Birelated defect states and their interaction with the host matrix VBM in GaBiP. Similar calculations for GaBiAs indicate that  $E_g$  decreases by 63 - 80 meV per % Bi for < 14% Bi and that we should encounter a crossover at 10 - 11% Bi, beyond which composition we have  $E_g < E_{so}$ , in agreement with recent experimental studies [2]. All calculations are performed using the NEMO 3-D NanoElectronic MOdelling software [3].

The  $E_g < E_{so}$  regime is of interest for optoelectronic device design since it presents the possibility of suppression of the CHSH Auger recombination process, a loss mechanism which plagues the efficiency of III-V multinary lasers operating at telecommunication wavelengths. It is therefore of particular interest to understand the GaBiAs band structure corresponding composition range to enable accurate modelling of dilute bismide optoelectronic properties. We present a modified form of the standard 8-band k.p Hamiltonian for zinc blende, derived from the TB calculations. The Hamiltonian accounts explicitly for BAC interactions in the alloys and provides an accurate description of the GaBiAs band structure in the vicinity of the band edges.

- [1] K. Alberi, et al., Phys.
- [2] Z. Batool, et al., in preparation
- [3] G. Kilmeck, et al., IEEE Trans. Electron. Dev. 54, 2079 (2007)

#### Strong carrier-phonon coupling in Ga(AsBi) single quantum wells

Alexej Chernikov<sup>1</sup>, Verena Bornwasser<sup>1</sup>, Martin Koch<sup>1</sup>, Stephan W.Koch<sup>1</sup>, Sangam Chatterjee<sup>1</sup>, Xianfeng Lu<sup>2</sup>, Shane R. Johnson<sup>2</sup>, Dan A.Beaton<sup>3</sup>, and Thomas Tiedje<sup>4</sup>

<sup>1</sup>Philipps Universität Marburg, Department of Physics, Renthof 5, Laborbau II, 35037 Marburg, Germany, <sup>2</sup>Center for Photonics Innovation and School of Electrical, Computer, and Energy Engineering, Arizona State University, Engineering Research Center, Rm#266, Tempe, AZ 85287, USA <sup>3</sup>Department of Physics and Astronomy, University of British Columbia, Vancouver, British Columbia V6T 1Z4, Canada

<sup>4</sup>Department of Electrical and Computer Engineering, University of Victoria, Victoria, British Columbia V8W 3P6, Canada

We present a study of phonon-assisted emission of 12 nm thick GaAs<sub>1-x</sub>Bi<sub>x</sub> single quantum wells with Bi concentrations up to x=0.055. The samples are investigated by continuous-wave photoluminescence as function of lattice temperature and excitation density. Pronounced phonon-sidebands of the main emission peak are observed. These sidebands originate from the recombination of an electron-hole pair under simultaneous emission of longitudinal optical phonons. The strength of the carrier-phonon coupling in the GaAs<sub>1-x</sub>Bi<sub>x</sub> quantum wells is quantified by the Huang-Rhys factor up to 0.3 and is unusually strong for a GaAs-based material. Carriers bound to isoelectronic impurities, i.e. Bi clusters, are identified to be the origin of the efficient carrier-phonon scattering. Our findings propose a potential application of the diluted bismides for extremely low threshold lasers utilizing the phonon-assisted emission by exploiting the well-established III-V technology.

#### Developments in molecular beam epitaxy growth of GaAsBi/GaAs(100)

#### Faebian Bastiman and J.P.R. David

#### The University of Sheffield, Electronic and Electrical Engineering, Mapping Building, Mappin Street, Sheffield, S1 3JD, UK

GaAs<sub>1-x</sub>Bi<sub>x</sub>/GaAs(100) has received much recent interest due to the large band gap bowing (88 meV/%) and spin orbit splitting. Molecular beam epitaxy (MBE) growth of high quality crystalline material is non-trivial and requires precise control of both fluxes and sample temperature. Bi compositions from ~0.1-14% have been grown, covering wavelengths from near GaAs to beyond 1.6µm utilising a growth temperature range from 325 to 450°C.

Growth temperature in particular is found to strongly influence epitaxy allowing control of maximum composition, rate of Bi incorporation and evaporation and droplet formation, crystal quality and room temperature photoluminescence (RT-PL) full width half maximum (FWHM). The latter is of particular interest, since RT-FWHM of GaAsBi is typically three times greater than binary GaAs. Work has been performed to maximise the Bi content and reduce the FWHM for a given growth temperature in 0.1µm thick bulk GaAsBi layers and compare them to 5nm QWs. Results indicate that the bulk FWHM varies significantly from 0.1-1% Bi, then reaches a steady state value of around 75 meV for 2 - 13% Bi. QW from 2 - 13% exhibit minimal RT FWHM of 65 meV, but alloy fluctuations, atomic ordering and clustering causing significant variation in this value. This work presents scanning tunnelling microscopy, transmission electron microscopy, x-ray diffraction and PL of the MBE grown samples.

#### High Bismuth Content GaAsBi Growth on GaAs, GaSb and InAs Substrates

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GaAsBi Alloys with Bi content in excess of 10 % are of particular interest for applications in midinfrared devices. To date, most GaAsBi has been grown on GaAs substrates; however, the large amount of lattice mismatch in high Bi concentration GaAsBi films would prevent the growth of thick, unrelaxed layers and compressive strain may inhibit bismuth incorporation. In this regard, larger lattice constant substrates, such as InP, InAs and GaSb may be more suitable for accommodating high concentration GaAsBi.

