Optical and X-Ray Charactorization of $Ge_{1-y}Sn_y$ alloy on GaAs

Haley Woolf,[1] Matt Kim,[2] Carola Emminger,[1] Carlos Armenta,[1] Stefan Zollner[1]

1. Department of Physics, NMSU, Las Cruces, NM
2. QuantTera, Scottsdale, AZ

College of Arts and Science Department of Physics

This work was supported by Air Force Office of Scientific Research under award number FA9550-20-1-0135.

FA9550-20-1-0135

BE BOLD. Shape the Future.®
New Mexico State University

Outline

- Background:
  - UV ellipsometry and x-ray diffraction
- Abstract
- X-ray diffraction data:
  - Omega rocking curves, and reciprocal pace maps on (004), (224), & $(\bar{2}\bar{2}4)$
- Lattice constants
- Optical data:
  - Pseudodielectric function, optical constants, & 2^{nd} der. of dielectric function
- Theoretical E_1 & $E_1+\Delta_1$ with tin content
- Conclusion

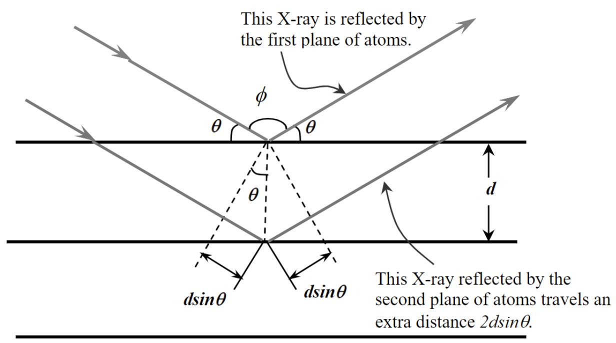
Background

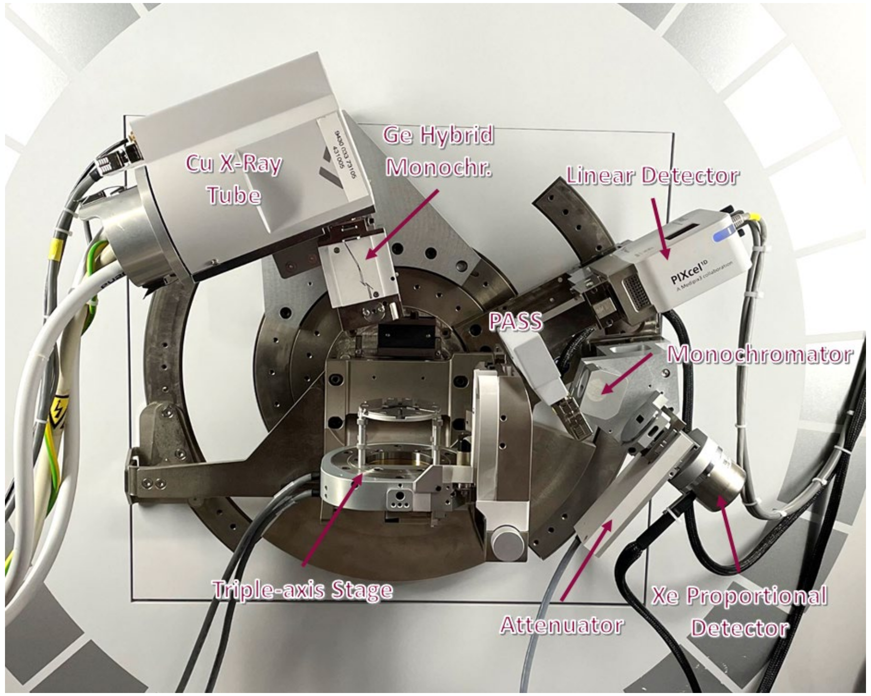
X-ray diffraction uses Bragg's Law to determine the characteristics of different materials. Omega Rocking curves were used to determine the lattice constants and reciprocal space maps were used to determine the strain and relaxation.

