Calculation of miniband structure in strain-balanced type-II GaAsBi/GaAsN superlattice

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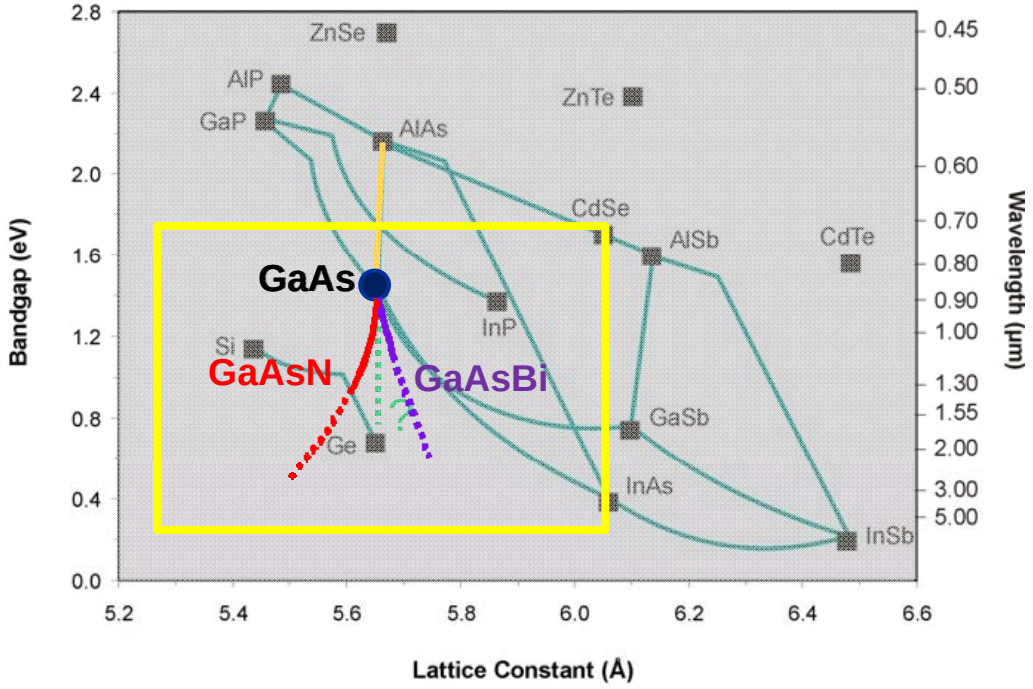
Outline

- **Motivations for GaAsBi/GaAsN Type-II SLS**
- **Study Objectives**
- **Calculation Methodology**
  - Strain-Balanced Criteria
  - Band alignment and Strain effect
  - Schrödinger – Poisson Self-Consistent Equation
- **Results**
- **Future work**
- **Conclusion**

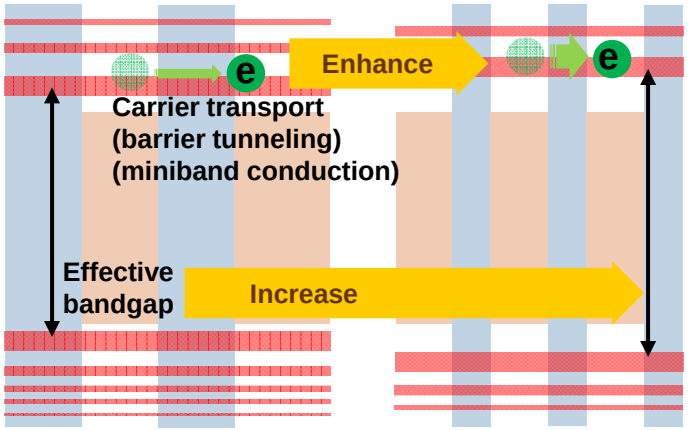
Motivations for GaAsBi/GaAsN

- **Desire narrow bandgap material with effective lattice match to GaAs**
  - Key for low-cost GaAs technology
  - Particularly important for optoelectronic devices such as detectors where thick active regions required
  - Lasers
  - Photodetectors
  - Solar Cells

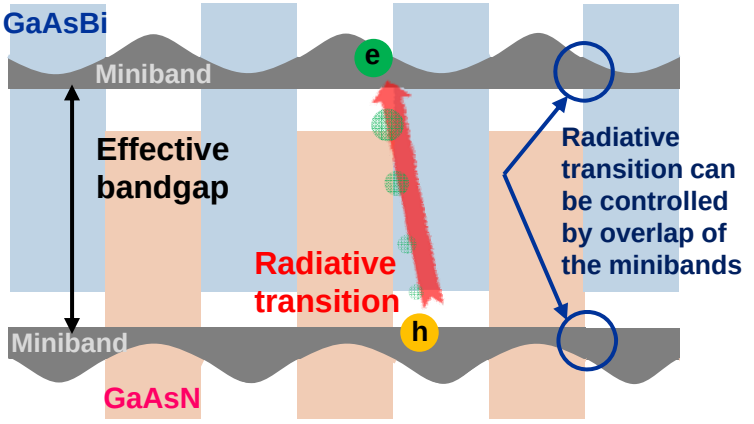


Motivations for Type-II SLS

- **Advantages of superlattices – Bandstructure engineering**
  - Effective bandgap
  - Electronic transport
  - Controlled by layer thickness