GaAsBi epilayers have been grown on GaAs, GaSb and InAs substrates. Bi incorporation up to 15.9 %, with good compositional uniformity has been achieved on GaAs by growing below the Bi melting point at substrate temperatures as low as 225°C. Growths done with a relatively large bismuth flux (Bi:Ga BEP ratio 0.6) and As2:Ga flux ratios as low as 0.25 are believed to show the maximum bismuth incorporation that is possible at a given temperature, which increases with decreasing temperature. These samples show excess Bi and Ga on the surface in the form of submicron bimetallic droplets. Reciprocal space mapping of an 18 nm thick 12.8% sample shows that the film is pseudomorphic. Growth on GaSb and InAs substrates has also been attempted. Up to 25% Bi incorporation has been achieved on GaSb substrates and up to 20% on InAs substrates under similar growth conditions to those on GaAs. These films have a bigger lattice mismatch with the substrate and a sample containing 25% Bi on GaSb was found to be relaxed. Little is known so far about the properties of these large Bi concentration alloys, including the bandgap.

#### Molecular Beam Epitaxy Growth of InSb<sub>x</sub>Bi<sub>1-x</sub>

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It is theoretically predicted that incorporation of Bi in normal III/V semiconductor materials can provide a large bandgap bowing effect and spin-orbit split which can be utilized to improve the performance of electronic and optoelectronic devices. Intensive research has been implemented in GaAsxBi1-x system using Molecular Beam Epitaxy (MBE). InSb<sub>x</sub>Bi<sub>1-x</sub>, which has large potentials for applications in long wavelength IR optoelectronics, is much less investigated.

We have studied the growth conditions for InSbxBi1-x using MBE and obtained large incorporation of Bi in InSb layer. The 200nm InSb<sub>x</sub>Bi<sub>1-x</sub> layers were metamorphcally grown on GaAs (001) substrates with a composite buffer consisting of 30nm InSb/ 200nm GaSb. Due to the weak bonding of Bi in competition with Sb, the Sb/In flux ratio should be kept as small as possible while the Bi/Sb as large as possible. To raise Bi incorporation, we use a low InSb growth rate of 0.2  $\mu$ m/h. The critical Sb/In flux ratio is judged by the formation of In droplets in RHEED. To avoid formation of Bi droplets, the beam equivalent pressure of Bi must be smaller or close to the Bi vapor pressure at a particular growth temperature. With these growth constraints, the lowest temperature for Bi incorporation is found at 350°C and the Bi composition quickly increases with the growth temperature and tend to saturate at above 360°C. Surprisingly, a large peak shift of 2000 arcsec toward a high angle in XRD was observed indicating lattice contraction of InSbBi with respect to InSb.

#### Molecular Beam Epitaxy of GaN<sub>1-x</sub>Bi<sub>x</sub> with high Bi content

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Recently it was demonstrated that it is possible to grow GaAs1-xBix alloys with a limited Bi content by metal-organic vapour phase epitaxy (MOVPE) and by molecular beam epitaxy (MBE). The band gap bowing as well as the electronic properties observed in GaAs1-xBix alloys can be explained within the band anticrossing (BAC) model.

It is more difficult to incorporate Bi into GaN layers than into GaAs layers, because the differences in electronegativity and atomic radii between N and Bi are larger than between As and Bi. Therefore only limited information is currently available on the growth and properties of  $GaN_{1-x}Bi_x$  alloys. At normal MOVPE and MBE growth temperatures for GaN there is no significant incorporation of the Bi into the bulk of the GaN layer.

Recently we have studied the MBE growth of  $GaN_{1-x}Bi_x$  alloys at extremely low temperatures down to ~100°C. We have grown layers on sapphire substrates under a wide range of Bi fluxes and under different Ga to N ratios. We found that with carefully controlled growth parameters, it is possible to incorporate up to 20% of Bi in GaN. The resulting GaNBi alloys are typically amorphous with the presence of crystalline phase on the nanometer scale. A dramatic reduction in the optical band gap from 3.4 eV in GaN to below 1.2 eV is observed in GaN<sub>1-x</sub>Bix alloys with x>0.11. This band gap reduction can also be qualitatively understood by the formation of a narrow band originating from an anticrossing interaction between Bi localized states and the extended states of the GaN matrix. In this talk we will review our prior efforts in using Bi as surfactant in MBE growth of GaN and compare Bi incorporation during the MBE growth of the GaN layers under Ga-rich and N-rich growth conditions.

#### Luminescence Dynamics in Ga(AsBi)

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We investigated the temporal evolution of the low temperature spectrally resolved photoluminescence of a Ga(AsBi) sample. Experimental data were analyzed using a kinetic Monte-Carlo simulation. The measured photoluminescence transients show the typical asymmetric behavior of disorder-dominated samples, i.e., the decay on the high-energy side is much faster than the decay on the low-energy tail. We reproduce both the temperature-dependent time-integrated photoluminescence and the low temperature dynamics by using the approach of two energy scales. We now explain the whole set of dynamic and time-integrated measurements using a model with only a very small number of parameters to which we then attribute actual physical meaning. The two energy scales are interpreted as alloy disorder and Bi-clusters. As an upper limit for the carrier capture time into the Bi clusters we obtain an average value of 5 ps which is much faster than the transitions between the individual cluster sites.

#### Photoluminescence Characterization of GaAsBi Quantum Wells Grown on GaAs

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Temperature and pump power dependent photoluminescence measurements are performed on GaAs1-xBix/GaAs quantum wells grown by molecular beam epitaxy. At low temperature the spectra are broad and exhibit large blue shifts in the peak position as the pump intensity is increased from 0.01 to 100 mW. Furthermore, transient intensity changes are observed with respect to illumination time that persist down to very low excitation powers. These results are consistent with reports of multiple energy levels near the band edge attributed to Bi clustering. Further details of this work will be reported at the workshop.