Bragg's Law:

$$2d\sin\theta = n\lambda$$

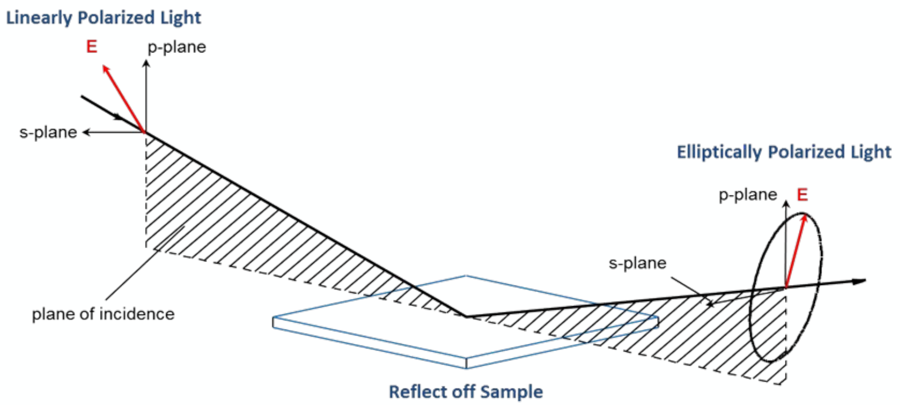
- $2d$ → Distance between layers of atoms
- $\sin\theta$ → Angle between incident beam and the surface of the crystal
- $n\lambda$ → Wavelength of the rays $\lambda_{X-rays} = 1.5406$ Å

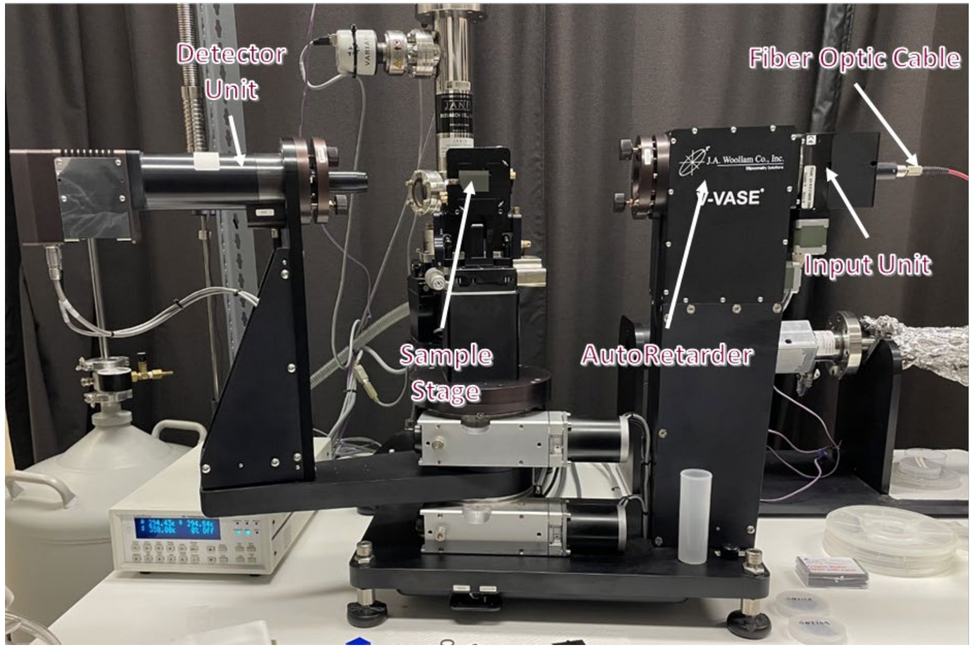




Background

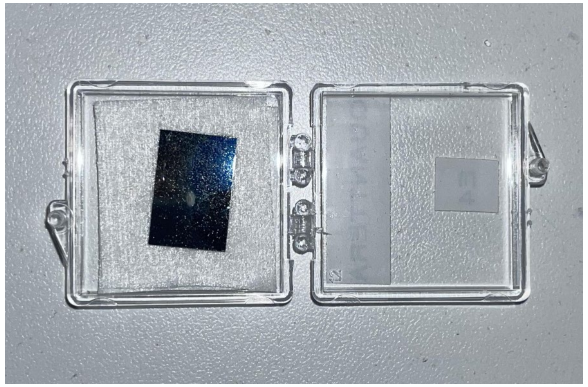
In UV ellipsometry, light is reflected/transmitted from a material causing the polarization to change. ψ is the amplitude ratio and Δ is the phase difference of the light. ψ and Δ depend on the material's optical properties and thicknesses.