- **Advantages of GaAsBi/GaAsN Type-II superlattice**
  - Effective lattice match to GaAs
  - Minibands in conduction/valence band can be independently controlled
  - Radiative transitions (lifetime, absorption) can be controlled



Study Objectives

- **Develop method for calculating electronic structure**
- **Determine range of transition energies for SLS**
  - Strain balanced structures
  - “Reasonable” Bi and N content (up to 5% Bi and N composition)
  - Varying thickness for GaAsBi, GaAsN layers
- **Initial objective to determine criteria to achieve “1 eV” material for photovoltaics**

Simulation Methodology

1 Strain-balanced Criteria

- Determine precondition of concentrations of Bi and N using the strain-balanced criteria on a GaAs substrate

2 Band alignment of GaAsBi/GaAsN superlattice

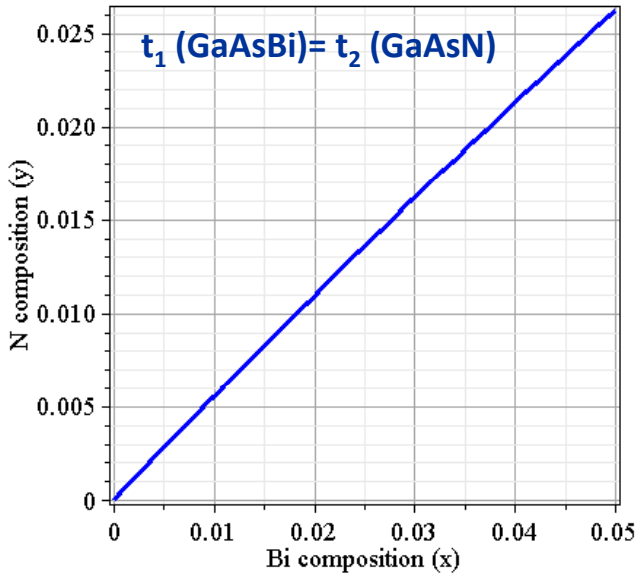
- Obtain band edge discontinuity of the heterostructure based on GaAsBi and GaAsN band alignment
- Consider strain effect due to lattice mismatch

3 Miniband calculation using Schrödinger – Poisson equation

- Simulate energy states in the superlattice using self consistent Schrödinger – Poisson equation
- Transfer matrix algorithm used to solve Schrödinger equation

Strain-Balanced SLS

- **Strain - balanced criteria on GaAs substrate**
  - Balancing compressive strain (GaAsBi) and tensile strain (GaAsN)
  - Condition of zero average in-plane stress[1]



$$\frac{\partial U_{av}}{\partial \epsilon_1} = \frac{2}{t_1 + t_2}\left(t_1 A_1 \epsilon_1 + t_2 A_2 \epsilon_2 \frac{a_1}{a_2}\right) = 0$$

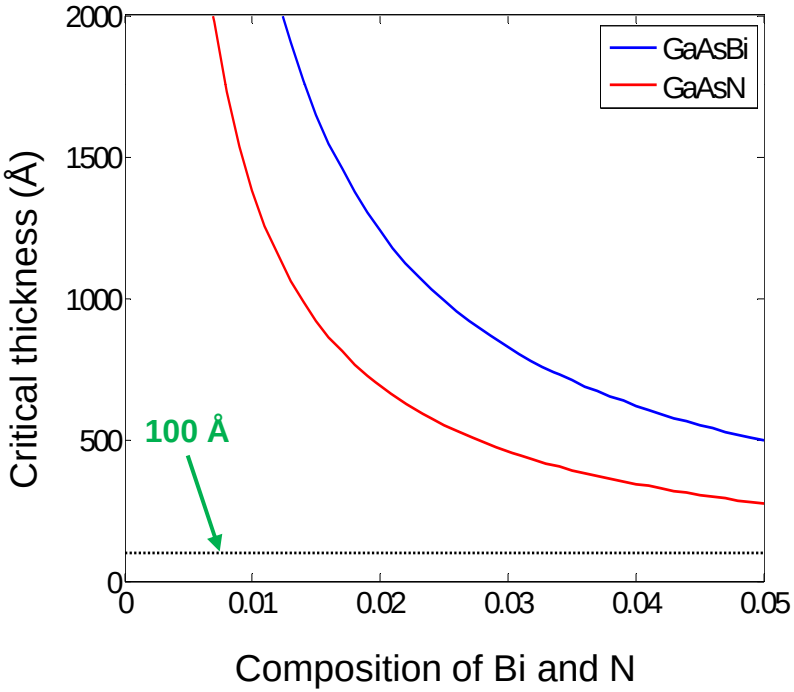
Results: $GaAs_{1-x}Bi_x$ / $GaAs_{1-y}N_y$