#### Resonance of bandgap and Spin orbit Splitting in GaAsBi / GaAs Alloys

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Room temperature (RT) photomodulated reflectance (PR) studies have revealed that the cross over between band gap ( $E_g$ ) and spin orbit splitting energy ( $\Delta_o$ ) occurs at 9.2% bismuth for strained and >10% for unstrained GaAsBi /GaAs epilayers. For a the bismuth concentration for which  $\Delta_o$  is greater than  $E_g$  Auger recombination involving the split-off band (CHSH) and inter-valence band absorption should be suppressed. Samples with Bismuth fractions lying on either side of cross over can be tuned in and out of this Auger resonance by employing temperature dependent PR. The idea of a resonance effect is supported by an increase in linewidth close to resonance and a lower decrease in the intensity of the PR signal with increasing temperature when the band gap is tuned into resonance with the spin orbit splitting energy. PR and Surface Photo Voltage (SPV) measurements can also help to reveal the Bi concentration of unknown samples by measuring both the band gap and spin-orbit splitting energies.

To investigate the possibility of Auger suppression further power dependent photoluminescence (PL) at room temperature as well as at low temperature (150K) was performed in order to determine the dominant recombination mechanism in GaAsBi/GaAs. We find that samples with Bi concentrations of 4.5% and an emission of 1.1µm show the highest intensity and are mainly dominated by radiative recombination. Samples with < 4.5% Bi show defect related recombination and samples with >4.5% Bi show additional non-radiative processes. For samples around the technological interesting wavelength of 1.5 µm we find additional evidence for tuning into an Auger resonance as shall be discussed.

#### Mechanism of enhanced photoluminescence in GaAs<sub>(1-x)</sub>Bi<sub>(x)</sub> alloys

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The optical properties of GaAs(1-x)Bi(x) alloys with Bi compositions up to 0.06 have been studied by photoluminescence (PL). The samples were grown at 380 - 400 °C using molecular beam epitaxy. At room temperature, the incorporation of Bi in GaAs reduces the bandgap by ~65 meV/%Bi with peak wavelength of 1.2  $\mu$ m for x = 0.06. It was found that higher Bi composition leads to higher PL intensity at room temperature but weaker PL intensity at 10 K. Power dependent measurements were carried out at room temperature to analyze the dominant carrier recombination mechanisms. The results indicate that the PL emission for low Bi content samples were dominated by non-radiative recombination (m = 2) but becomes more radiative (m = 1.6 and 1.4) with further increases in Bi contents. The enhanced PL intensity with increasing Bi content at room temperature may due to the reduction in defect density in the samples. The low Bi content samples have greater PL intensity at 10 K possibly due to greater localization energy which efficiently trap carriers rather than due to better crystal quality.

#### Optical Characterization of GaAsBi Films using Spectroscopic Ellipsometry

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Alloying bismuth with III-V materials results in a large reduction in bandgap energy. Recent growths of GaAsBi films with Bi content in excess of 10% give credence to the potential of this material system for mid and long wavelength device applications. Furthermore, device design using bismuth containing III-V materials requires a detailed set of optical characteristics. While photoluminescence is a technique used to probe the bandgap energy of a sample, spectroscopic ellipsometry is a technique used to probe the absorption features of various optical transitions including the fundamental bandgap. This technique can also provide the refractive index, extinction coefficient, and the complex dielectric function. Recent work on the optical characterization and measurement of the optical functions of GaAsBi films grown by molecular beam epitaxy will be reported.

#### Compositional evolution of Bi-induced acceptor states in GaAsBi alloys

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Recent measurements of the exciton reduced mass and short-range ordering of Bi-atoms in  $GaAs_{1-x}Bi_x$  alloy in a large range of Bi concentration (x up to ~11%) have displayed a surprising, anomalous dependence of these properties on the alloy composition: For x < ~5%, the exciton reduced mass increases with x and Bi-atoms display a short-range ordering; for x > ~5% the exciton reduced mass largely decreases and begins to follow a regular k·p behavior, while a random anion distribution is restored [1,2]. These results indicate a transition in GaAsBi from a nonconventional- to a conventional-alloy behavior for Bi concentration around 5%.

In the present work, we report on the first evidence of Bi-induced acceptor states in nominally undoped GaAsBi alloys, and their unexpected compositional evolution. By performing far-infrared absorption spectroscopy for magnetic fields up to 30 T, we observe the Lyman series of an acceptor in nominally undoped GaAsBi layers. The involved acceptor states are characterized by an exceedingly high value of the ground state g-factor ( $g_{eff} = 14.9$ ), which points to Bi as the origin of these states. The Bi-induced acceptor states dominate the absorption spectra of samples for Bi concentrations below 5%, while they suddenly disappear at higher Bi concentrations. Such a behavior reveals an electronic or structural transition in the same concentration range in which the exciton reduced mass and short-range order recover a conventional-alloy behavior in this same alloy. We discuss the likely origin of the Bi-induced acceptor states in terms of Bi-clusters formation and/or of the peculiar characteristics of Bi to behave as a mixed valence element, namely, either as a group-III or a group-V element.

[1] G. Pettinari et al., Phys. Rev. B 81, 235211 (2010).

[2] G. Ciatto et al., Phys. Rev. B 82, 201304(R) (2010).

## Photoinduced carriers type determination in GaBiAs epitaxial layers by contactless surface photovoltage spectroscopy

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We present contactless surface photovoltage spectroscopy (SPS) studies of 1  $\mu$ m thick GaBiAs layers grown by MBE technique on semi-insulating GaAs substrate. The investigated structures differ in arsenic flow during growth process. The different growth conditions influences the bismuth concentration in GaBiAs layer and its optical quality. The red-shift of absorption edge in SPS spectra is clearly visible due to increase of Bi content. It was observed that besides the absorption edge shift, the growth conditions have also influence on the band bending close to the surface. The curvature of SPS signal changes for different samples, which means that SPS signal originates from different type of carriers. The annealing influence on investigated structures was also studied.