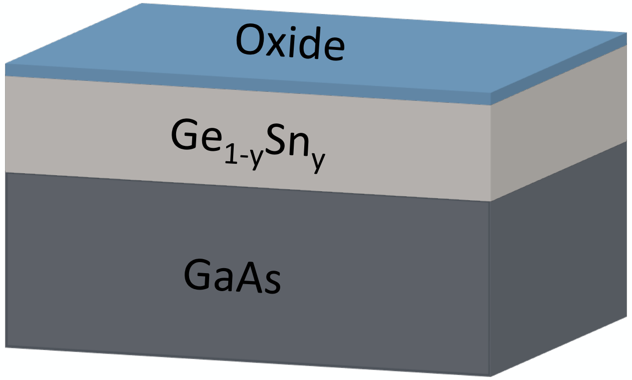


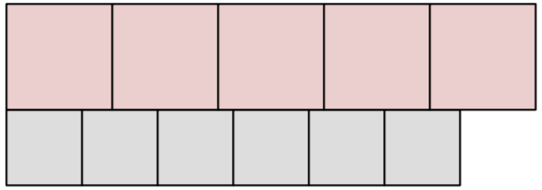


Introduction

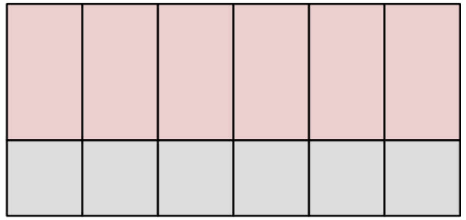
- $Ge_{1-y}Sn_y$ layer is 1600 nm thick and was grown on GaAs by chemical vapor epitaxy. The tin content can be found with (004) reciprocal space map and omega rocking curves.
- (224) and $(\bar{2}\bar{2}4)$ reciprocal space maps will determine the strain and relaxation of the epitaxial layer
- UV ellipsometry can determine the sample’s optical properties, including the dielectric function and the optical constants.
- GeSn is often used in lasers and inferred detectors.





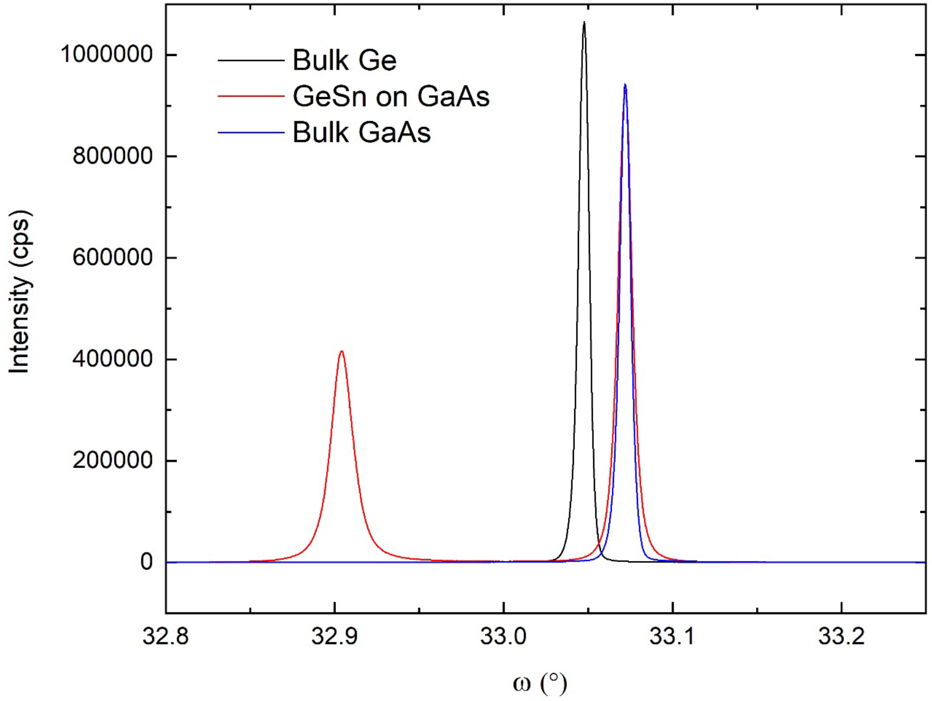


Relaxed epitaxial layer



Pseudomorphic/strained epitaxial layer

(004) Rocking Curves (Open Detector)



