Novel Lattice-matched ε-Ge, GeSn/InAl(Ga)As Heterostructures for Optoelectronics by MBE

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5^{th} Tri-Service Workshop on GeSn and GeSiSn

Ack: NSF **ECCS-2042079**

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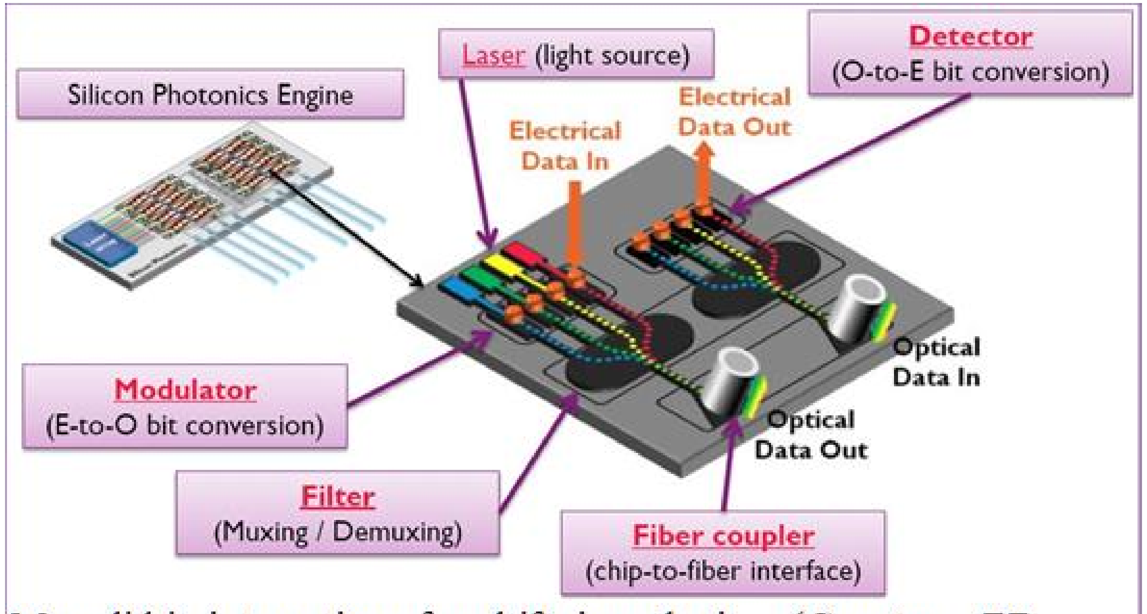
*Views expressed herein do not necessarily represent the views of the U.S. Department of Energy or the United States Government

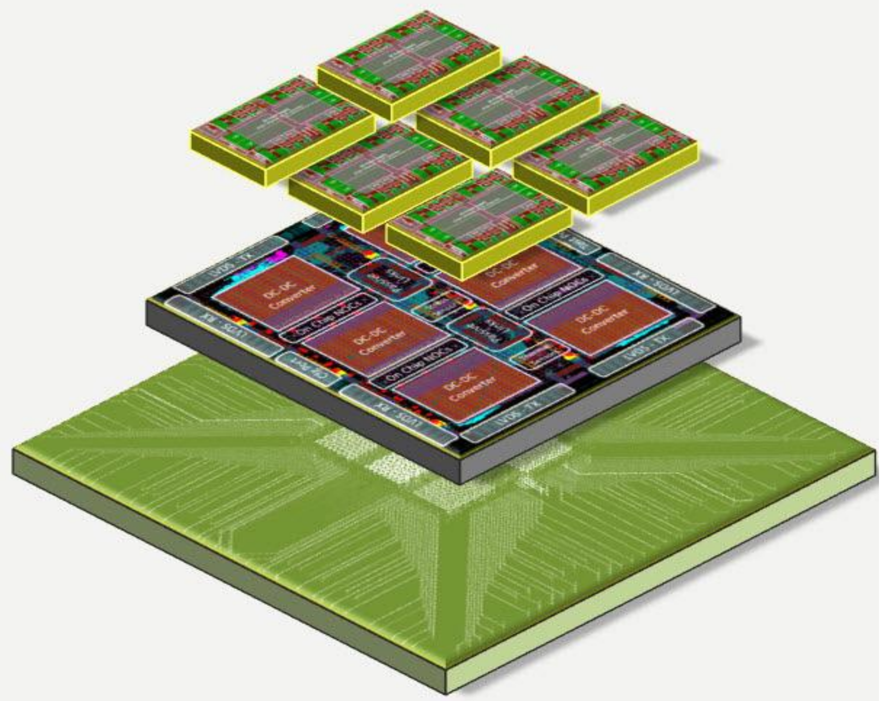
Outline

- Objective
- Epitaxial Tensile strain Ge (ε-Ge) and GeSn Material Synthesis by MBE
- Material Analysis
  - Crystallinity →HR-XRD and Reciprocal Space Maps
  - Defects properties → Cross-sectional TEM and PV-TEM
  - Minority carrier lifetime → μ–PCD Technique
- X–ray photoelectron spectroscopy (XPS) analysis
  - Energy band alignment
  - Band offset: Atomic Interdiffusion and Benchmarking
- Summary

Group-IV based Integrated Optoelectronic System



Monolithic integration of multifarious devices (*Courtesy: EE Times, October 15, 2013*).

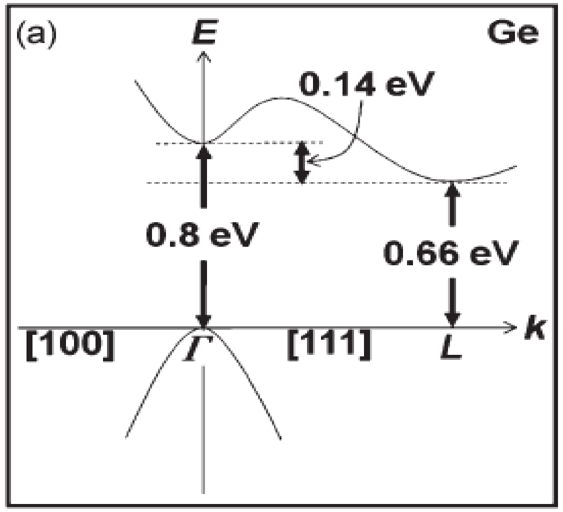


Courtesy CEA-Leti

Heterogeneous IC integration

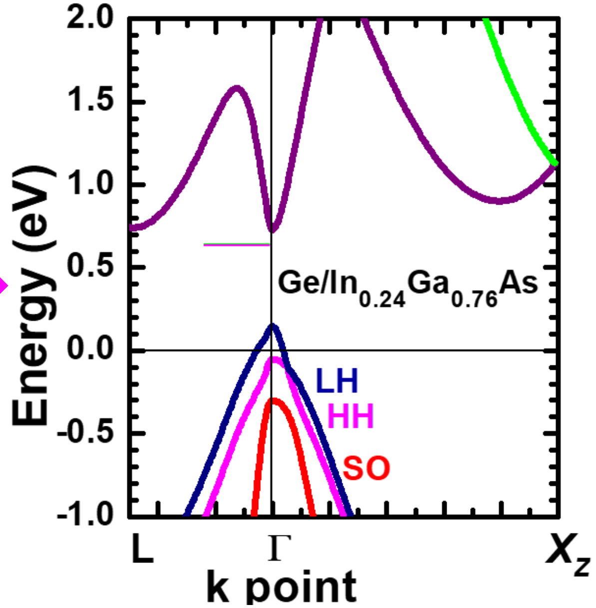
- Aims to achieve **Group-IV** based devices compatible to Si photonics

Approaches to Make Indirect →Direct Bandgap!



K.-H. Kao *et al.*, *TED*, **59**, 2012

❶



M. K. Hudait *et al.*, *ACS AEM*, 2021, **3**, 4535–4547

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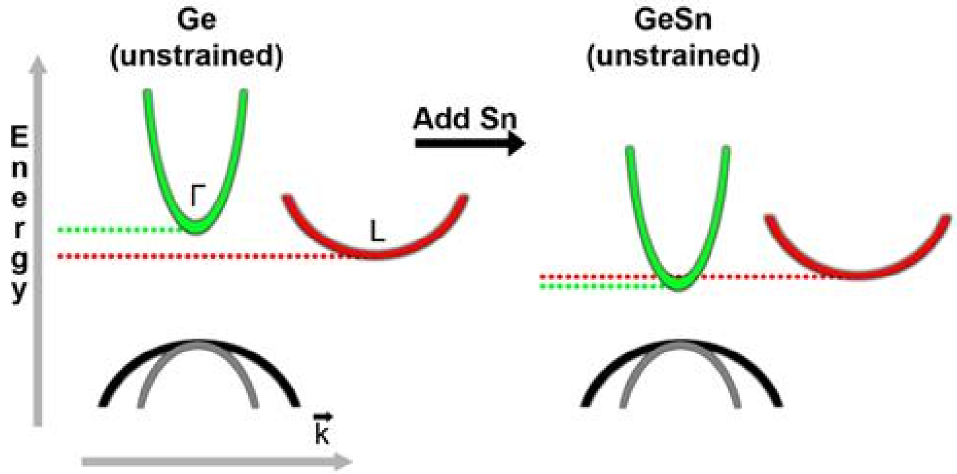

Ge alloyed with α-Sn

R.Chen *et al.*, *Nano Lett.*, 2014, **14**, 37-43.

Indirect Bandgap:

- Phononic interactions
- Auger recombination
- Low *IQE*
- High J_{th}

Direct Bandgap:

- ✓ Optical Transitions ↑
- ✓ Detector Responsivity ↑
- ✓ Lasing Threshold Current ↓
- ✓ Mobility ($m_{eff,\Gamma} > m_{eff,L}$) ↑

Tensile Strained Germanium

→ DIRECT at ~1.6% strain

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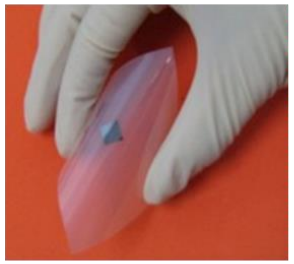
Ge/AlAs/GaAs as-grown by MBE

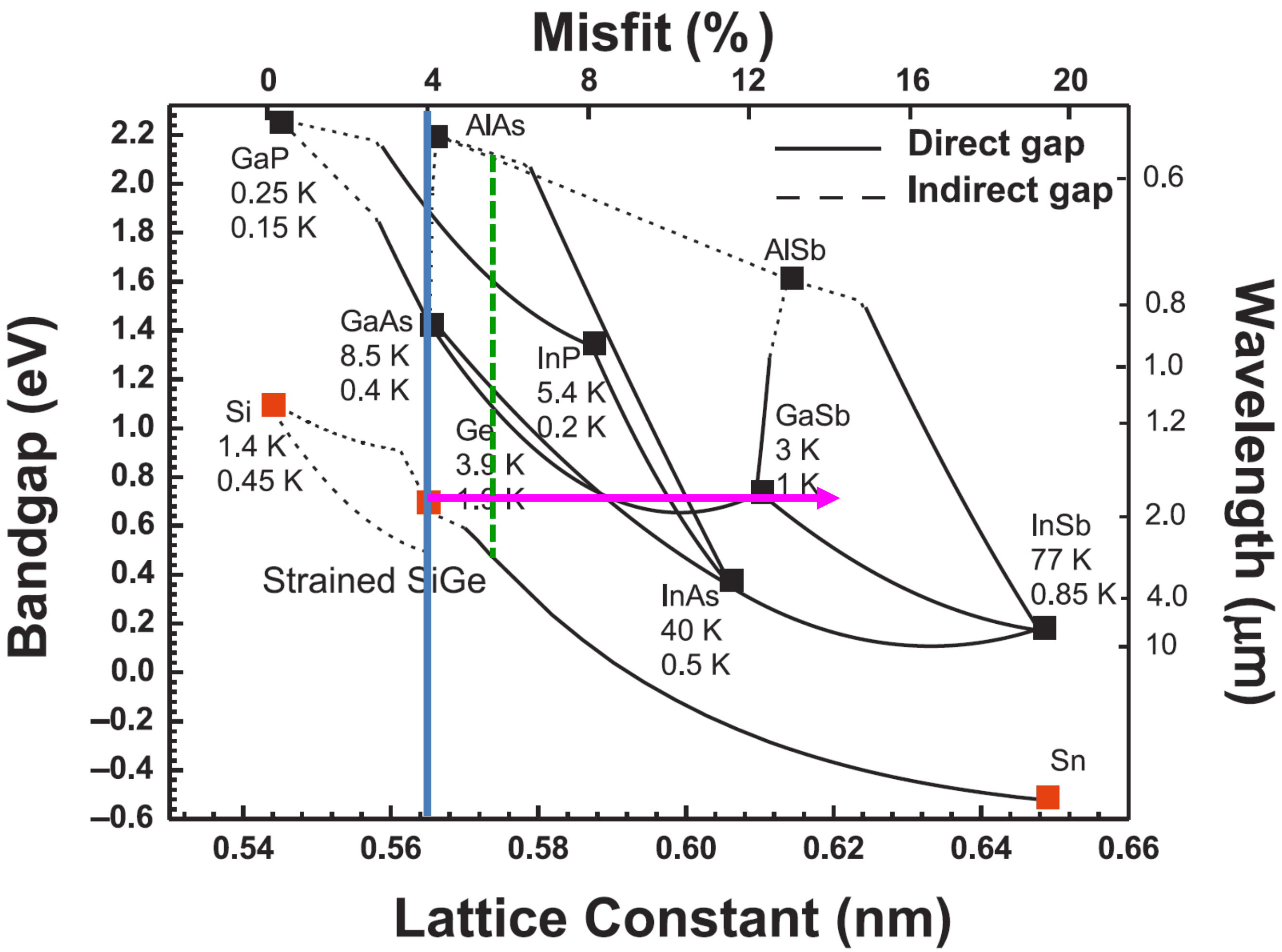


Released **Ge** layer mounted on a Hybridsil® thin film

1µm-thick Si membrane encapsulated in a Hybridsil® thin film

ELO Ge on flexible substrate

Epitaxial ε-Ge and GeSn: Lattice Mismatch Issues



C.W. Liu *et al.*, *MRS*, 2014, **39**, 658.