#### Effect of Bi alloying on the transport properties of the dilute bismide alloy, GaAsBi

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We studied the effect of Bi incorporation on the electron and hole mobility in the dilute Bismide alloy, GaAsBi using electrical transport (Hall) and PL techniques. We observed no significant degradation in the electron Hall mobility with Bi incorporation in GaAs, up to a concentration of 1.2%. At higher Bi concentration (≥1.6%) some degradation of the electron mobility was observed, although there is no apparent trend. Our measurements show that the hole Hall mobility decreases with increasing Bi concentration. Analysis of the temperature dependant Hall transport data of p-type GaAsBi epilayers along with low-temperature PL measurements of p-doped and undoped epilayers suggests that Bi incorporation results in the formation of several trap levels above the valence band which we attribute to Bi-Bi pair states. The decrease in hole mobility with increasing Bi concentration as being caused by scattering at the isolated Bi and the Bi-Bi pair states.

#### Atomic Structure of Bi-induced GaAs (001) Surfaces

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Bi readily surface segregates in III-V alloys, smoothing the surface via atomic reordering on the surface. The reconstruction of Bi-terminated GaAs has been studied using experimental and computational methods. Bi deposition via molecular beam epitaxy onto the GaAs (001)  $\beta$ 2(2x4) and c(4x4) reconstructions at a substrate temperature of 440°C produces (1x3) and (2x3) reflective highenergy electron diffraction (RHEED) patterns, respectively. After depositing 2.4 ML of Bi onto the β2(2x4) surface, in vacuo scanning tunneling microscopy (STM) reveals a disordered row reconstruction with a row spacing of 3x the GaAs surface lattice parameter along the [110]. Deposition of 0.6 ML of Bi onto the c(4x4) reconstruction induces a mixed reconstruction consisting of the  $\beta^2(2x4)$  reconstruction and the disordered row reconstruction. The Bi-induced stability of the disordere d row reconstruction relative to the GaAs  $\beta$ 2(2x4) and c(4x4) reconstructions has been determined using density functional theory and the cluster expansion method. A surface reconstruction phase diagram of Bi-containing (4x3), c(4x4), and  $\beta 2(2x4)$  reconstructions shows that the GaSb (001) (4x3) reconstruction (consisting of rows of V-V dimers separated by a Ga-V kinked dimer at every fourth dimer, where V is either As or Bi) is predicted to become stable in Biterminated GaAs as the Bi chemical potential increases. The predicted stable surface structures compare favorably with the observed STM of the 3x periodic surface, with the disorder likely arising from the various configurations of Bi within the (4x3) reconstruction.

The transformation to a Bi-induced (4x3) reconstruction produces a change in step energies that alters the step density. The (4x3) reconstruction has a higher step density, but they alternate in type. That is, trains of dissimilar steps (i.e., up/down/up/down,) are favored, while suppressing trains of successive steps (i.e., up/up/up or down/down/down). While this increases step-height density on the 1nm length scale, the overall roughness decreases.

#### Structural Characteristics of Bi-containing III/V semiconductors

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Bismuth (Bi)-containing III/V semiconductors are interesting from the application point of view, as Bi increases the spin-orbit splitting in conventional III/V semiconductors and hence certain Auger loss processes could be suppressed in future laser devices using these materials as active layers. From fundamental point of view, these alloys are interesting, as Bi has a significantly larger covalent radius than all the other group V atoms, which are replaced by Bi. Consequently, Bi-containing III/V semiconductors are highly metastable and tend towards structure formation.

We examine several Ga(BiAs)/GaAs heterostructures, which were grown by molecular beam epitaxy and have nominally different Bi contents using transmission electron microscopy (TEM). High angle annular dark field imaging as well as conventional chemical sensitive dark field imaging was used to address the composition and the homogeneity of the element distribution. In addition, high resolution TEM was applied to examine elemental ordering on a small length-scale.

We will show, that – depending on growth conditions – there can be a strong tendency towards phase separation in these alloys. Nevertheless, Bi-concentrations up to 20% can be realized. In addition we find CuPt-ordering on the {111} group V lattice planes in some of the samples. The presentation will summarize the structural characteristics in dilute Bi-containing GaAs in dependence on the growth conditions as well as on the Bi-fraction in the material.

#### Transmission Electron Microscopy characterization of InAs(Bi)/GaAs QDs

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The heteroepitaxial growth of Bi-containing InAs quantum dots (QDs) on GaAs(100) substrates is desirable in order to take advantage of the 88 meV per at.% redshift caused by Bi incorporation, as observed in the GaAsBi/GaAs system. Bi acts as a surfactant, affecting the wetting layer growth morphology. Furthermore, the presence of Bi during the SK transition alters the size, shape, density and internal composition of the QDs.

The present work aims to study the structural and compositional differences between InAs/GaAs QDs when growing with and without Bi overpressure in a molecular beam epitaxy (MBE) reactor. Preliminary TEM analytical results show indications of Bi atoms incorporated in the QD structure. Additionally, PL results indicate up to a 130 meV shift in the peak position with no apparent broadening of the PL spectra linewidth. These results are consistent with a Bi content of 1.5 % Bi within the QDs. Despite the difference in atomic volume, this incorporation does not affect the crystalline quality of the heterostructure.

#### Mechanisms of Droplet Formation during Ga(In)AsBi Molecular Beam Epitaxy Growth

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Due to the significant bandgap reduction associated with Bi incorporation, Ga(In)AsBi alloys have been proposed for high-efficiency solar cells and high performance infrared detectors. The performance of such devices is predicted to be improved by the incorporation of absorptionenhancing plasmonic structures. Interestingly, for both GaAsBi and InAsBi alloys, metallic droplets are often observed on the surface during epitaxial growth. In the case of GaAsBi and InAsBi, droplet sizes and densities are reported to be dependent on the Bi flux during growth [1], but the optical properties remain unknown. Here, we report on the formation mechanisms and optical properties of Ga(In)AsBi films with Ga(In), Bi and Ga(In)-Bi composite surface droplets. We have grown Ga(In)AsBi films by molecular beam epitaxy (MBE) and examined their surfaces with scanning electron microscopy and energy-dispersive x-ray spectroscopy. For GaAsBi, MBE growth at 300-350°C results in the formation of GaAsBi films containing a few percent Bi, along with Ga-Bi composite surface droplets. For standard growth rates (~1µm/hr), mono-modal distributions of droplets are observed, with average sizes ranging from 400 nm to 4µm for substrate temperatures ranging from 300 to 350°C. For low growth rates (~0.1µm/hr), a bimodal distribution of droplets is apparent, with droplet size distributions centered around 1 and 7  $\mu$ m. We will discuss the influence of V/III ratio, substrate temperature, and growth rate on the droplet formation and evolution. In addition, the optical properties of the droplets will be presented. We gratefully acknowledge the support of the National Science Foundation through Grant DMR-1006835.