Bi (x)	N (y)
0.01	0.006
0.02	0.011
0.03	0.017
0.04	0.022
0.05	0.028

[1] N. J. Ekins-Daukes, K. Kawaguchi, and J. Zhang, Crystal Growth & Design **2**, 287 (2002)

Strain-Balanced SLS

- **Critical thickness of GaAsBi and GaAsN on GaAs substrate**

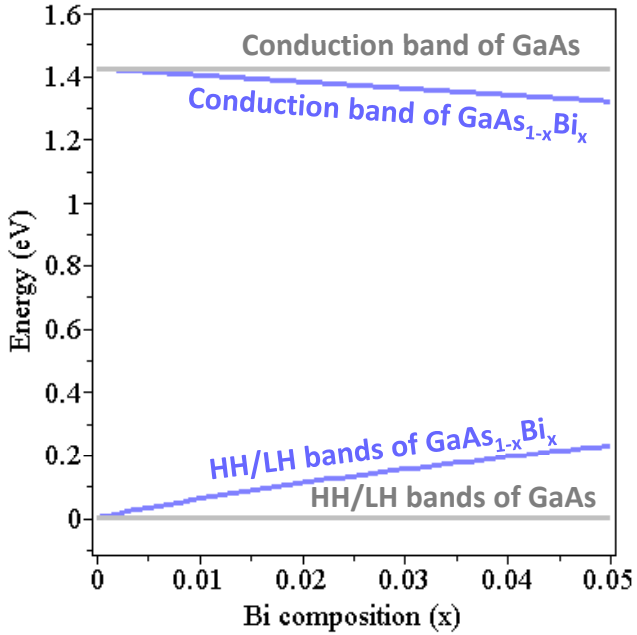


$$d_c \cong \frac{a_s}{2|\epsilon|}$$

Band alignment – Bi, N alloys

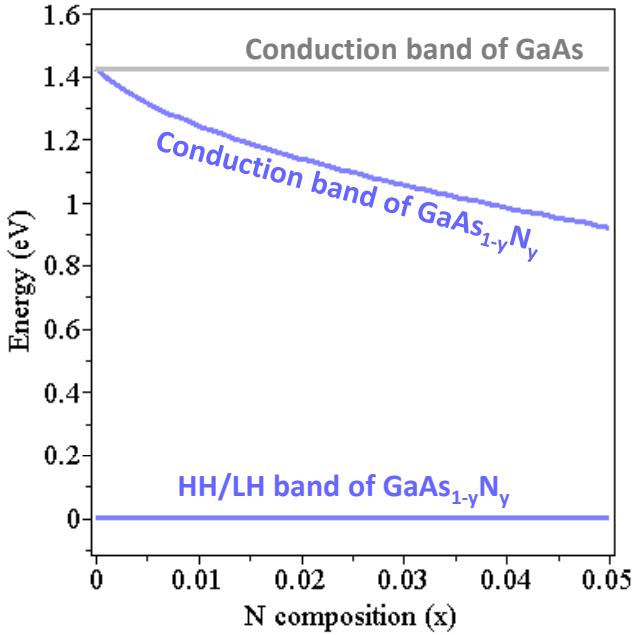
GaAsBi

- **Conduction and Valence band alignment[2]**



GaAsN

- **Conduction and Valence band alignment[3]**

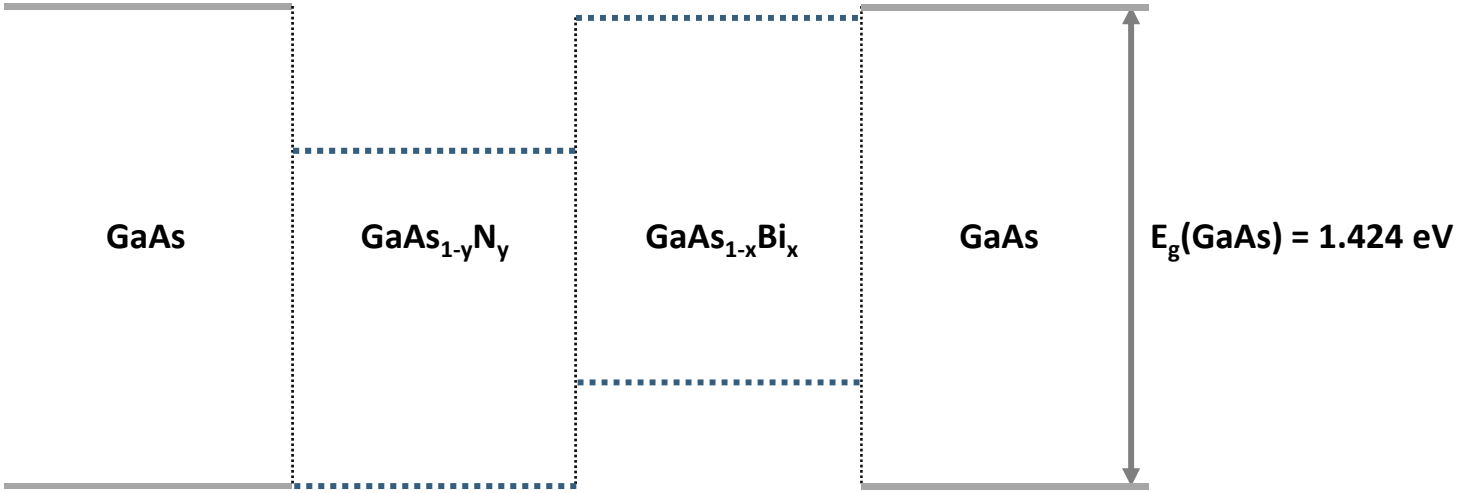