AlInAs, GaInAs, GaAsSb, GaInP, AlAsSb lattice matched layer options

Challenges:

- ~15% lattice mismatch between Ge and Sn
- Threading Dislocations Density (TDDs)
- Reduced carrier lifetime → affect device performance

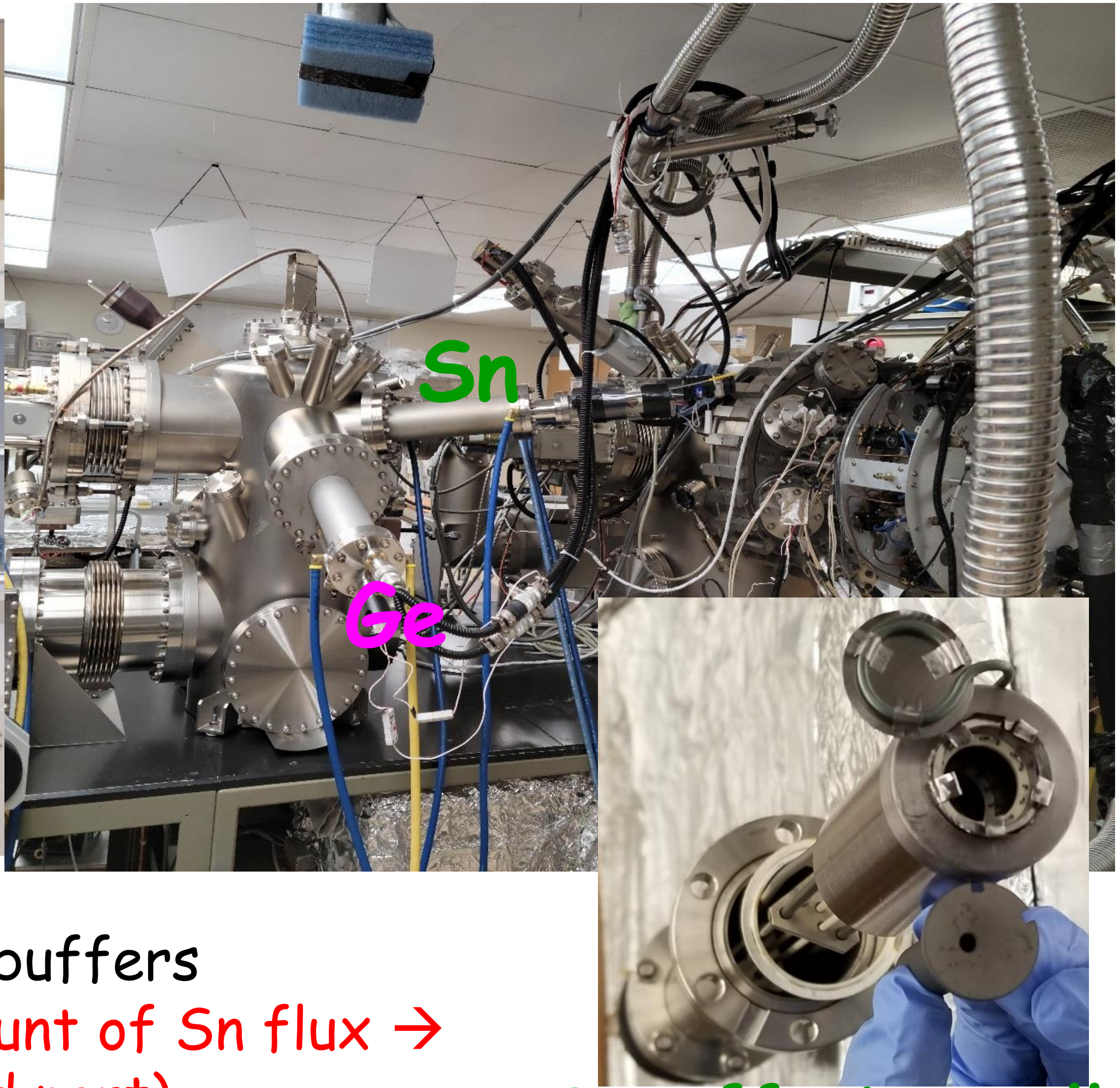
Required defects mitigation approaches:

❶ Lattice matched structure

❷ Pseudomorphic growth

❸ Epitaxial lift-off the device layer

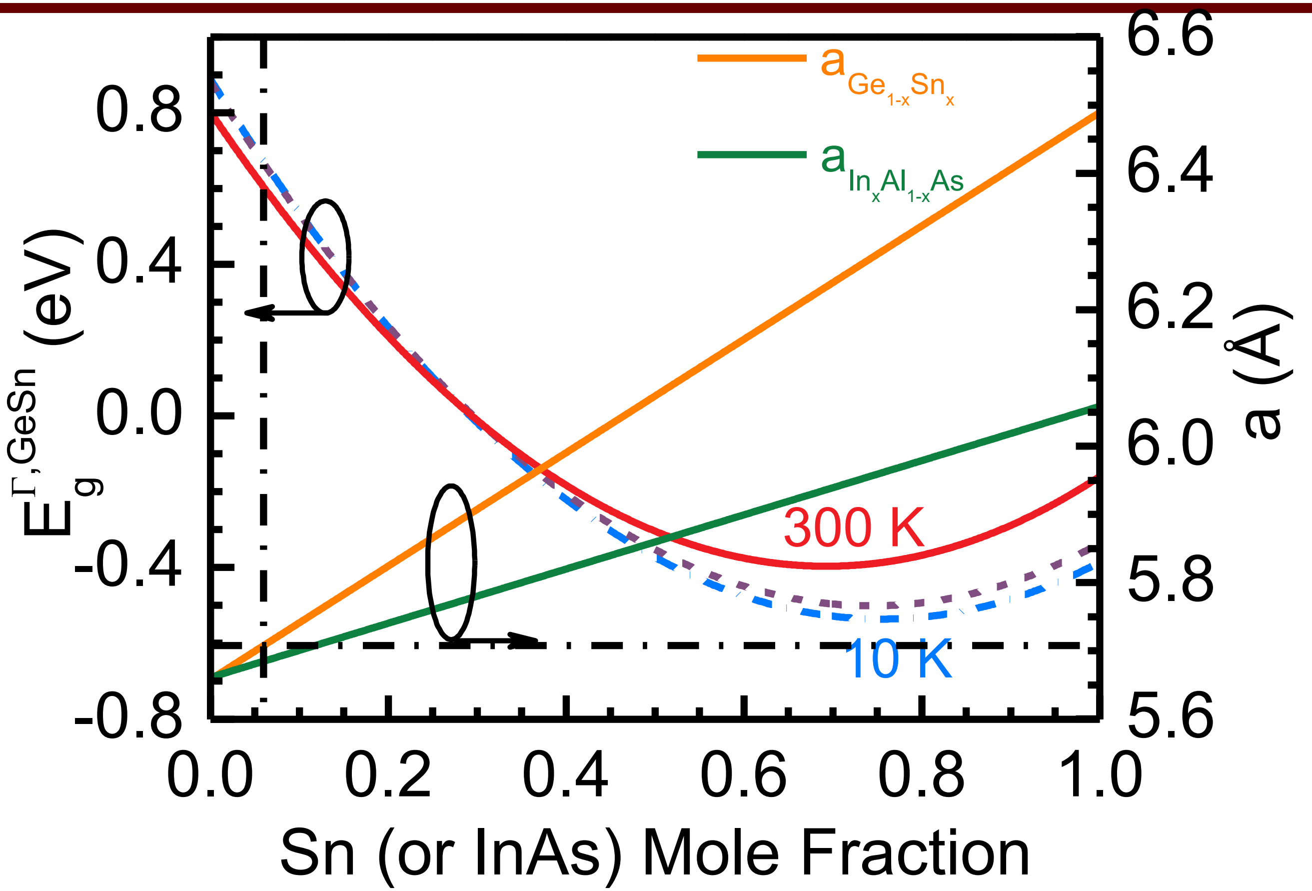
Dual Chamber MBE System for III-V and GeSn



Sn effusion cell

- ❑ No restriction for ε-Ge growth on III-V buffers
- ❑ Shallow angle Sn source restrict the amount of Sn flux → required to mount with Ge source (upward port)

Epitaxial GeSn : Address Lattice Mismatch



- ✓ **AlInAs or GaInAs lattice matched layer to GeSn**
- ✓ **GeSn/InAl(Ga)As heterostructures, *e.g.*, Sn = 12% & In = 24%**

M. K. Hudait *et al.*, *JMC-C*, 2022, **10**, 10530–10540.

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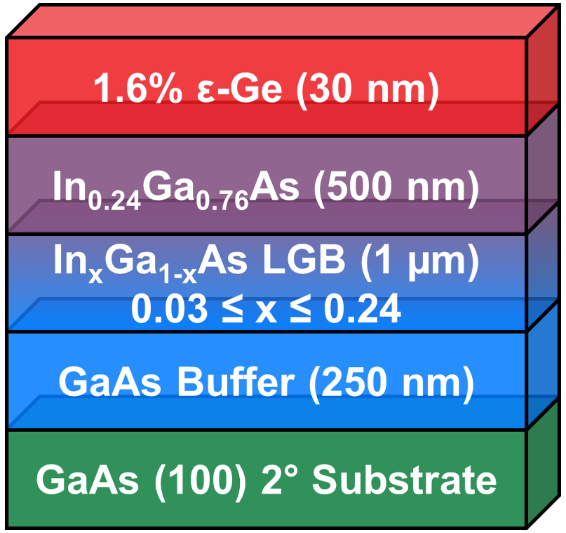
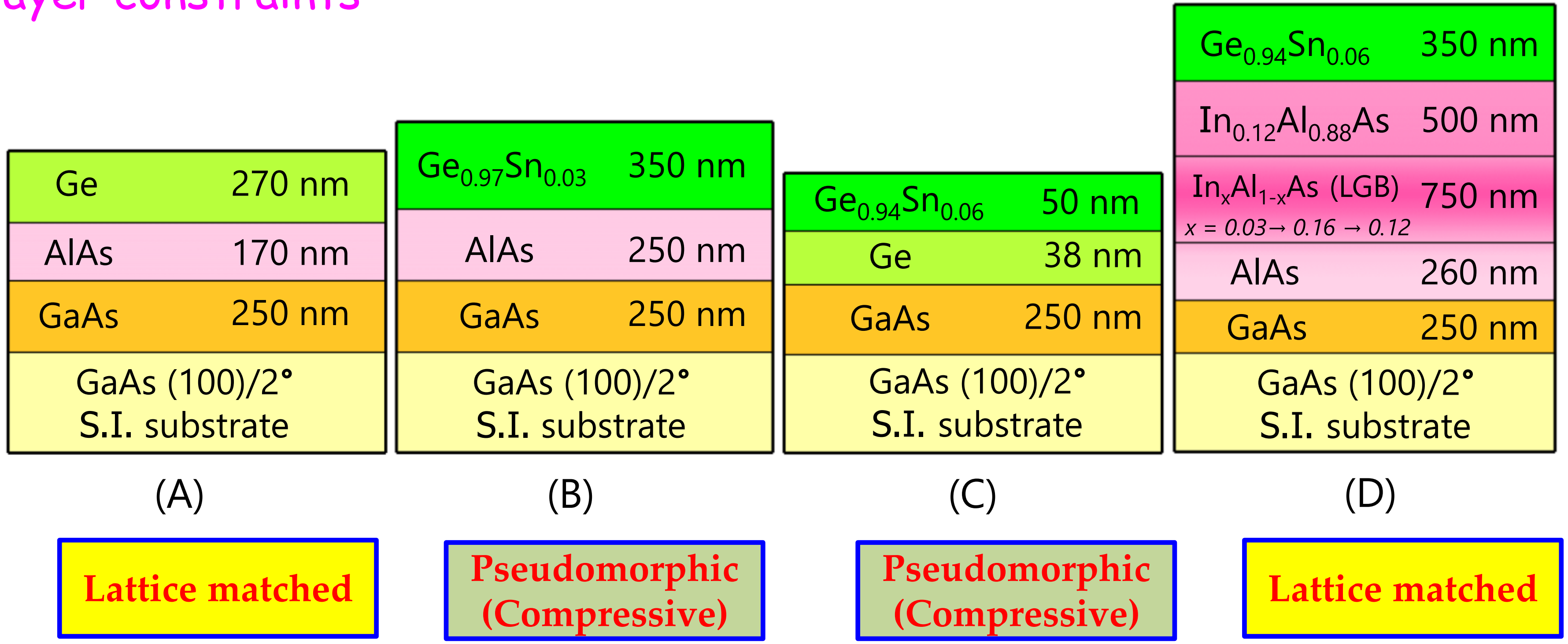
Epitaxial ε-Ge and GeSn Material Synthesis