[1] G. Ciatto, M. Thomasset, F. Glas, X. Lu, and T. Tiedje, Phys. Rev. B 82, 201304 (2010).

#### The Prospects for use of Highly Mismatched Alloys in Long-Wavelength Infrared Detectors

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The performance and feasibility of fielding strategic and tactical night-vision systems depends upon the infrared detector materials chosen for their design. System designers must accommodate the competing parameters of performance, cost, and availability. Although mercury cadmium telluride (MCT) compounds offer the best performance parameters, they have general synthesis issues and lack an appropriate substrate in terms of size and availability. II-VI materials in general do not have the benefits of commercial leveraging to bring down costs. Therefore, a III-V based materials alternative to MCT is highly desirable for Army applications.

Based on the assumption that III-V compounds do not have an inherently small bandgap enabling operation out to 10 micron, the long wave infrared (LWIR) range, there has been substantial research investment in superlattice approaches. However, superlattices present their own shortcomings, namely low quantum efficiency and operating temperature for quantum well infrared photodetectors (QWIP), and very short minority carrier lifetimes for strained layer superlattice (SLS) detectors.

Recently there has been renewed interest in unipolar barrier designs. The performance of such devices in the MWIR has revived interest in the search for direct-bandgap III-V compounds suitable for LWIR. Introducing Bi and/or N in dilute concentrations to certain III-V host compounds allows for bandgap reduction. In this presentation, we will review potential approaches for highly mismatched alloys to create LWIR detector materials. So far more work has been done with N, which has been added to GaSb, InSb and InAs. In most cases, however, this leads to significant reductions of the minority carrier lifetimes. We will compare the relative benefits of N and Bi and discuss possible designs that take advantage of these elements' bandgap narrowing effects, in relation to the expected bowing parameter in the InAsSb system, as well as the lattice-hardening properties of highly mismatched alloys.

#### Novel GaInAsSbBi Materials for Mid-Infrared Type-I Quantum Well Lasers

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It has been shown that Bismuth has great possibility to engineer the band gap and band alignment of III-V alloys. The giant band gap reduction, the uplifting of valence band maximum, and the large spinorbit splitting, make bismides promising material for mid-infrared light emitting sources in the 3-4µm wavelength range. Where for instance, GaInAsSbBi/GaInAsSb active regions offer type-I quantum wells with a superior hole and electron confinement balance when compared to convention mid-infrared Sb based materials. Non-radiative recombination can also be possibly suppressed. Preliminary results show Bi can be incorporated into GaSb by MBE growth at low temperature. More results and analysis will be presented.

#### Spectral and Thermal Properties of GaAs<sub>1.x</sub>Bi<sub>x</sub> LEDs

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The incorporation of Bismuth in GaAs leads to band gaps in the near- and mid-infrared range with potential applications in lasers and optical amplifiers. Furthermore, the large spin-orbit splitting provides an opportunity to suppress non-radiative loss processes. In a first step towards developing lasers, we investigate the carrier recombination processes occurring in GaAs<sub>0.986</sub>Bi<sub>0.014</sub>/GaAs p-i-n light emitting diodes (LEDs) via temperature and pressure dependence of the light-current characteristics and an analysis of the electroluminescence spectra. The emission wavelength of the p-i-n structures is measured to be ~936 nm at 260K. The emission wavelength shows a low temperature coefficient of emission peak shift of 0.17 nm/K from 80-260K, which may be attributed to band-anticrossing and/or carrier localization effects. A rapid decrease in emission efficiency with increasing temperature implies that loss processes play a role in these structures. In order to investigate this further, high pressure measurements were utilized. The pressure coefficient of the GaAs<sub>0.986</sub>Bi<sub>0.014</sub> band gap was measured to be 11.8±0.3 meV/kbar compared with 10.7meV/kbar for GaAs. The electroluminescence emission shows that while the overall emission intensity decreases with increasing pressure, the emission in the GaAs barrier region increases as pressure is applied suggesting carrier overflow into the GaAs. This together with a decrease in efficiency with increasing pressure is attributed to electron leakage and subsequent recombination in the GaAs due to a decrease in band offset between GaAsBi and GaAs with increasing pressure. This provides evidence that the GaASBi/GaAs conduction band offset is type I, highlighting its potential for laser applications.

#### Lasing in GaAsBi with low temperature dependence of oscillation wavelength

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Development of semiconductor laser diodes with temperature-insensitive oscillation wavelength is expected to open up a new era of wide spread application of wavelength-division-multiplexing telecommunication network systems. Semiconductor materials with a temperature-insensitive band gap are attracting attention, as they are expected to create a laser whose lasing wavelength remains stable in the face of variations in ambient temperature.

GaAs<sub>1-x</sub>Bi<sub>x</sub>/GaAs laser has been realized for the first time by photo-pumping. A GaAs<sub>0.975</sub>Bi<sub>0.025</sub> active layer was grown at a very low temperature of 350°C by molecular beam epitaxy (MBE). The characteristic temperature of the laser was 83 K between 160 and 240 K. The lasing emission peak energy decreased at a constant rate of 1.8 meV/K, which is only 40% of the temperature coefficient of the GaAs bandgap in the temperature range. Above 240 K, the lasing threshold pumping power increased sharply, and the lasing emission peak energy started shifting to shorter wavelengths. These phenomena might be explained by carrier behaviors at the GaAs<sub>0.975</sub>Bi<sub>0.025</sub>/GaAs hetero-interface in which a large valence band offset and an almost flat conduction band offset is expected.