	FWHM
Bulk Ge	0.0074°
GaAs	0.0098°
GeSn	0.0155°
Bulk GaAs	0.0076°

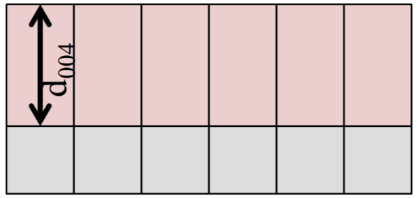
Braggs's Law:

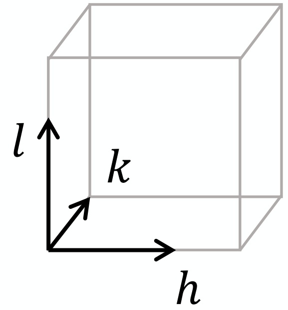
$$2d\sin\theta = n\lambda \quad n = 1$$

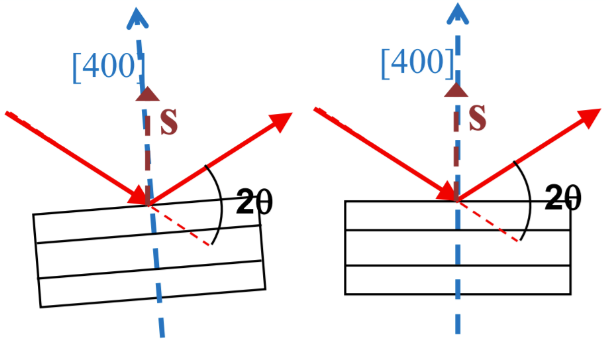
Lattice Constant:

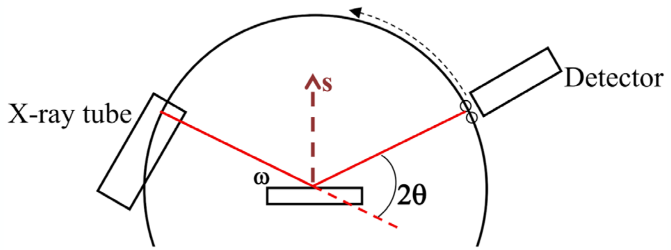
$$a = d\left(\sqrt{h^2 + k^2 + l^2}\right)$$