$Ge_{1-y}Sn_y$ grown on $In_xAl_{1-x}As$

- ☑ Large band offsets
- ☑ Superior confinement
- ☑ Lattice matched (virtually defect-free)
  - No critical layer constraints

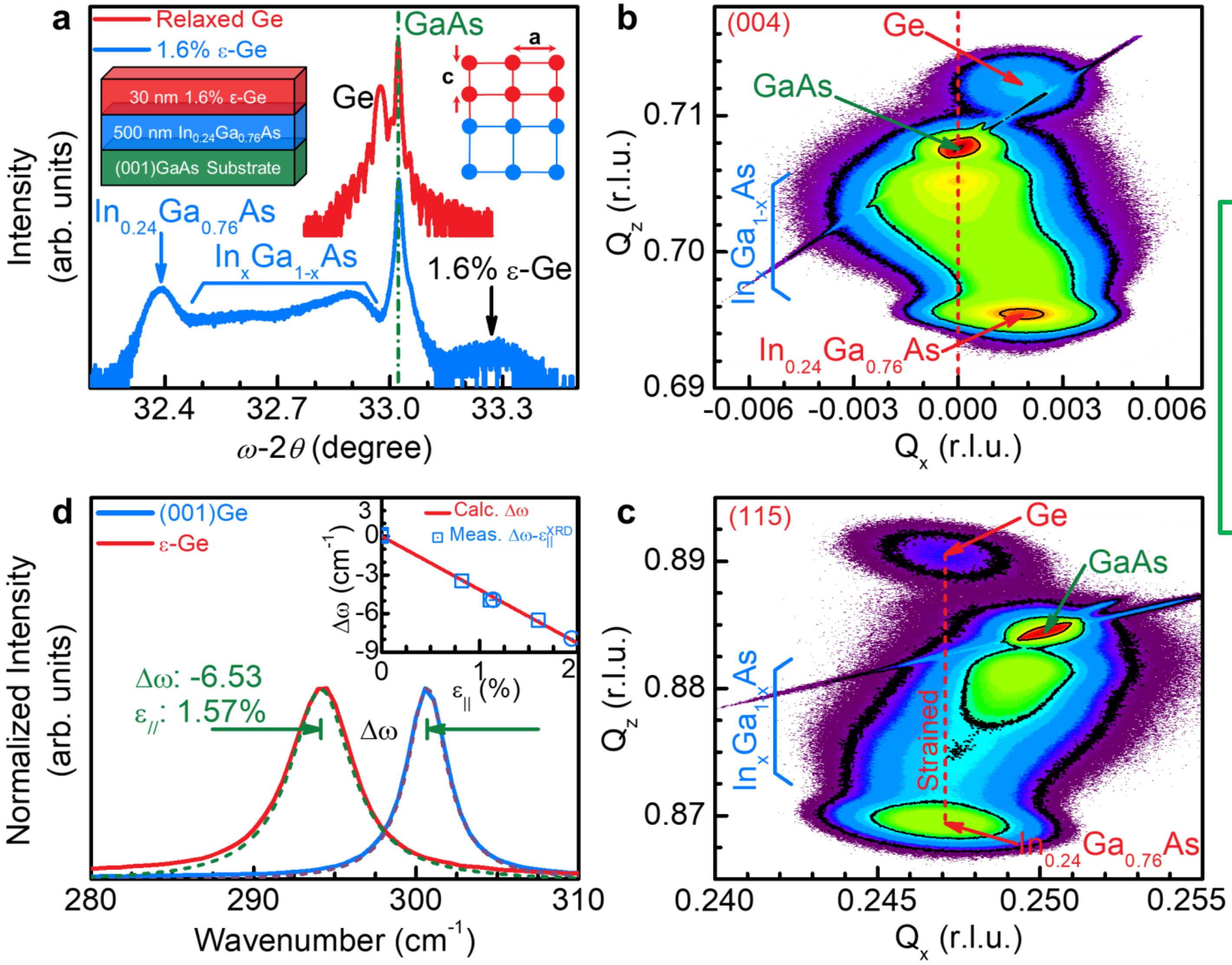


ε-Ge (1.6%)/InGaAs



0-6% Sn in GeSn/In(Al)As

Group−IV Optoelectronics: Epitaxial 1.6% ε-Ge

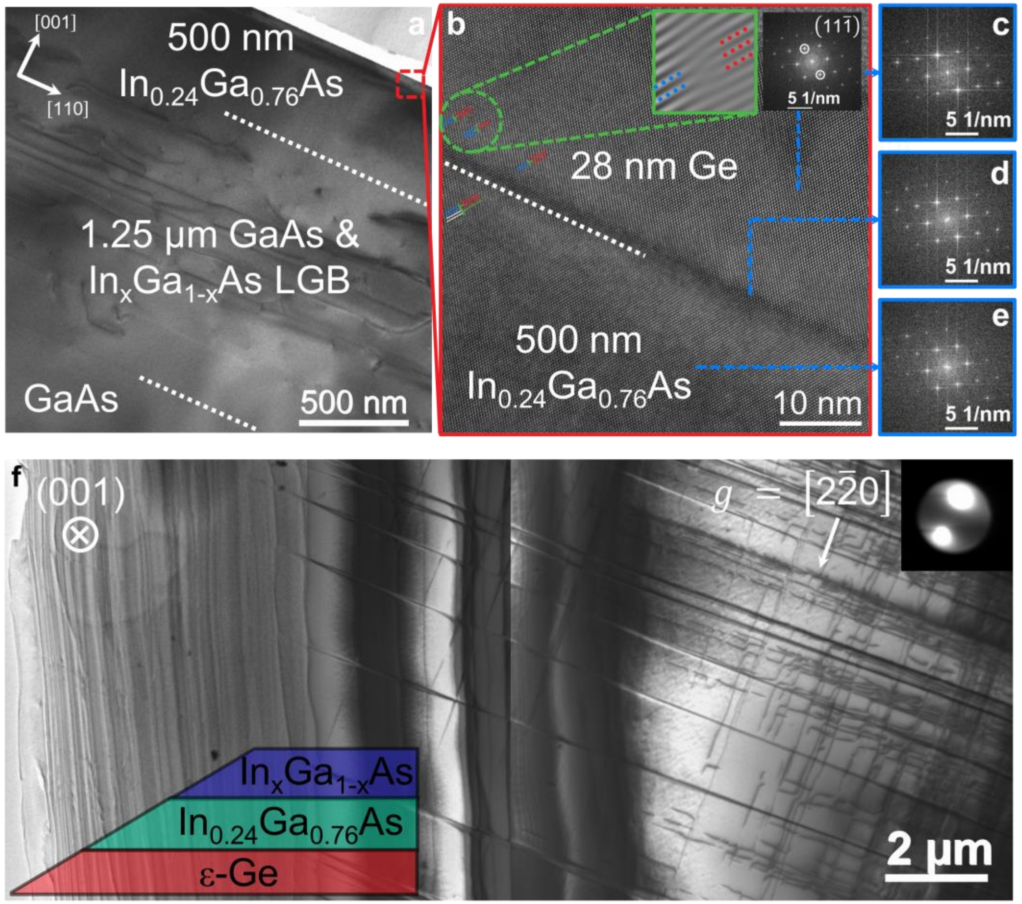


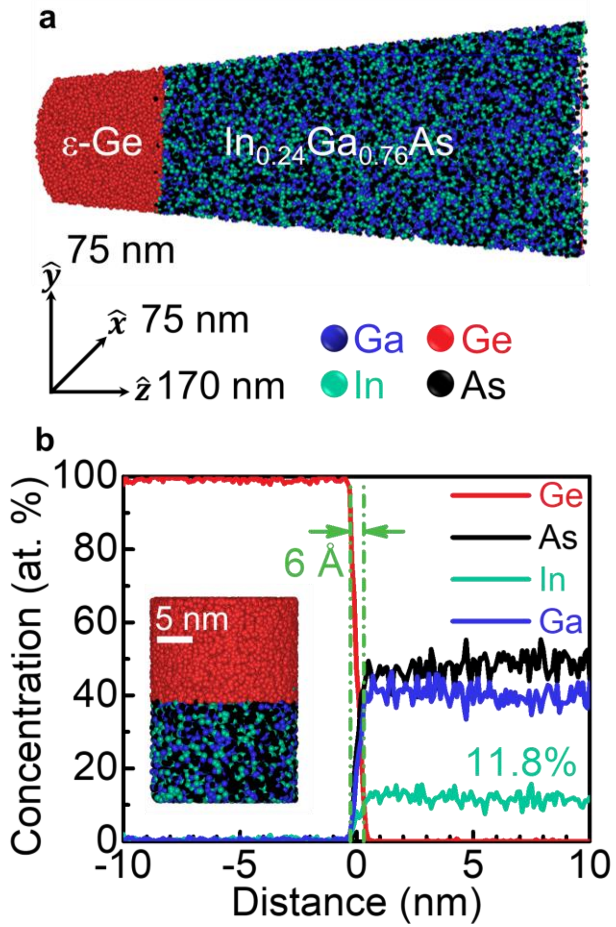
1.6% ε-Ge on $In_{0.24}Ga_{0.76}As$

- ☑ RSMs confirms the ε-Ge
- ☑ X-ray and Raman analysis corroborate each other in strain analysis