[2] K. Alberi, J. Wu, W. Walukiewicz, K. M. Yu, O. D. Dubon, S. P. Watkins, C. X. Wang, X. Liu, Y. –J. Cho, and J. Furdyna, Phys. Rev. B. 75, 45203 (2007)

[3] W. Shan, W. Walukiewicz, K. M. Yu, J. W. Ager III, E. E. Haller, J. F. Geisz, D. J. Friedman, J. M. Olson, S. R. Kurtz, H. P. Xin, and C. W. Tu, Phys. Stat. Sol 223, 75 (2001)

Band alignment- Bi, N Alloys

- **General Band alignment of $GaAs_{1-x}Bi_x$ (x=0~0.05) , $GaAs_{1-y}N_y$ (y=0~0.05), and GaAs**



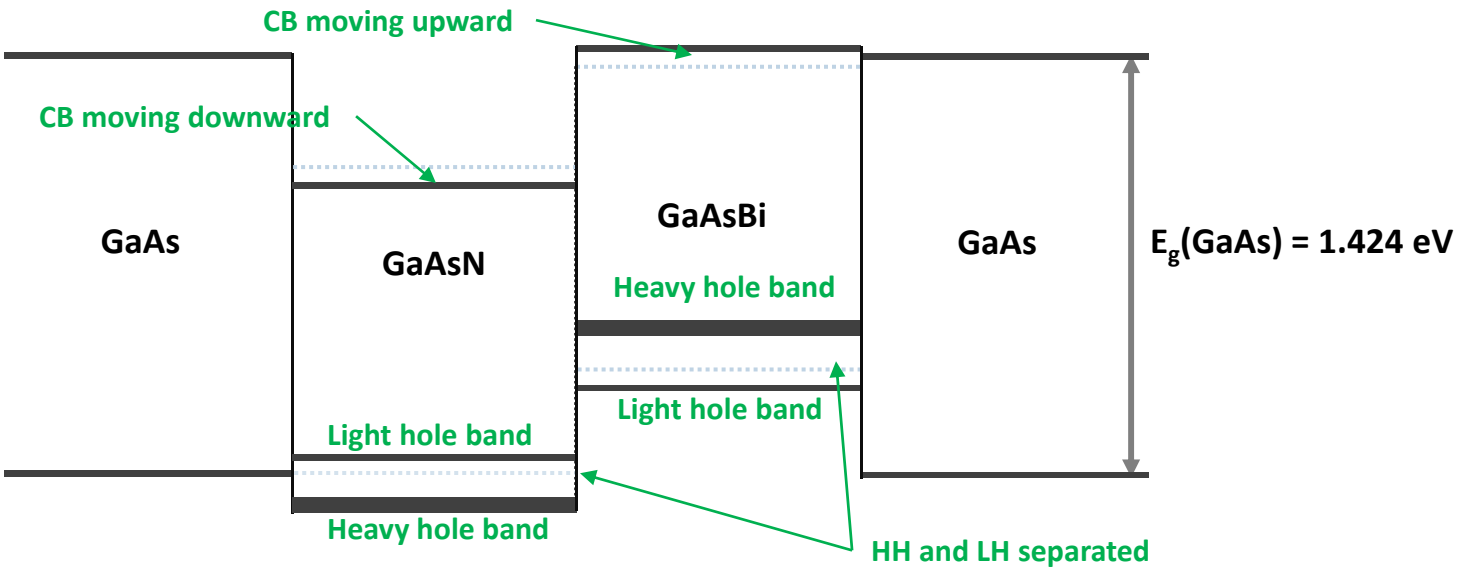
Band alignment - Strain effect

Strain effect on band alignment

- GaAsBi: Compressive strain / GaAsN: Tensile strain
- Pseudomorphically grown on a (100)-oriented substrate