a_{GeSn} = 5.679 Å
a_{GaAs} = 5.653 Å
a_{Ge} = 5.658 Å
a_{Sn} = 6.489 Å



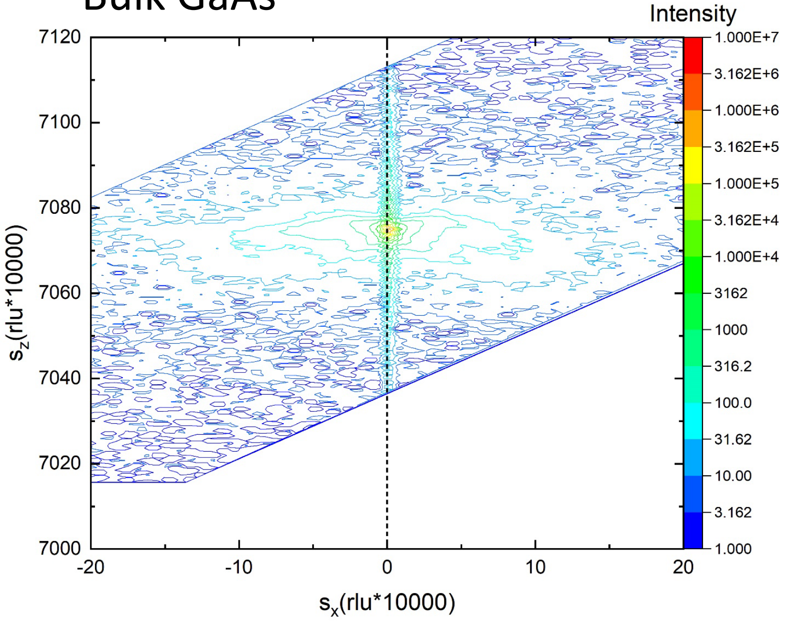




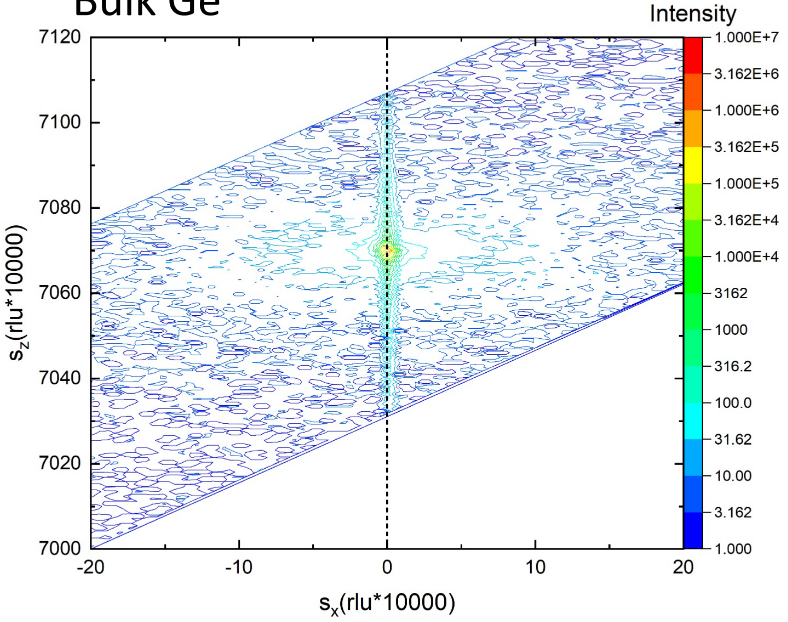


(004) Reciprocal Space Maps

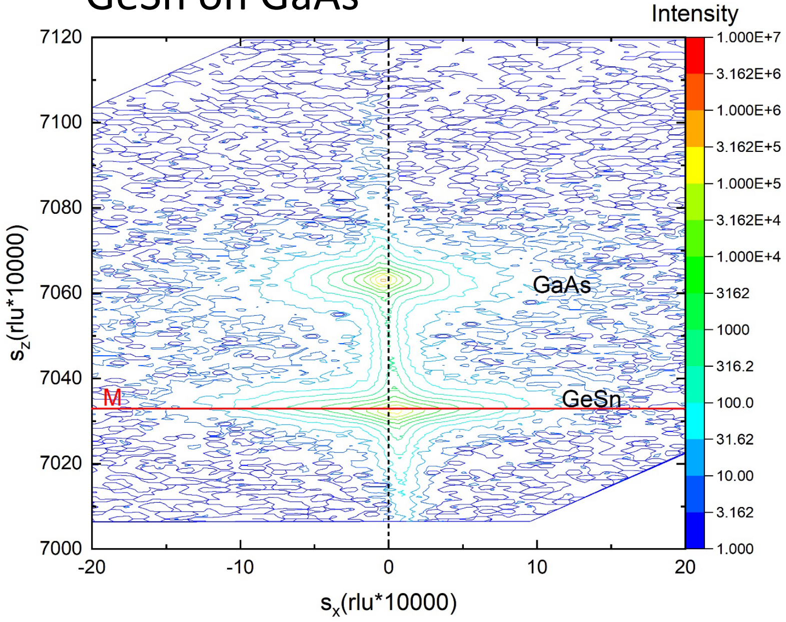
Bulk GaAs

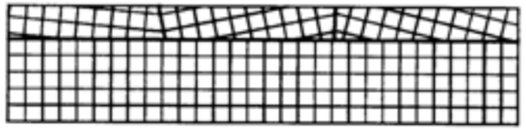


Bulk Ge



GeSn on GaAs





Dashed line drawn through substrate peak

M-Mosaic Spread (Relaxation Line)