M. B. Clavel *et al*, *Phys. Rev. Appl.*, 2022, **18**, 064083-1-12 (December 27th).

Defect Microstructures & Interface Abruptness: Epitaxial 1.6% ε-Ge





☑ Defects are confined within the graded $In_xGa_{1-x}As$ buffer

☑ PV-TEM confirms the "virtually defect-free" ε-Ge layer

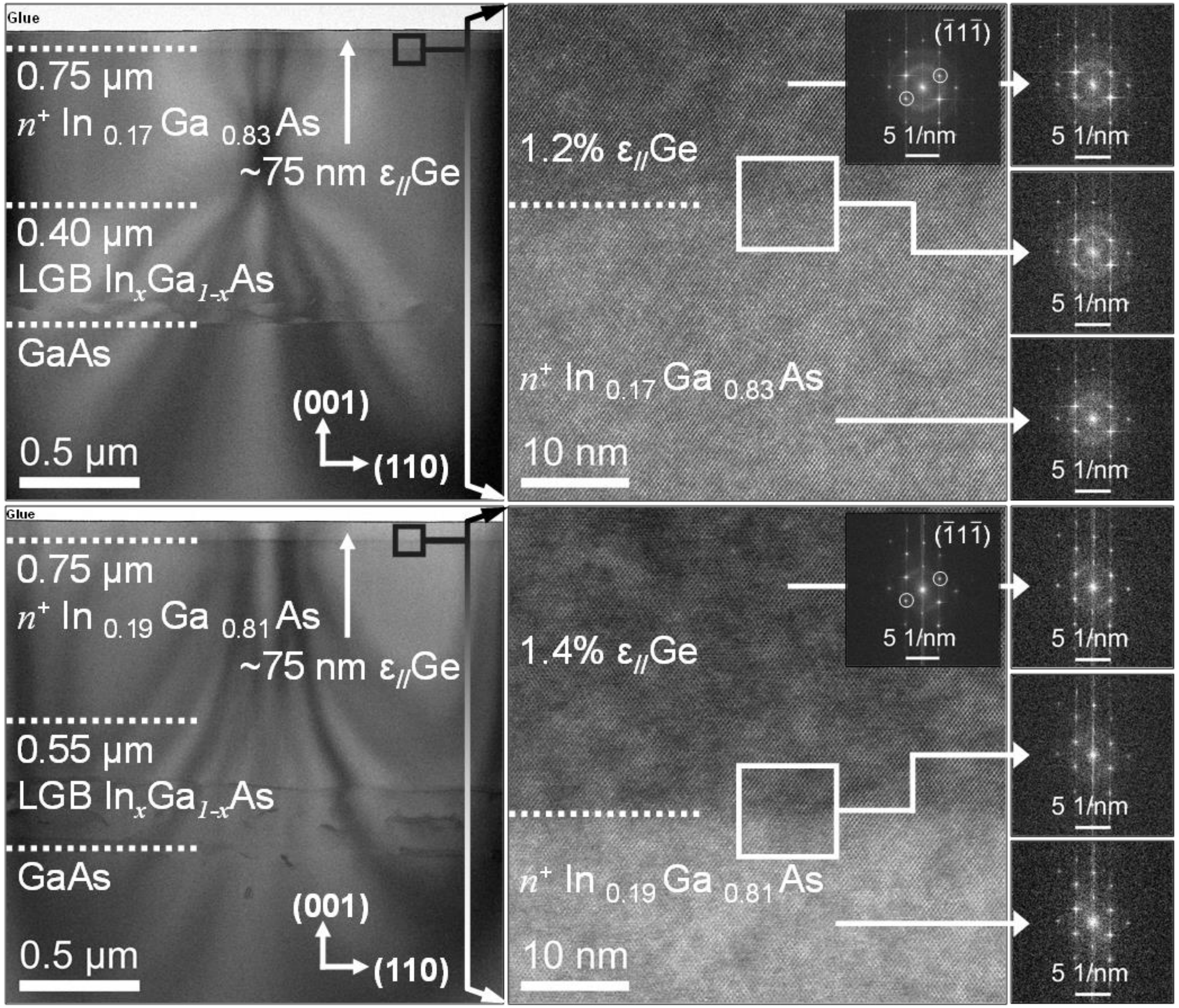
☑ Only 6 A interdiffusion by atom probe tomography

M. B. Clavel *et al*, *Phys. Rev. Appl.*, 2022, **18**, 064083-1-12.

Defect Microstructures : Epitaxial Tunable ε-Ge

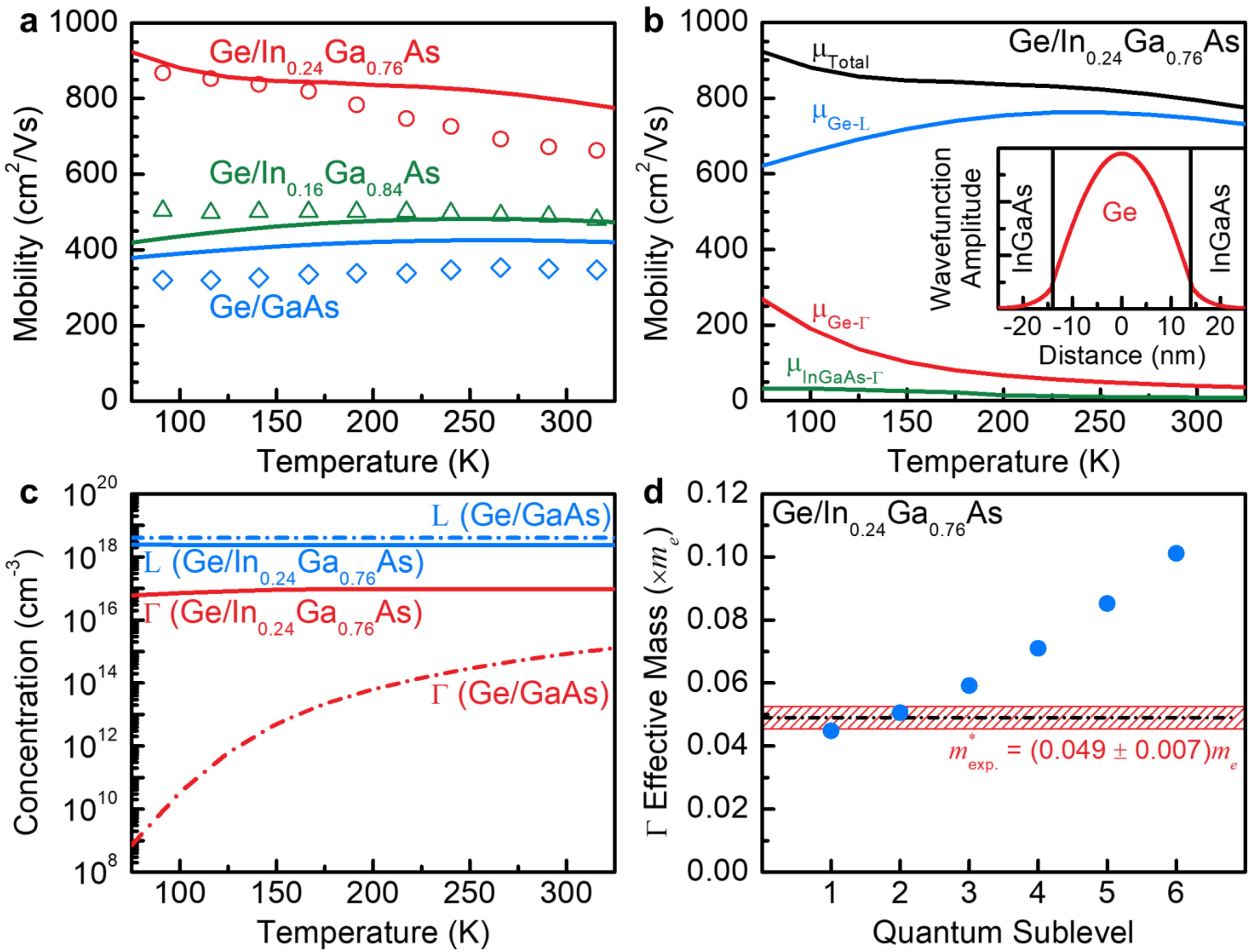
1.2% ε-Ge

1.4% ε-Ge



S. Bhattacharya *et al, ACS Nano (To be submitted, 2023)*

Carrier Transport: Ge and Tunable ε-Ge



1.6% ε-Ge on $In_{0.24}Ga_{0.76}$As

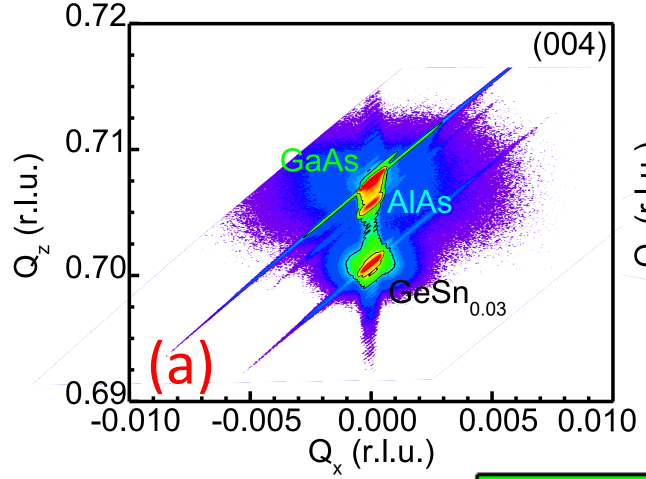
- ☑ 2 × μ_n boost compared to unstrained Ge
- ☑ Increase in mobility of L-valley electrons !!
- ☑ Carriers are confined within the 1.6 % ε-Ge
- ☑ No mobility contribution from underlying $In_{0.24}Ga_{0.76}$As stressor layer
- ☑ Effective mass of 0.049 m_e

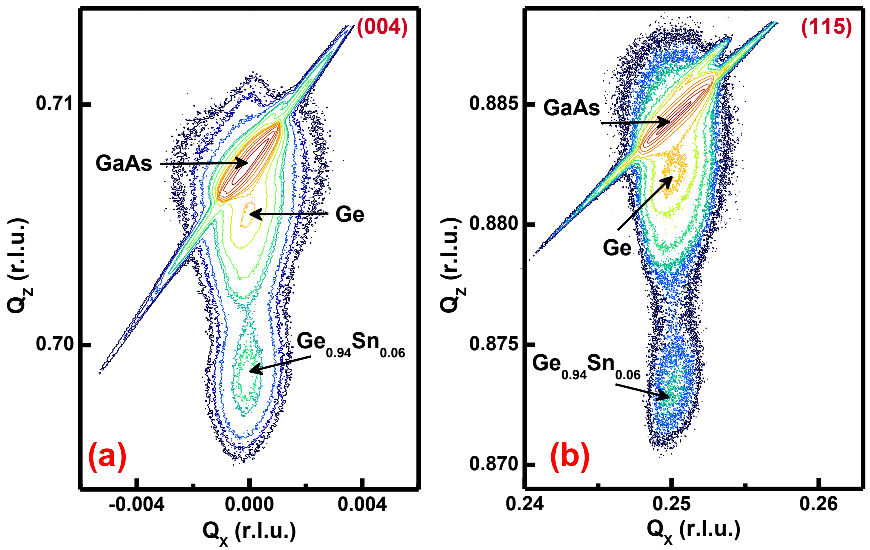
M. B. Clavel *et al*, *Phys. Rev. Appl.* ,2022, **18**, 064083-1-12.

Material Analysis of GeSn: X-ray RSMs

Pseudomorphic (compressive)

Reciprocal Space Maps





$Ge_{0.97}Sn_{0.03}$	350 nm
AlAs	250 nm
GaAs	250 nm
GaAs (100)/2° S.I. substrate	

Sample B

$Ge_{0.94}Sn_{0.06}$	50 nm
Ge	38 nm
GaAs	250 nm
GaAs (100)/2° S.I. substrate	

Sample C

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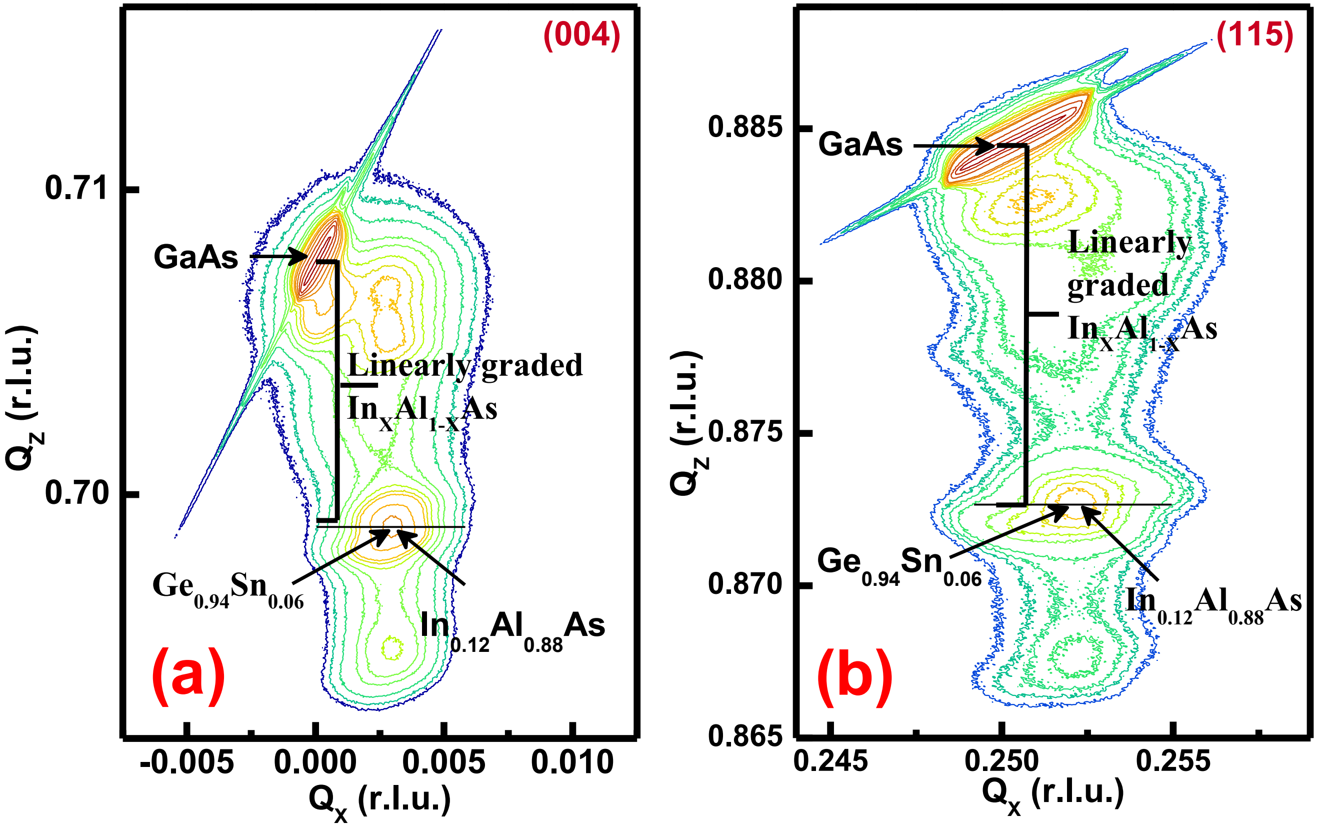
X-ray Analysis of Lattice matched $GeSn_{0.06}/In_{0.12}AlAs$