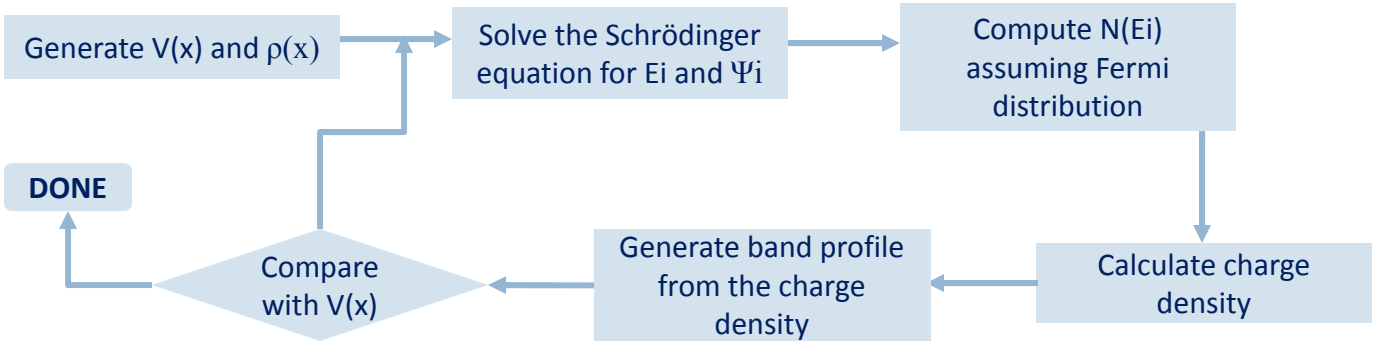
$$\mathbf{E_{C-HH}(k=0)} = \mathbf{E_g} + a(\epsilon_{xx} + \epsilon_{yy} + \epsilon_{zz}) - (b/2)(\epsilon_{xx} + \epsilon_{yy} - 2\epsilon_{zz})$$

$$\mathbf{E_{C-LH}(k=0)} = \mathbf{E_g} + a(\epsilon_{xx} + \epsilon_{yy} + \epsilon_{zz}) + (b/2)(\epsilon_{xx} + \epsilon_{yy} - 2\epsilon_{zz}) \qquad a = a_c - a_v$$