#### Challenges and prospects of metastable III/V-materials grown by MOVPE

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In recent years the class of dilute nitride III/V-semiconductors and corresponding heterostructures are gaining increasing interest both from fundamental as well as applied point of view. This is caused by their unique optoelectronic properties and in particular by the novel conduction band formation process leading to an extreme band gap bowing with increasing N-content in the crystal. As one potential application novel laser devices with improved characteristics on GaAs-, InP- and in recent years also monolithically integrated on Si-substrate are discussed.

Due to their metastable character these dilute nitride III/V compounds have to be grown under extreme non-equilibrium conditions at low growth temperatures. This communication summarizes the present understanding of the atomic incorporation efficiencies of the group-V-atoms as a function of detailed epitaxial growth conditions, i.e. growth temperature, V/III-ratio, V/V-competition processes, chemical composition, strain as well as precursor chemistry for the laser material systems (GaIn)(NAs) on GaAs- as well as Ga(NAsP) on GaP-substrate applying metalorganic vapour phase epitaxy (MOVPE). In addition, surfactant effects applying Sb as additional growth species will be elucidated. Based on all of these findings, implications for the future epitaxial growth of Ga(NAsBi) by MOVPE will be discussed.

### Atmospheric-pressure metalorganic vapour phase epitaxy of GaAsBi alloy on different oriented GaAs substrates

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Metalorganic vapour phase epitaxial growth of GaAsBi alloy on different oriented GaAs substrates has been carried out at atmospheric pressure in horizontal geometry reactor. Trimethyl-gallium, trimethyl bismuth (TMBi), and arsine were used as precursor sources at a growth temperature of 420°C within a very narrow range of V/III ratios and molar flow rates of TMBi.We performed high-resolution X-ray diffraction (HRXRD) and photoreflectance (PR) measurements in order to characterize the structural and optical properties of the as-grown GaAsBi layers. The analysis of the HRXRD data show that GaAsBi growth rate is particularly lower in (511)A epilayer than in (100), (111)A and (411)A. This behaviour follows the gap shrinkage obtained by PR spectroscopy. In analyzing the surface morphology, scanning electron microscopy (SEM) was used to qualify films properties. Our result suggests that the density of Bi islands exhibits some dependence on GaAs substrate orientations.

#### Growth and Characterization of high quality InSbBi layers grown by Liquid Phase Epitaxy

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InSbBi alloys have attracted interest for potential applications in the infrared spectral region. Addition of small quantities of of Bi to III-V semiconductors results in a substantial reduction in the energy band gap of the parent semiconductor, thus opening up the possibility of easy control of the operating wavelength of optoelectronic devices made therefore.

Liquid phase epitaxy (LPE) provides a simple and low cost technique to grow this material with high crystalline perfections. We have grown InSbBi layers on (100) InSb substrates in a horizontal LPE reactor at 340-345oC under a melt supercooling of 10-12°C and a cooling rate of 0.2°C/min. The melt contained high purity In metal saturated with polycrystalline InSb to which upto 2.2 at% 6N pure Bi was added.

The surface morphology and thickness of the grown layers were characterized respectively by scanning electron microscopy (SEM) and Nomarski interference contrast microscopy. Energy dispersive x-ray analysis (EDAX) spectrum of InSbBi layer clearly showed distinct Bi peak confirming incorporation of same in the material. High resolution x-ray diffraction (HRXRD) pattern resolved two distinct peaks due to the substrate and the InSbBi layer. X-ray compositional mapping showed that Bi was uniformly distributed over the surface of the grown layer. We have also performed room temperature Fourier transform infrared (FTIR) absorption measurements on the material. The result indicated a red shift of the absorption edge as Bi incorporation in the material is increased and a band gap reduction upto ~10meV was obtained.

## Optical characterization of GaBiAs/GaAs and InGaBiAs/InP epitaxial layers

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Dilute bismides are considered as promising materials for advanced semiconductor sources in the near- and mid-infrared spectral ranges for the applications in telecommunications and sensing. In this contribution we will report on the investigations of the energy structure and the photoluminescence spectra in dilute bismides grown on GaAs and InP substrates and emitting at  $1.55 \,\mu\text{m}$  and longer wavelengths.

The thickness of the GaBi<sub>x</sub>As<sub>1-x</sub> /GaAs and In<sub>y</sub>Ga<sub>1-y</sub>Bi<sub>x</sub>As<sub>1-x</sub> /InP layers grown in the SVT-A MBE reactor was 30-100 nm, their growth temperature was varied over the range from 330°C to 220°C. The layers were grown on lattice-matched with the substrate buffer layers of GaAs and InGaAs, respectively. The layers grown on GaAs substrates were strained. Their carrier lifetimes were long – of the order of several hundreds of picoseconds and did not decrease after the annealing. Optical properties of the layers were investigated by photoluminescence, photomodulated reflectance, surface photovoltage, and optical transmittance spectroscopies. The efficiency of the photoluminescence from the GaBiAs layers emitting in the 1.55  $\mu$ m range significantly increased after their post-growth annealing at 600°C and higher temperatures. On the other hand, the growth of In<sub>y</sub>Ga<sub>1-y</sub>Bi<sub>x</sub>As<sub>1-x</sub> with y=0.5 on InP at the temperatures of 280-300°C has resulted in the incorporation of approximately 3% Bi and the reduction of the energy bandgap to ~0.7 eV.