Lattice matched



$Ge_{0.94}Sn_{0.06}$	350 nm
$In_{0.12}Al_{0.88}As$	500 nm
$In_xAl_{1-x}As$ (LGB) $x = 0.03 \rightarrow 0.16 \rightarrow 0.12$	750 nm
AlAs	260 nm
GaAs	250 nm
GaAs (100)/2° S.I. substrate	

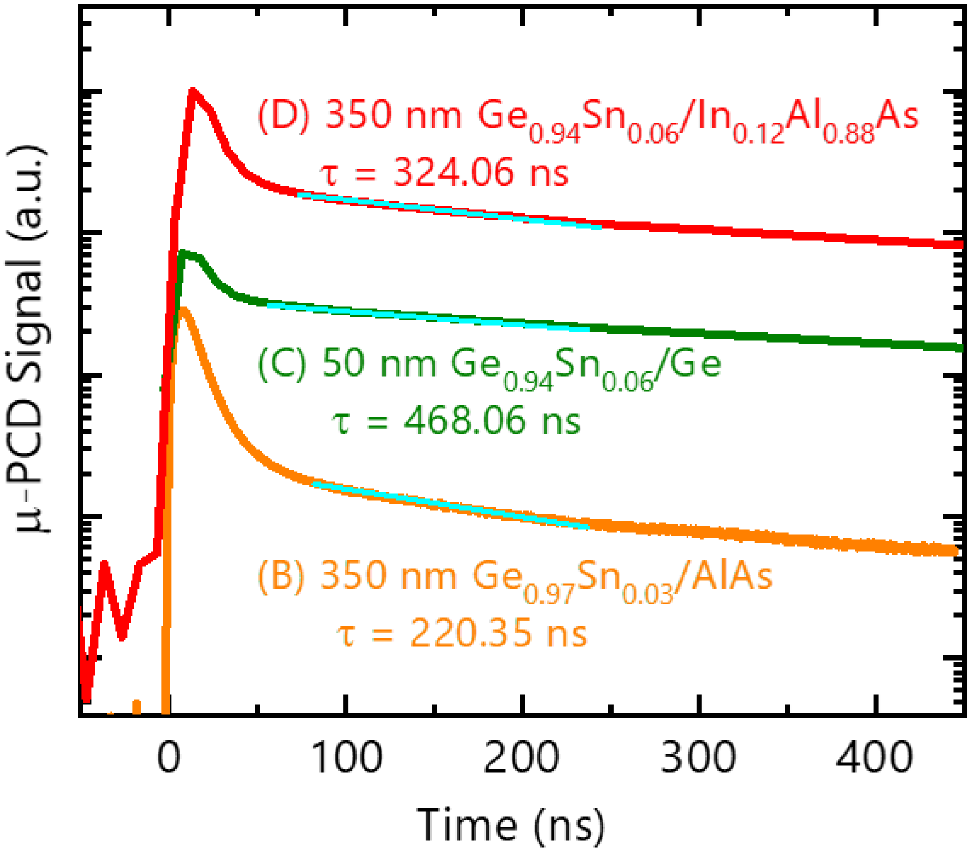
Sample D

- $Ge_{0.94}Sn_{0.06}$ overlapping with $In_{0.12}Al_{0.88}As$
  ↓
  lattice matched
  ($a_{Ge_{0.94}Sn_{0.06}}$ = 5.70786 Å at 300 K)
- Q_z and Q_x symmetricity at $Ge_{0.94}Sn_{0.06}$ shows no or minimal defects.
- $In_xAl_{1-x}As$ linearly graded buffer constraints mismatch induced defects.

Hudait *et al.*, *JMC-C*,2022, **10**, 10530–10540.

Minority Carrier Lifetime of GeSn (0-6% Sn)

Microwave Reflection Photoconductive decay (μ−PCD) technique

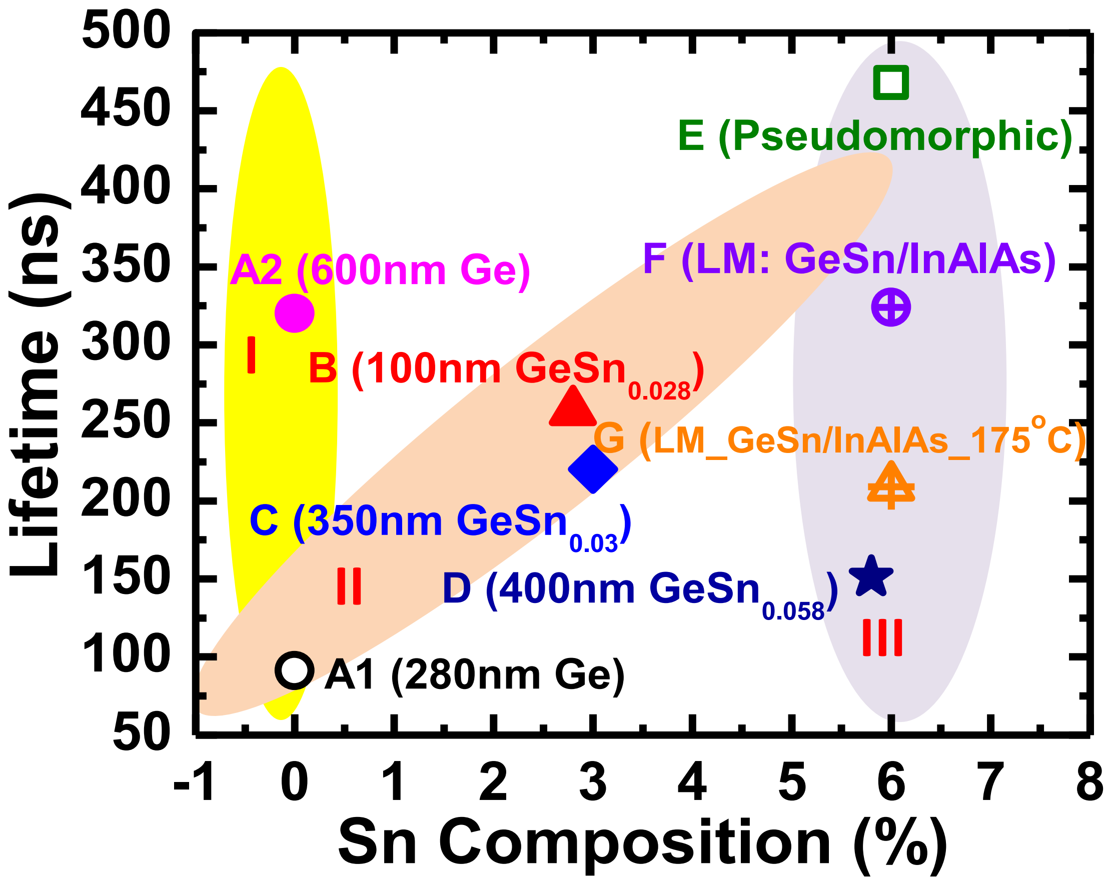


- ❑ λ =1500 nm (20 mW, ~10^{13} cm^{-3} injection density), E_{ph} ≈ 0.83 eV carriers in *L*- and *Γ*-valleys
- ❑ Low surface states induced recombination → high lifetime
- ❑ SRH recombination (defect assisted) reduces carrier lifetime
- ❑ High minority carrier lifetimes of 220 ns to 468 ns.

Low defects !!! ☑

High carrier lifetime !!! ☑

Minority Carrier Lifetimes of Ge and GeSn



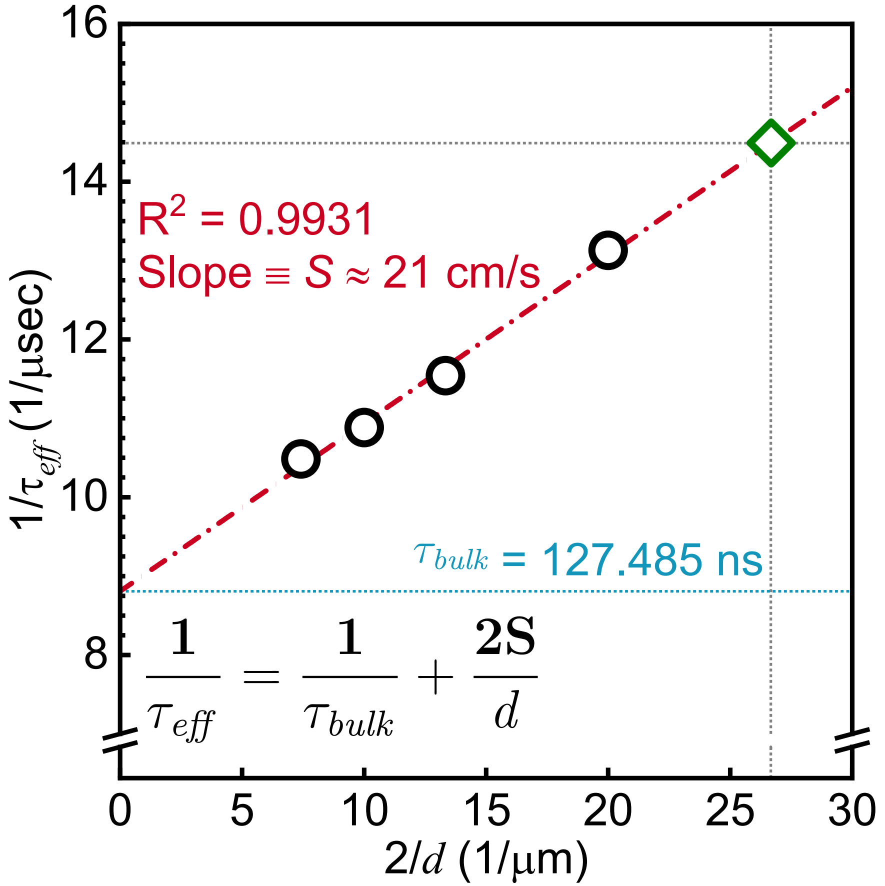
GeSn advantages:

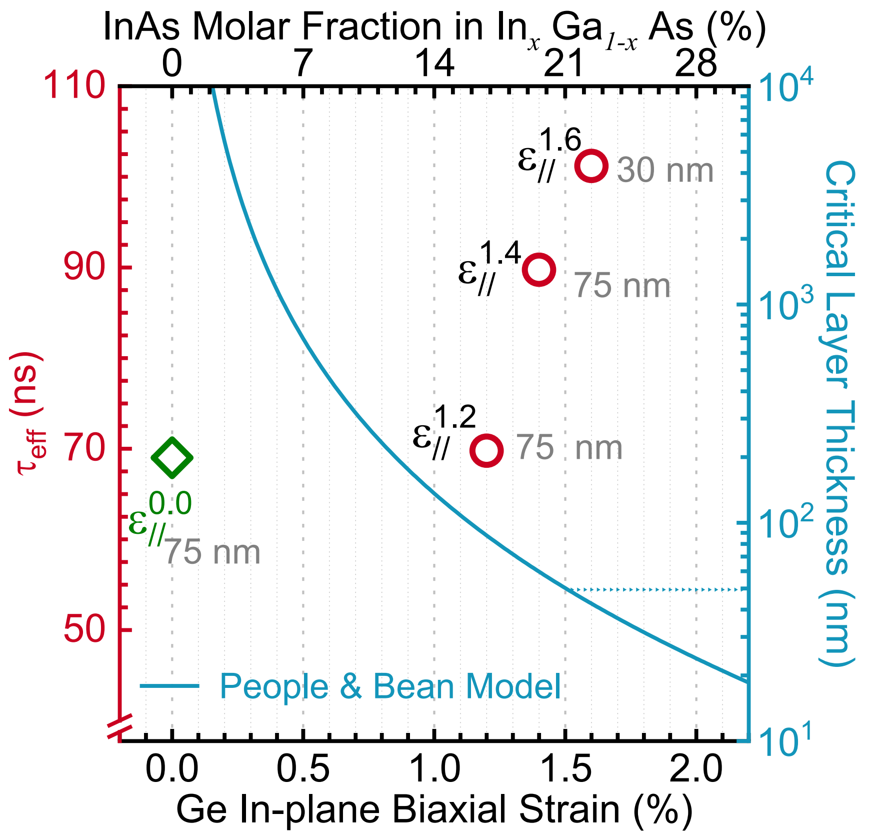
- ✓ Improved Optical Transitions
  - ✓ Detector Responsivity (absorption)
  - ✓ Lasing Threshold Current (emission)
- ✓ Mobility Boost – high ON current
- ✓ Increased carrier lifetime (reduced surface roughness)
- ✓ Silicon compatible