Electronic Structure Calculation

- **Coupled Schrödinger – Poisson Equation[4]**

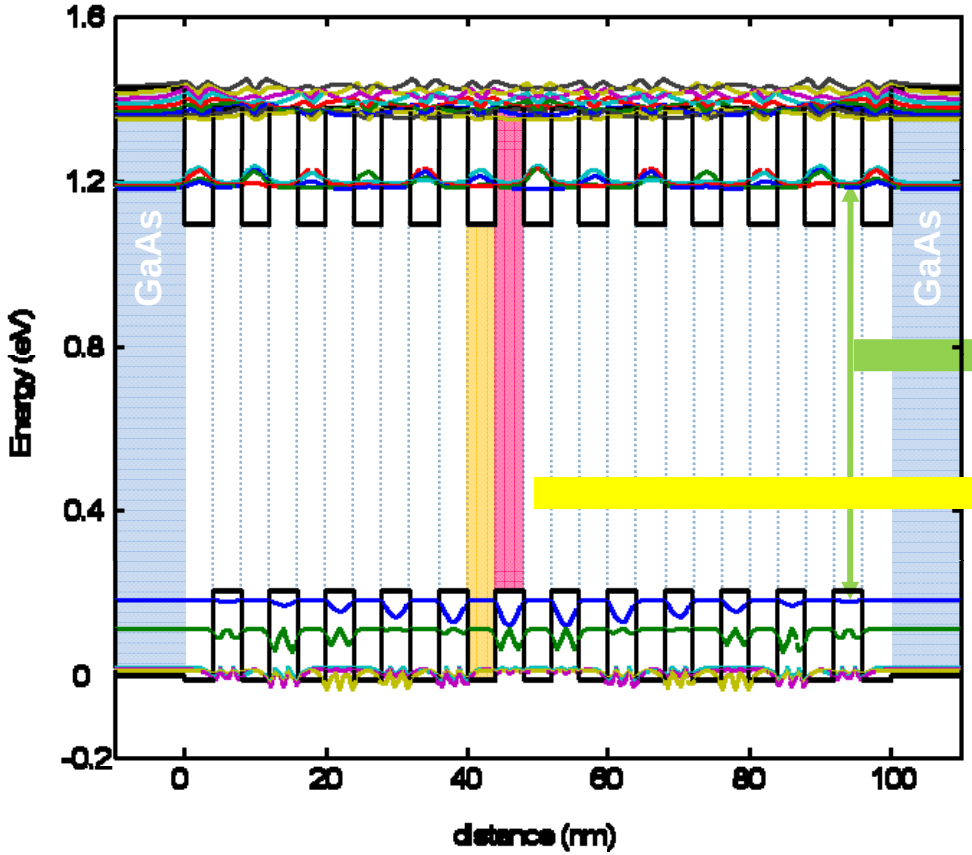


- **Solving Schrödinger equation**
  - Calculate subband structure in the superlattice
  - Transfer matrix approach[5] used

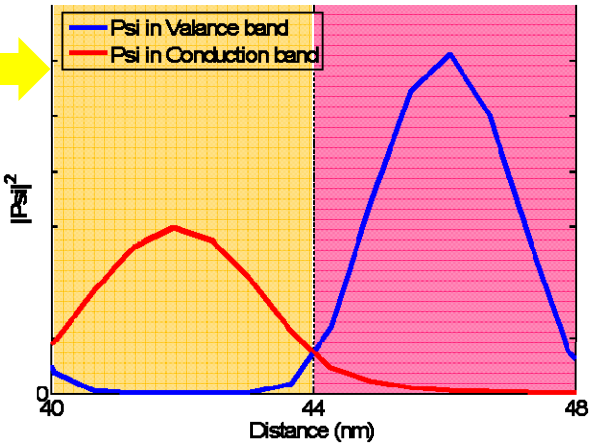
[4] C. H. Fischer IV, Ph.D. dissertation. University of Michigan (2004)
[5] E. Anemogiannis, E. N. Glytsis, and T. K. Gaylord, IEEE Journal of Quantum Electronics 29, 2731 (1993)

Miniband structure of SLS

- **Miniband of $GaAs_{0.96}Bi_{0.04}$ / $GaAs_{0.979}N_{0.021}$**



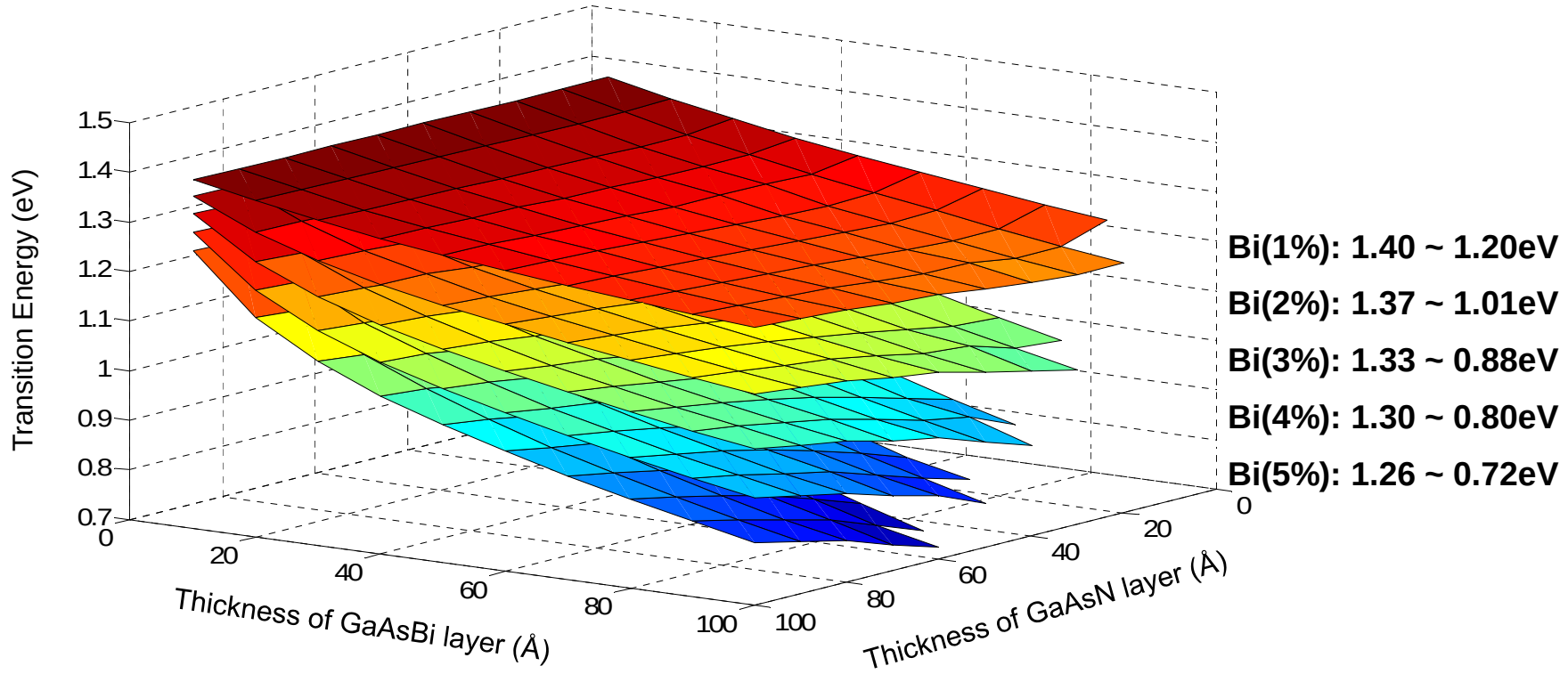
Layer thickness	
$GaAs_{0.96}Bi_{0.04}$	40 Å
$GaAs_{0.979}N_{0.021}$	40 Å
# of layers	25
Total thickness of SLS	100nm
Effective band gap	1.0011 eV