## Growth of dilute nitride (GaIn)(NAs) on InP by MOVPE

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Current optoelectronic devices operating at  $1.55\mu$ m emission wavelength consist of (GaIn)(AsP)/(GaIn)(AsP) MQW systems grown on InP substrate. The energy efficiency of such devices which are used for data transfer in telecommunication networks is very low. On one hand, a lot of input energy is wasted as heat due to significant auger recombination. On the other hand these devices show a poor temperature stability caused by insufficient electron confinement and the highly temperature dependent bandgap. In this work, we will concentrate on higher temperature stability of 1.55  $\mu$ m optoelectronic devices to minimize the need of active cooling.

The incorporation of a small amount of nitrogen (N) into (GaIn)As host material causes a reduction of the conduction band due to band anti crossing. Therefore, the replacement of the active layer of current devices by dilute nitride containing (GaIn)(NAs) increases the confinement of electrons and accordingly the temperature stability. Furthermore, the incorporation of N reduces the temperature dependence of the bandgap.

The challenge growing (GaIn)(NAs) lattice matched to InP by metal organic vapour phase epitaxy (MOVPE) is the low incorporation efficiency of N into the host material which is further reduced with increasing indium content.

We will present investigations of the MOVPE growth of dilute nitride containing (GaIn)(NAs)/(GaIn)(AsP) MQW structures on InP substrate. Furthermore the structural and optoelectronic properties of these layers will be analyzed and discussed.

#### Bismide-nitride alloys — promising candidates for near- and mid-infrared photonics

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Both dilute-N and Bi-alloys have become hot topics in near-infrared photonics in recent years. Such considerable interest arises mainly due to two key points. Firstly, due to the interesting physics of significant band structure shrinkage by adding either highly mismatched nitrogen or bismuth atoms into GaAs, which are described well by the band anticrossing (BAC) model [1]. Secondly, it is shown that they are promising candidates for near-infrared photonic applications, due to their potential to improve the temperature sensitivity of devices compared to conventional InP-based GaInAsP and GaInAlAs alloys. It is therefore important to determine theoretically the potential operating wavelength range of these alloys and the extent to which the band structure may be optimised to minimise Auger recombination processes which typically dominant long-wavelength lasers.

Here we present the calculated key material parameters such as band gap/optical transition energy, band offsets, spin-orbit splitting energy,  $\Delta_{SO}$ , and strain for GaAs-based bulk GaAsBiN and GaAsBiN/GaAs quantum well structures with different N- and Bi-compositions at various well thicknesses utilising the BAC model [1-3]. The relative alignment of band edges between the quantum well and barrier is calculated using model-solid theory [4]. Band structures are calculated with a self-consistent approach by solving a modified 6-band k·p Hamiltonian matrix with Poisson's and Schrödinger's equations. Numerical results show that this material system covers a wide energy range from 0.4eV to 1.2eV, which makes GaAsBiN suitable for a wide spectral range from near-infrared to mid-infrared. Furthermore, because  $\Delta_{SO}$  increases superlinearly with Bi-content,  $\Delta_{SO}$  will be larger than  $E_g$  if high Bi content (> 10%) is used in GaAsBiN, providing an opportunity to suppress CHSH Auger recombination and inter-valence band absorption losses in the near- and mid-infrared. Further scope for type-II band alignments and other potential Bi/N alloys will be discussed.

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#### **INVITED:**

#### Imposing changes in band and spin-orbit gaps in GaNBi alloys

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We present first-principles pseudopotential plane-wave calculations and large 64-atoms relaxed supercells to explore the effects of alloying of non conventional III-V compound GaN with bismuth. We found a highly nonlinear reduction of the energy gap of GaN for small Bi composition. Consequently the optical band gap bowing is found extremely important and composition dependent. The stronger contribution is due principally to structural and to less extent to charge transfer effects. Moreover, because of strong relativistic effects caused by bismuth, we found a giant bowing for the spin-orbit splitting energy of valence band, by far the largest of any III-V ternary alloys.

# Electronic Structure Calculations for Supercells containing Dilute 'Bi' inside GaAs – An Atomistic Tight-Binding Approach

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We report an atomistic model established for electronic structure calculations of GaBi(x)As(1-x) (0 < 1x < 12%) alloys based on empirical tight binding parameters. Alloy supercells consisting of 1000 (3x3x3nm^3) and 8000 (6x6x6nm^3) atoms are relaxed using the Valence Force Field (VFF) method [1], including anharmonic corrections to the Keating potential [2]. Nearest neighbor tight binding Hamiltonian is solved for electronic spectra by representing each atomic site with sp3s\* parameters including spin orbit coupling (ten band model). The sp3s\* tight binding parameters are designed to reproduce previously reported bulk band structures for GaAs and GaBi. The calculated GaBi bulk band structure shows the good agreement with previously reported LDA+C calculations [3]. Our calculations of alloy supercells indicate a reduction of ~63-80 meV/%Bi in the band gap of GaBi<sub>x</sub>As<sub>1-x</sub>. Recent experimental data [4] indicates a crossing between the energy gap (Egap) and spin-orbital coupling ( $\Delta o$ ) for x~10.5% which closely matches with our calculations. Our results for a Ga500Bi1As499 structure confirm a band-anticrossing interaction between Bi resonant defect states and the valence band maximum. The computed energy and charge density distribution  $|\psi|^2$ indicate that the Bi-related resonant state lies ~250meV below the valence band edge and is ~60% localized on the Bi site and its four nearest Ga neighbours. The close agreement of our calculations with the experimental data for periodic GaBi(x)As(1-x) supercells allows us to extend our study to strained GaBi<sub>x</sub>As<sub>1-x</sub> grown on top of GaAs substrates. The simulations are performed using NanoElectronic MOdeling tool, NEMO 3-D [5].

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# Energy broadening of the perturbed valence band states in GaAs<sub>1-x</sub>Bi<sub>x</sub>

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In general the interaction of a localized impurity state with the delocalized host states imposes a strong anticrossing behavior of the perturbed mixed states. Within the Anderson impurity model1 these perturbed states correspond to the real solutions of the Green's functions of the delocalized states. The advantage of the Anderson model is that we can obtain further information from the imaginary component of the Green's functions2. In other words, this imaginary component is associated with an energy broadening of the real solutions and physically represents the localized character of the mixed states.