Leverage by superior growth

M. K. Hudait *et al.*, *JMC-C*, 2022, **10**, 10530–10540.

Carrier Recombination: Ge & Tunable ε-Ge





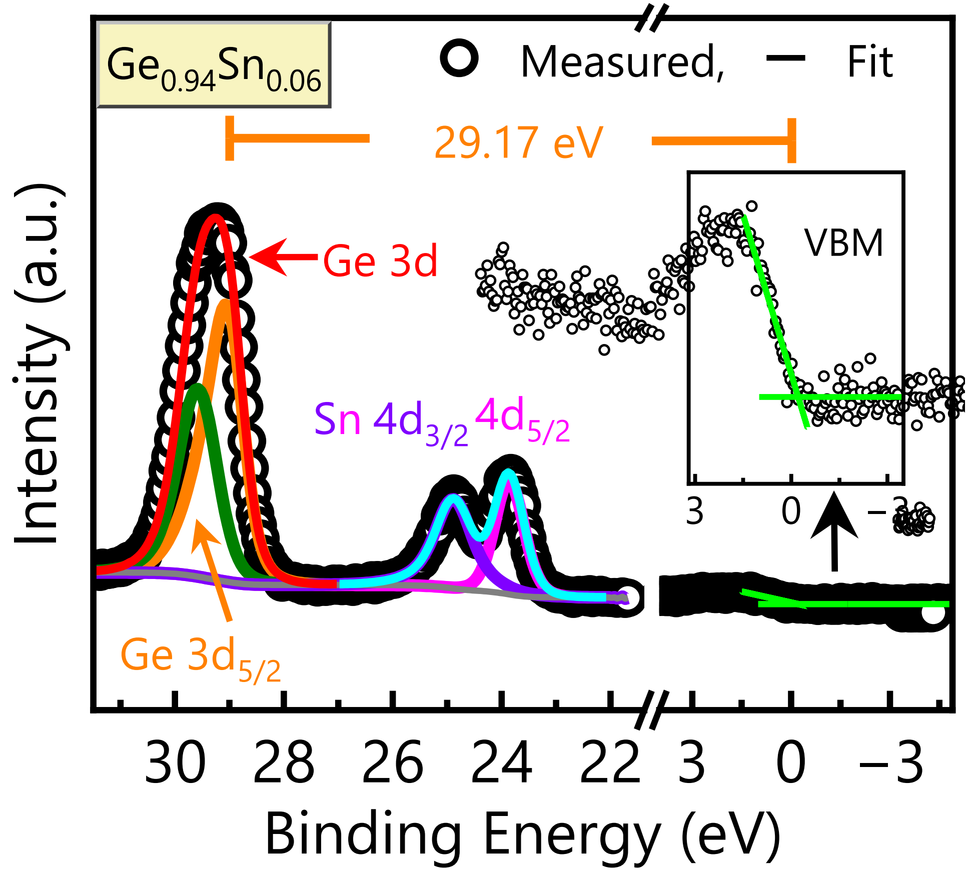
☑ **SRV of 21 cm/s was achieved from unstrained Ge**

☑ **Bulk lifetime of ~127 ns was determined**

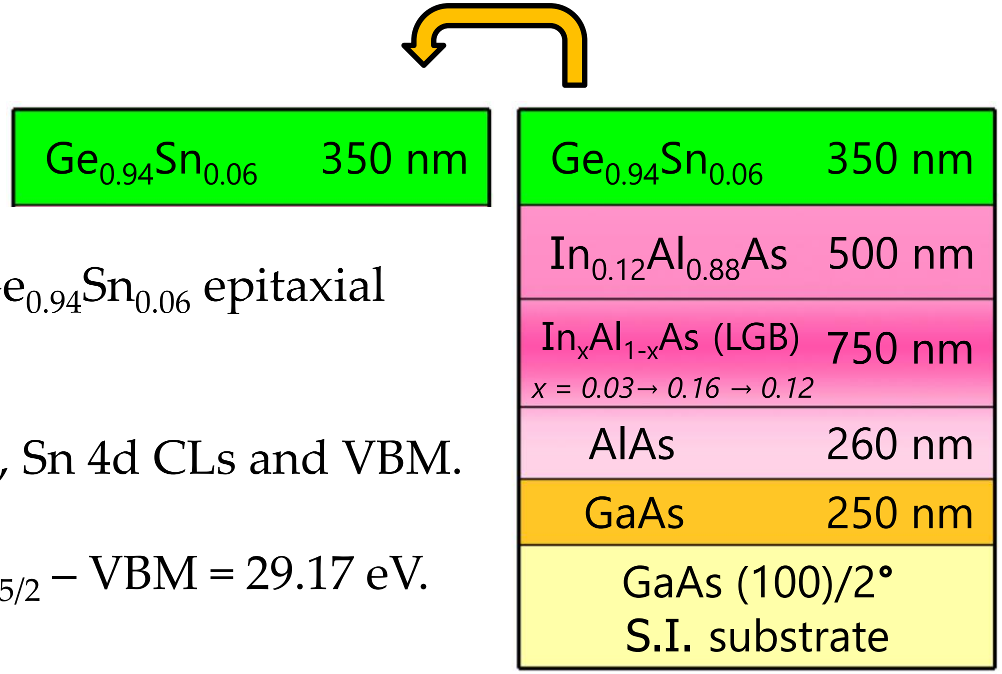
☑ ***Carrier lifetime increases with increasing strain***

Bhattacharya *et al, ACS Nano (To be submitted, 2023)*

Energy band alignment of GeSn – Regions (1)



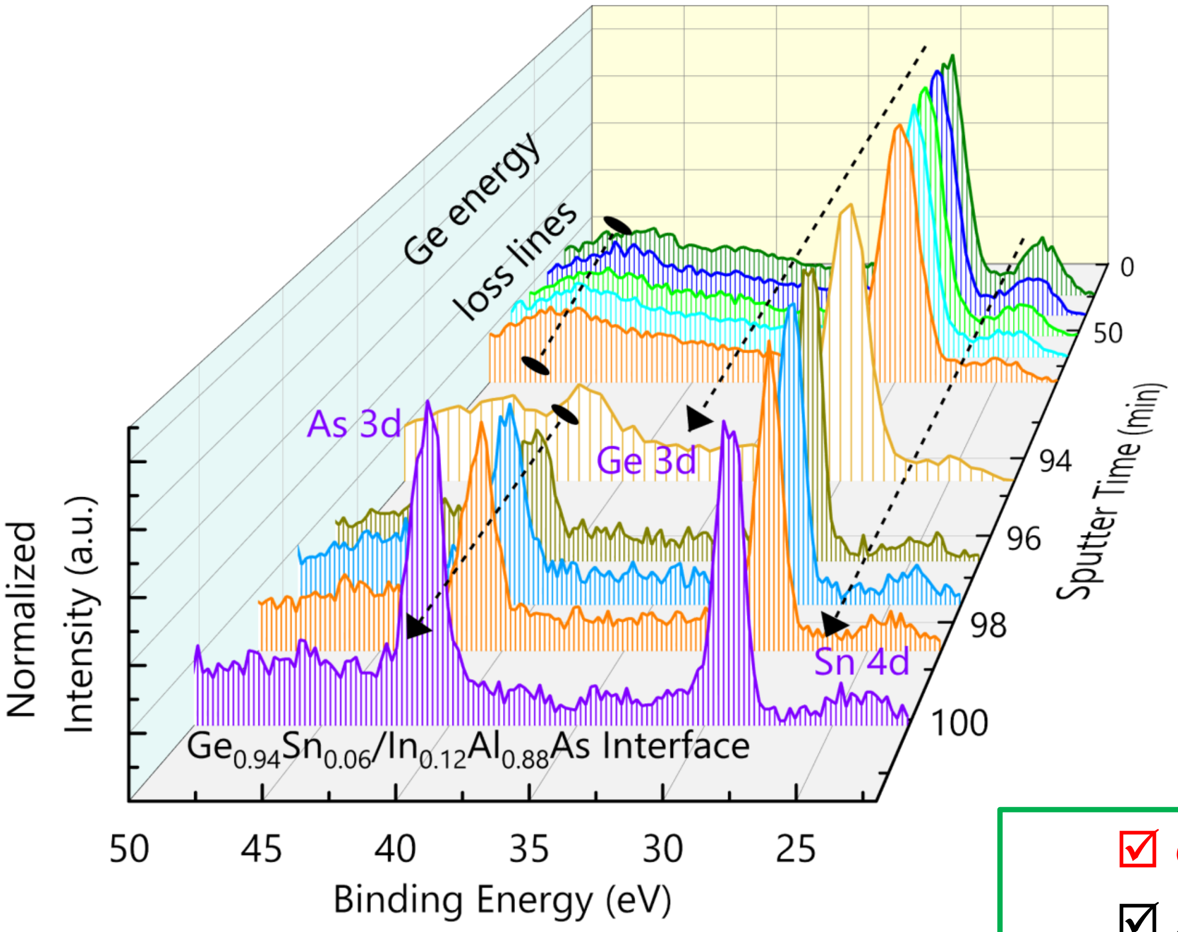
Sample D - $Ge_{0.94}Sn_{0.06}/In_{0.12}Al_{0.88}As$



- Top $Ge_{0.94}Sn_{0.06}$ epitaxial layer.
- Ge 3d, Sn 4d CLs and VBM.
- Ge $3d_{5/2}$ – VBM = 29.17 eV.

S. Karthikeyan *et al.*, *JMC-C (to be submitted, 2023)*

Energy band alignment of GeSn – Regions (2)



Sample D - $Ge_{0.94}Sn_{0.06}/In_{0.12}Al_{0.88}As$

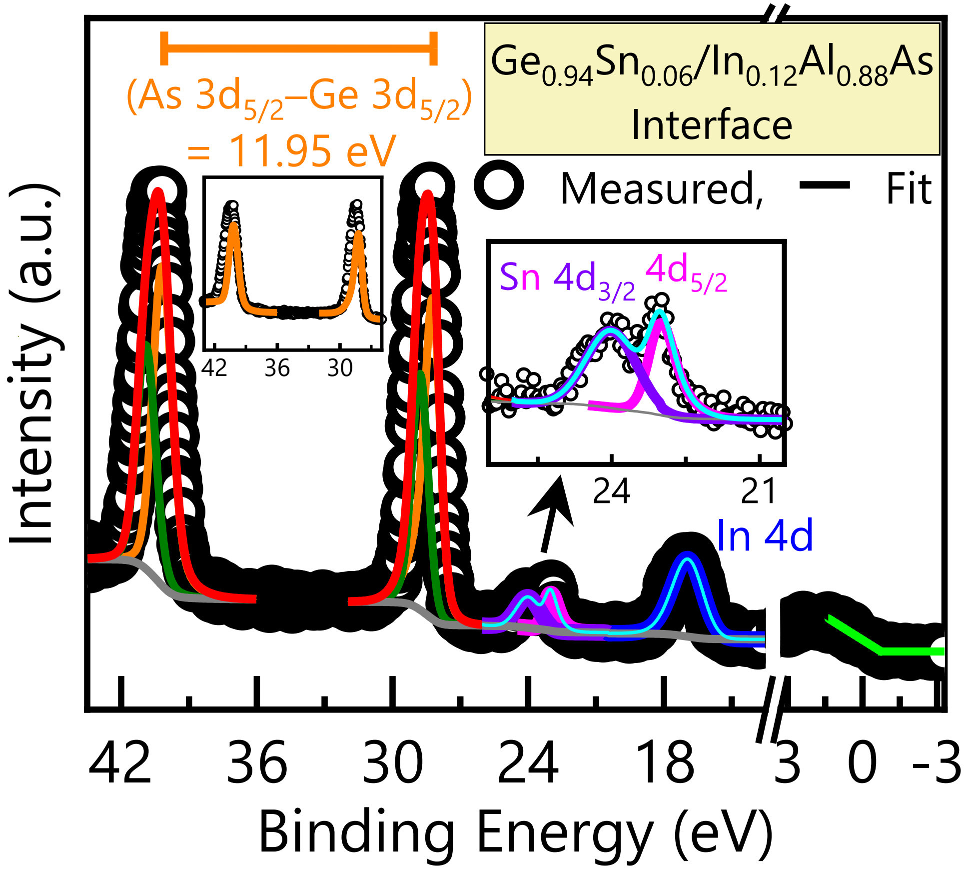
- ❑ Sputter etch 350 nm thick $Ge_{0.94}Sn_{0.06}$ epitaxial layer.
- ❑ Depth profile Ge 3d, Sn 4d and As 3d CLs.