Transition energy of SLS

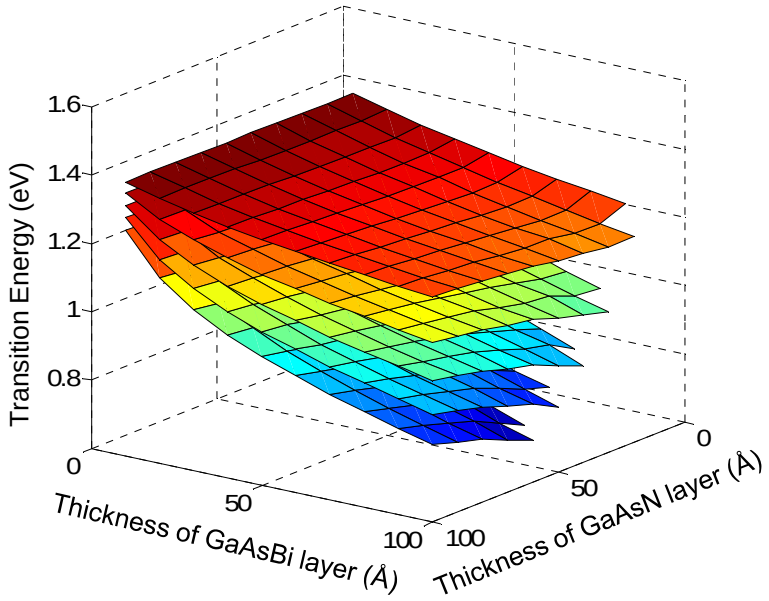
- **Transition energy range for different Bi composition**