This approach has worked well in the dilute nitrides. For example, by using the Green's functions the mixed density of states2,3,4 have been calculated successfully around the impurity level exhibiting an s-type behavior.

We shall use the same methodology for the GaAs1-xBix alloys. We use as an input the energy of the valence band states of GaAs and the energy of the localized states of Bi accounting explicitly for their imaginary component which relates to the impurity broadening as this is described within the Anderson model.

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# Band gap, spin orbit splitting and radiative transitions of GaNAsBi layers matched on GaAs substrates

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GaNAsBi quaternary containing small concentrations of N and Bi are highly electronegativity mismatched alloys (HMAs) belong to III-N-V-Bi compounds semiconductors which can be lattice matched to GaAs substrates. These dilute nitride-bismides can represent the active zone of temperature intensitive wavelength (1.55 micron) laser diode intended for optical fiber communication. In this work, we have studied theoretically the electronic band structure (BS) of GaAsBi and GaNAsBi within the framework of the band anti-crossing model (BAC). In fact, using the valence-BAC, the conduction-BAC and the k.p method, BS was calculated near the Brillouin zone center (gamma point) for three non-equivalent directions (delta, lambda and sigma). We have determined also the variation of energy levels and inter-band transitions with Bi content, in particular the band gap energy. In addition, we have treated the case of GaNAsBi leading to the wavelength emission of 1.55 micron. Finally, we note the possibility to obtain the resonance of band gap and spin orbit splitting when Bi content increases.

# Nonequilibrium carrier trapping and recombination in GaBiAs layers

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The heteroepitaxial growth of Bi-containing InAs quantum dots (QDs) on GaAs(100) substrates is desirable in order to take advantage of the 88 meV per at.% redshift caused by Bi incorporation, as observed in the GaAsBi/GaAs system. Bi acts as a surfactant, affecting the wetting layer growth morphology. Furthermore, the presence of Bi during the SK transition alters the size, shape, density and internal composition of the QDs.

The present work aims to study the structural and compositional differences between InAs/GaAs QDs when growing with and without Bi overpressure in a molecular beam epitaxy (MBE) reactor. Preliminary TEM analytical results show indications of Bi atoms incorporated in the QD structure. Additionally, PL results indicate up to a 130 meV shift in the peak position with no apparent broadening of the PL spectra linewidth. These results are consistent with a Bi content of 1.5 % Bi within the QDs. Despite the difference in atomic volume, this incorporation does not affect the crystalline quality of the heterostructure.

# The effect of Bi on the growth and performance of Type II strained layer superlattices for IR photodetectors

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Type II Strained Layer Superlattice (SLS) photodetectors offer an attractive alternative to Mercury Cadmium Telluride (MCT) infrared (IR) imaging devices. If Shockley Reed-Hall (SRH) minority carrier lifetimes are sufficiently long, then the SLS is theoretically predicted to outperform MCT due to the significant suppression of Auger recombination enabled through bandstructure engineering. Despite the lauded advantages, the SLS has yet to perform as theoretically predicted, or as well as MCT. While MCT has SRH lifetimes on the order of 1 µs, the best MWIR and LWIR SLS material has SRH lifetimes on the order of 35 and 75 ns, respectively. Low lifetimes persist despite extensive growth optimization studies in terms of strain balancing and controlling the nature and quality of the numerous interfaces. Current data indicates that strain, number and type of interfaces, and the growth conditions are not first-order effects. This implies that minority carrier lifetimes may be limited by defects in the binary constituents.

Our new approach is to use Bi during the growth of the SLS. The simplest approach is to expose the SLS to Bi throughout the entire growth. If Bi is beneficial, then exposure of one SLS constituent at a time could reveal which one is responsible for the short SLS lifetime. Our past studies indicate that GaSb has a shorter lifetime and is the most likely location of the unwanted recombination centers. Preliminary work shows an improved PL intensity for samples grown with the GaSb layers exposed to Bi, compared with a reference sample where there was no Bi exposure. Despite this finding, there is no improvement in the SRH lifetime. Imminent studies will include the growth and characterization of Bi-exposed bulk materials used in the SLS, GaSb and InAs, as well as optimization of other growth conditions related to the optimized use of Bi.

# Thermoelectric and Optoelectronic Properties of Dilute Bismuthide Materials on InP Substrates

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We present our latest experimental and theoretical results on the molecular beam epitaxy (MBE) growth of dilute bismuthide (a/k/a bismide) materials on InP substrates for both thermoelectric and optoelectronics applications. Thermoelectric power generation is an important technology for waste heat recovery, but practical application requires improved efficiency of thermoelectric materials. This is accomplished by increasing the thermoelectric figure of merit,  $ZT=S^2\sigma T/\kappa$ , where S is the Seebeck coefficient,  $\sigma$  is electrical conductivity, and  $\kappa$  is thermal conductivity. Dilute bismuthides are attractive candidates for thermoelectric for several reasons: (1) bismuth is heavy and therefore likely to decrease thermal conductivity, (2) bandgap narrowing and good electronic transport properties allow improvements in  $S^2\sigma$ , and (3) these materials are compatible with the int roduction of nanostructure to further optimize thermoelectric properties.

Using MBE, we have grown InGaBiAs on InP substrates and measured structural, electronic, and optical properties. We are currently studying thermoelectric properties. We have found that growth of bismuthides on InP requires low substrate temperature and nearly stoichiometric conditions, in good agreement with the larger body of GaBiAs work. We have found that incorporation of bismuth reduces bandgaps as expected and modeled this successfully using the valence band anti-crossing (VBAC) model. We have found high electron mobility and modest carrier concentration in unintentionally-doped bismuthide materials and are studying the effects of doping on these materials. Preliminary results confirm the potential of these materials to improve thermoelectric performance.

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# MAPS