$Ge_{0.94}Sn_{0.06}$	350 nm
$In_{0.12}Al_{0.88}As$	500 nm
$In_xAl_{1-x}As$ (LGB) $x = 0.03 \rightarrow 0.16 \rightarrow 0.12$	750 nm
AlAs	260 nm
GaAs	250 nm
GaAs (100)/2° S.I. substrate	

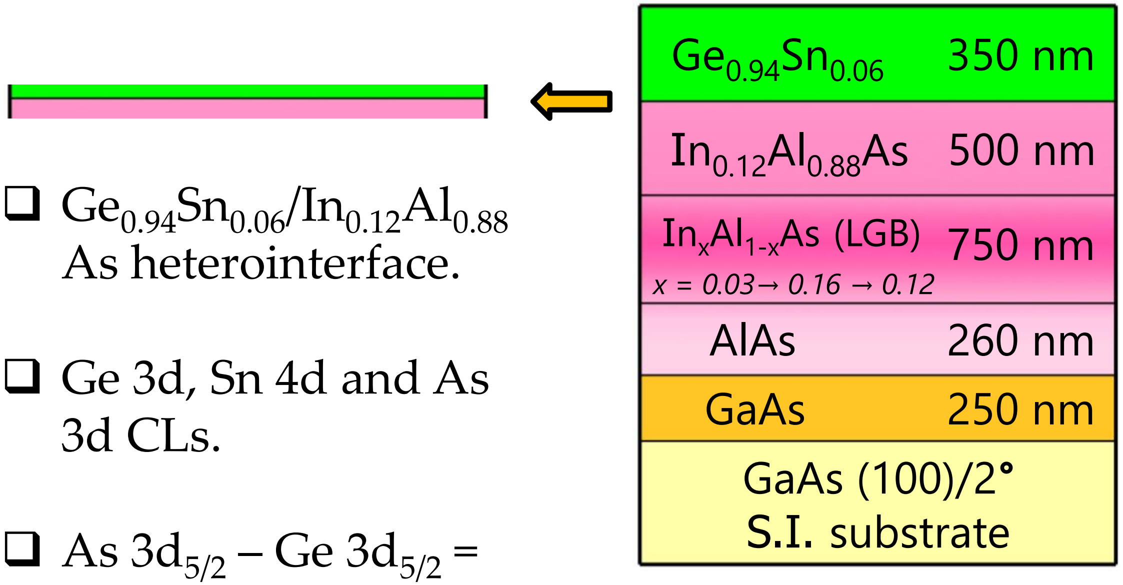
- ☑ ***Challenge to acquire interface signal***
- ☑ **Several iterations were needed since no information on sputter etch rate of GeSn**

Karthikeyan *et al., JMC-C (to be submitted, 2023)*

Energy band alignment of GeSn – Regions (2)



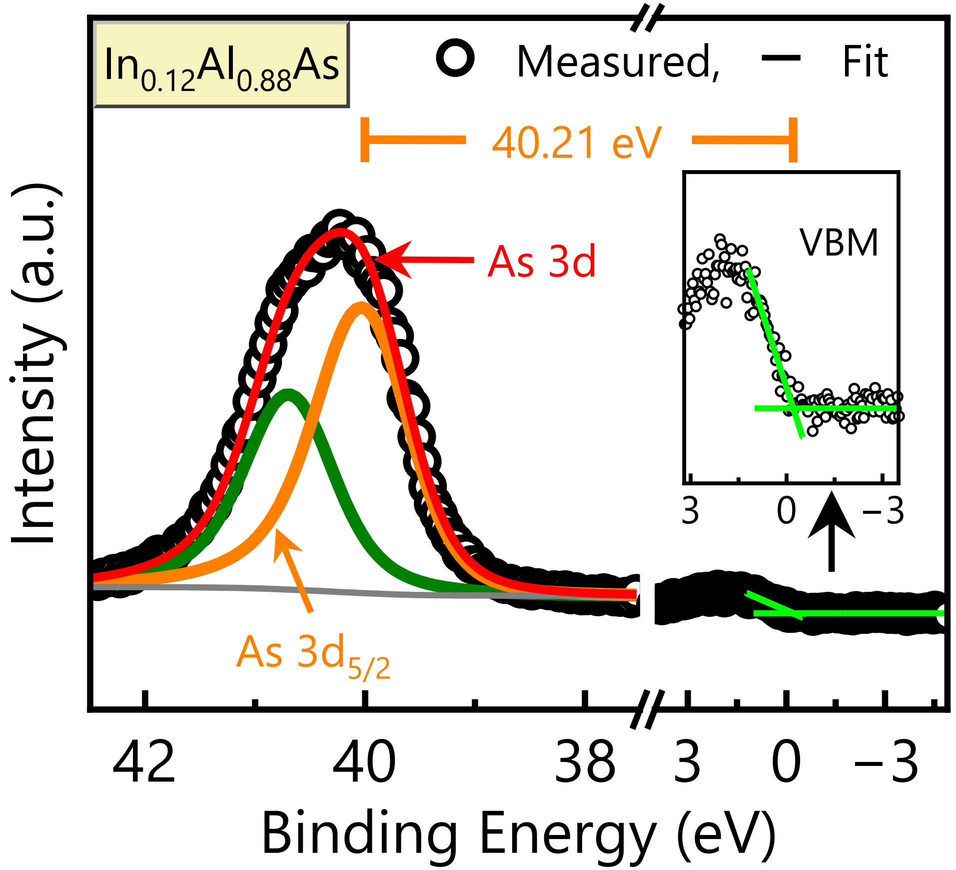
Sample D - $Ge_{0.94}Sn_{0.06}/In_{0.12}Al_{0.88}As$



- ❑ $Ge_{0.94}Sn_{0.06}/In_{0.12}Al_{0.88}$ As heterointerface.
- ❑ Ge 3d, Sn 4d and As 3d CLs.
- ❑ As $3d_{5/2}$ – Ge $3d_{5/2}$ = 11.95 eV.

Karthikeyan *et al., JMC-C (to be submitted, 2023)*

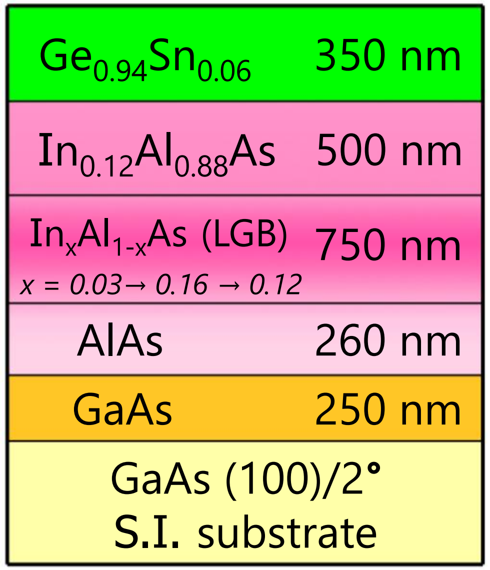
Energy band alignment of GeSn – Regions (3)



Sample D - $Ge_{0.94}Sn_{0.06}/In_{0.12}Al_{0.88}As$

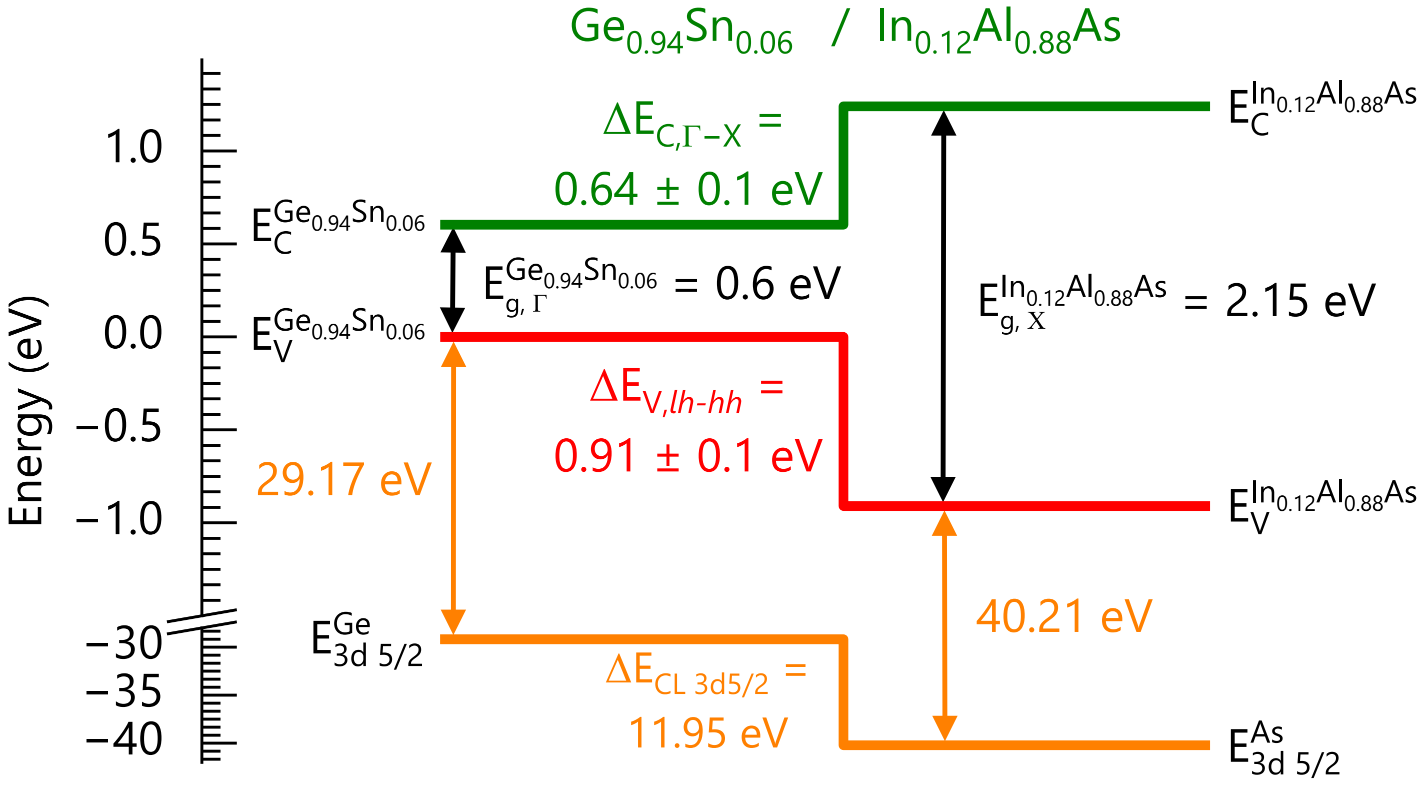
$In_{0.12}Al_{0.88}As$ 500 nm

- ❑ Underlying $In_{0.12}Al_{0.88}As$ buffer layer.
- ❑ As 3d CL and VBM.
- ❑ As $3d_{5/2}$ – VBM = 40.21 eV.