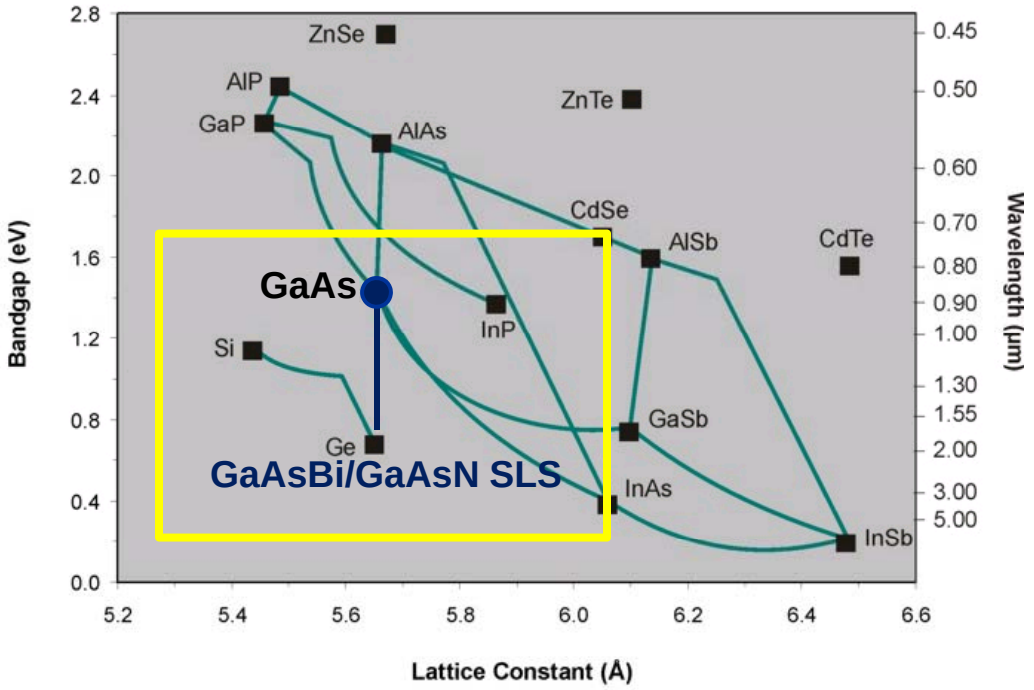
Composition of Bi and N: 0 ~ 5%



Transition energy of SLS

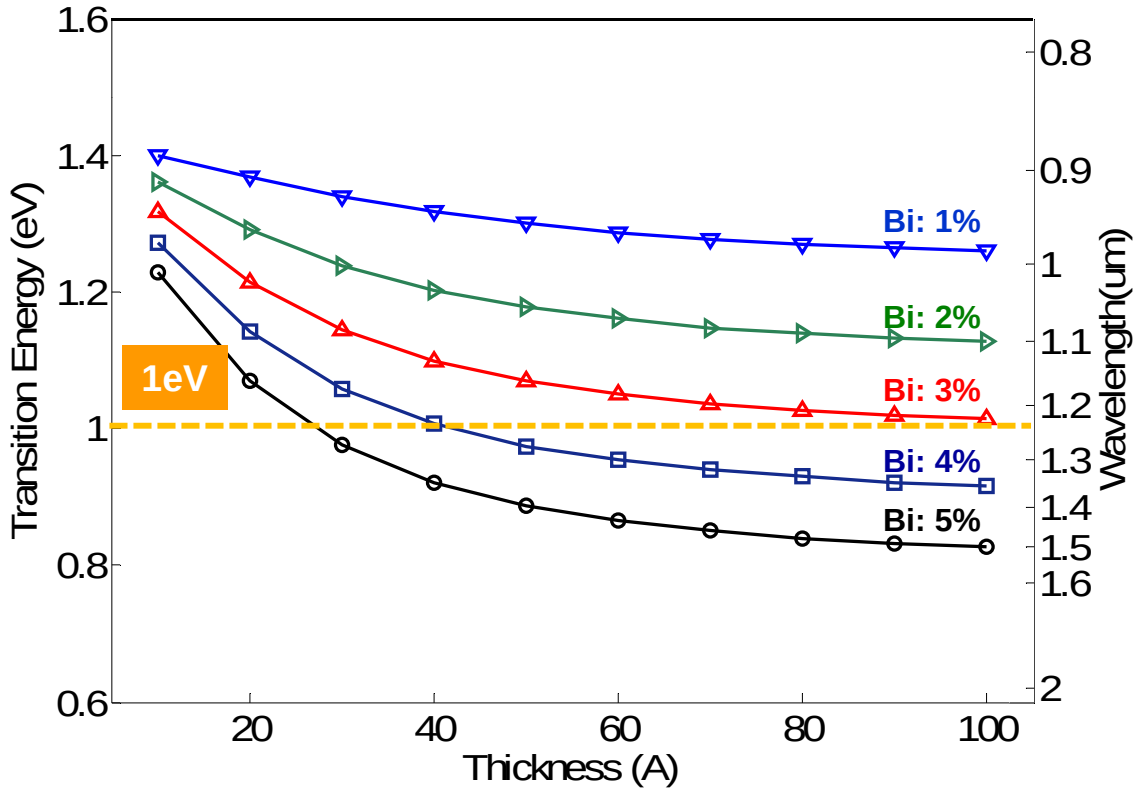
- **Transition energy range for different Bi composition**





Results

- **Thickness of individual layer vs. transition energy with different N and Bi composition ($t_{1,GaAsBi} = t_{2,GaAsN}$)**



Future work

- **Carrier transport simulation**
  - Tunneling probability
  - Carrier scattering probability via Monte-Carlo simulation
  - Determine electron transport in vertical and lateral directions
- **Radiative transitions**
  - Wavefunction overlap
  - Optical absorption/recombination lifetimes
- **Compare with experimental data**
  - Material parameters, band offsets, etc, used in simulation
  - Experimental SLS structures

Conlclusions

- **Electronic structure of GaAsBi/GaAsN superlattices were calculated for varying layer thickness and alloy composition**
- **GaAsBi/GaAsN superlattices offer a wide range of effective bandgap energy (~0.7 – 1.4 eV) for strain-balanced structures on GaAs**
- **Attractive for variety of optoelectronic devices, and need further experimental and theoretical research efforts**

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