Karthikeyan *et al.*, *JMC-C (to be submitted, 2023)*

Energy band alignment of GeSn → Type–I



Kraut *et al.* method:

$$\Delta E_V = \left(E_{Ge\ 3d\ 5/2} - E_{VBM}\right)^{Ge_{0.94}Sn_{0.06}} - \left(E_{As\ 3d\ 5/2} - E_{VBM}\right)^{In_{0.12}Al_{0.88}As} - \left(E_{As\ 3d\ 5/2} - E_{Ge\ 3d\ 5/2}\right)^{interface}$$

$$\Delta E_{C,\Gamma-X} = E_{g,X}^{InAlAs} - E_{g,\Gamma}^{GeSn} - \Delta E_V$$

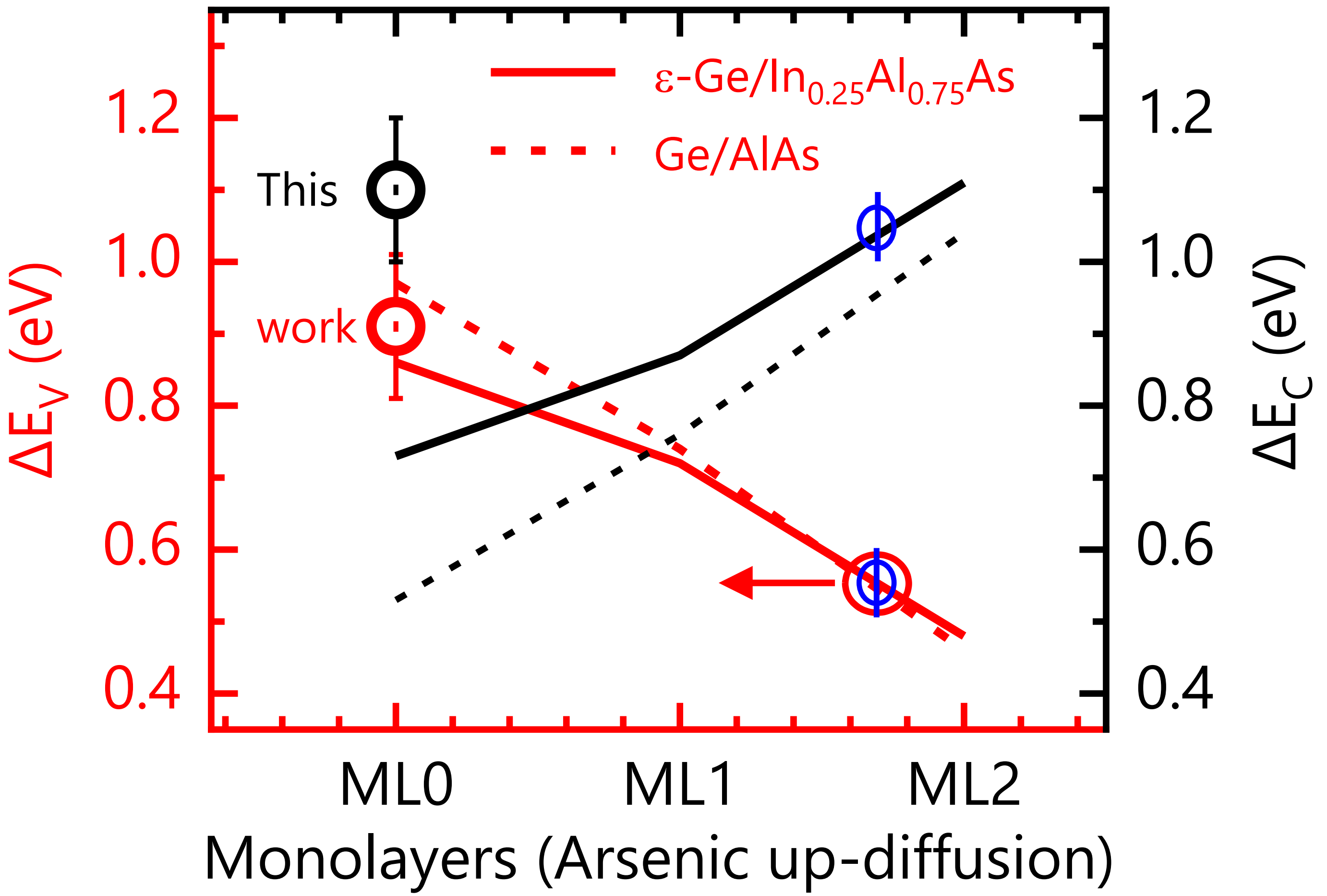
- ❑ Type –I!! ☑
- ❑ Large Band offsets!! ☑
- ❑ Superior confinement!! ☑

Sample D - $Ge_{0.94}Sn_{0.06}$/$In_{0.12}Al_{0.88}As$

Karthikeyan *et al., JMC-C (to be submitted, 2023)*

E. A. Kraut *et al.*, *Phys. Rev. Lett.*, 1980, **44**, 1620–1623.

Band offset – Atomic Interdiffusion



○ **1.75% ε-Ge on $In_{0.26}Al_{0.74}As$**

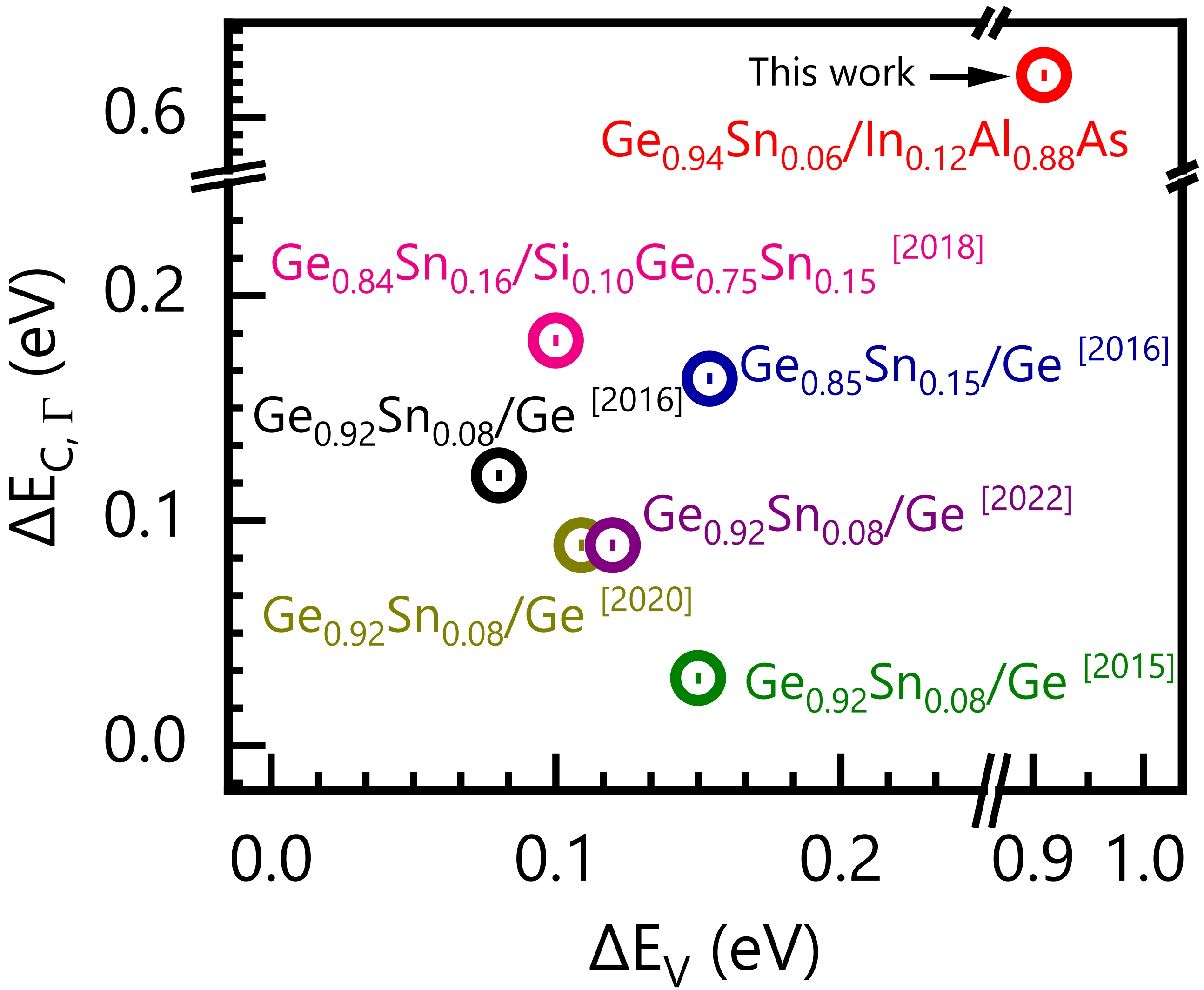
First principles calculation-based analysis:

- ❑ Abrupt interface ☑
- ❑ No interdiffusion ☑
- ❑ ΔE_V and ΔE_C large enough to hold carriers within $GeSn_{0.06}$ layer ☑
- ❑ GeSn (225˚C) lower growth temperature than Ge (400˚C) reduces interdiffusion ☑

G. Greene-Diniz and M. Grüning, *Phys. Rev. Appl.*, 2018, **10**, 044052-1-16

M. B. Clavel *et al*, *ACS Omega* , 2022, **7**, 5946

Band offset – Benchmarking



Large band offset of lattice matched $Ge_{0.94}Sn_{0.06}/In_{0.12}Al_{0.88}As$ Heterostructure:

- ❑ $\Delta E_V = 0.91$ eV.
- ❑ $\Delta E_{C,\Gamma-X} = 0.64$ eV.
- ❑ Band offsets of GeSn grown on Ge or SiGeSn < 0.2 eV.

[2015]: 10.1364/OE.24.001358
[2016]: scholarworks.uark.edu/etd/1824
[2016]: 10.1038/srep34082
[2018]: 10.1002/advs.201700955
[2020]: 10.1364/OE.389378
[2022]: 10.1109/TED.2022.3145776

S. Karthikeyan *et al.*, *JMC-C (to be submitted, 2023)*

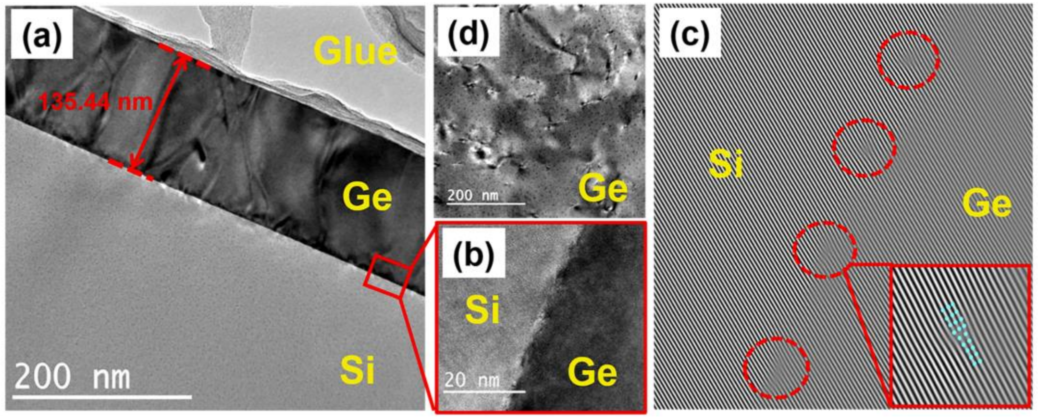
Summary

- ❑ Device quality epitaxial ε-Ge and GeSn can be realized by interconnected MBE chambers
- ❑ Defects and dislocations are confined within the III-V buffer layers for ε-Ge and GeSn
- ❑ Carrier transport of ε-Ge on InGaAs suggests carriers are confined within ε-Ge layer
- ❑ Lattice matched $Ge_{0.94}Sn_{0.06}/In_{0.12}Al_{0.88}As$ benefits:
  - ✓ Virtually defect-free
  - ✓ High minority carrier lifetime (324 ns)
  - ✓ Type-1 band alignment
  - ✓ Large band offsets (ΔE_V = 0.91 eV, $\Delta E_{C,\,G\text{-}X}$ = 0.64 eV)
  - ✓ Abrupt interface
- ❑ Required Sn source re-configuration for higher Sn (> 6%) compositional GeSn materials

- **EXTRA**

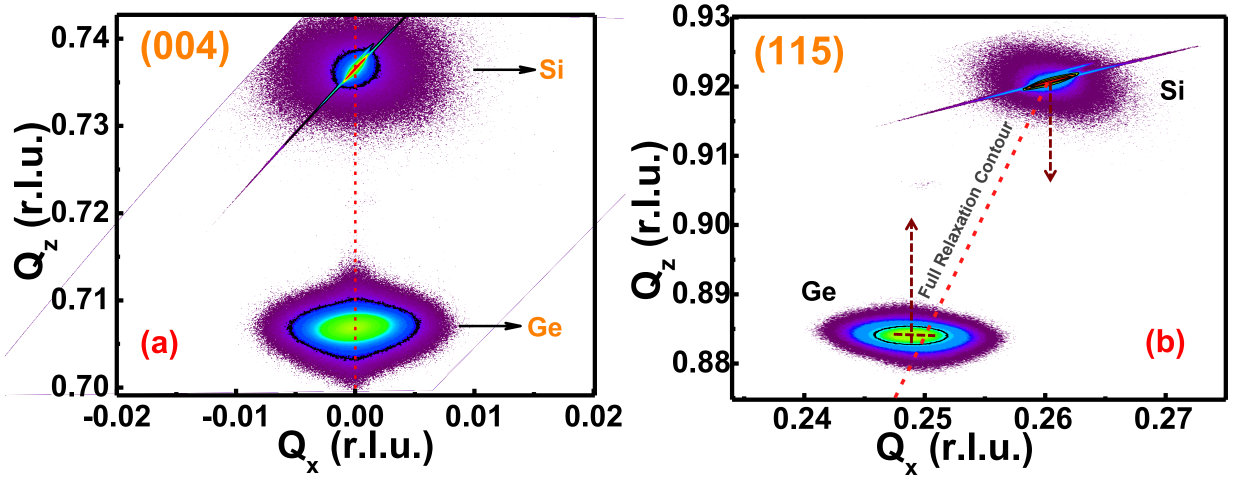
Epitaxial Ge on Si

MBE Growth (Ge-on-Si)



A.Ghosh *et.al*, *AIP Adv.*, 2017, **7**, 095214.

(i): XTEM



(ii): RSMs

(iii): Carrier recombination