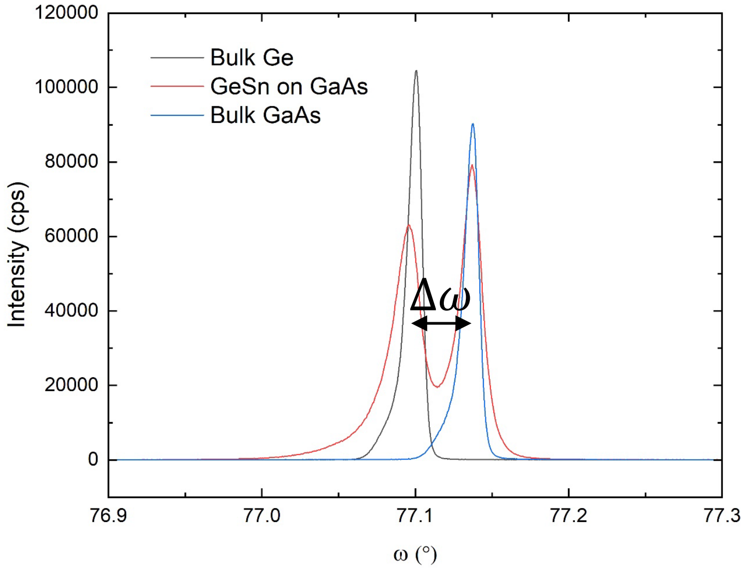
$$s_x = \frac{q_x}{2\pi} = \frac{1}{\lambda}[\cos(\omega) - \cos(2\theta - \omega)]$$

$$s_z = \frac{q_z}{2\pi} = \frac{1}{\lambda}[\sin(\omega) + \sin(2\theta - \omega)]$$

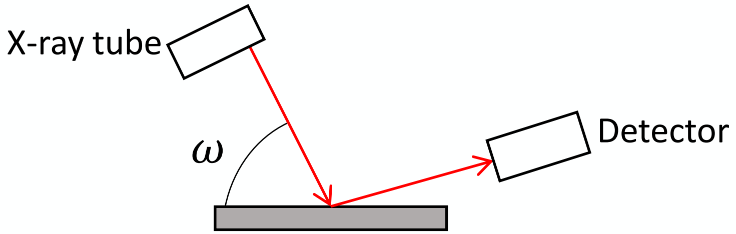
$$\lambda = 1.5406\ \text{Å}$$

$(\bar{2}\bar{2}4)$ & (224) Rocking Curve (Open Detector):

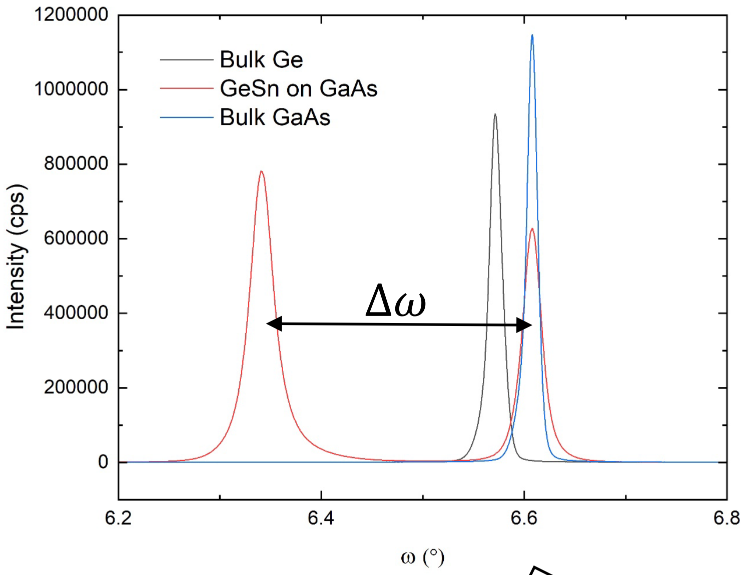
Grazing Exit:



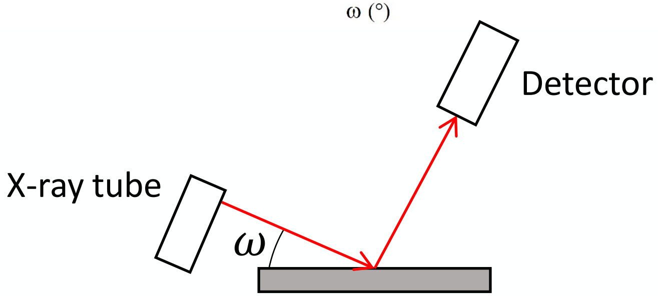
	FWHM
Bulk Ge:	0.0109°
GaAs:	0.0117°
GeSn:	0.0225°
Bulk GaAs:	0.0114°



Grazing Incidence:

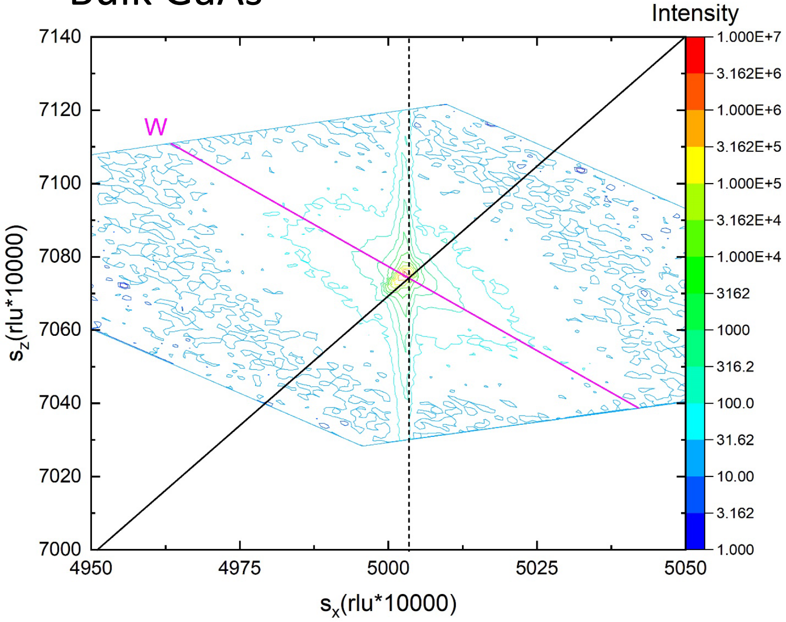


	FWHM
Bulk Ge:	0.0149°
GaAs:	0.0221°
GeSn:	0.0281°
Bulk GaAs:	0.0125°

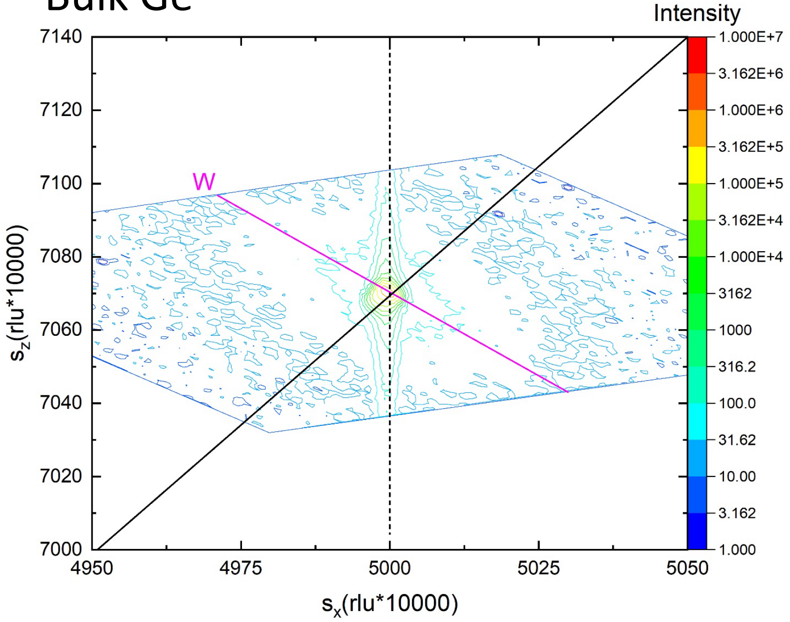


(224) Grazing Incidence Reciprocal Space Map

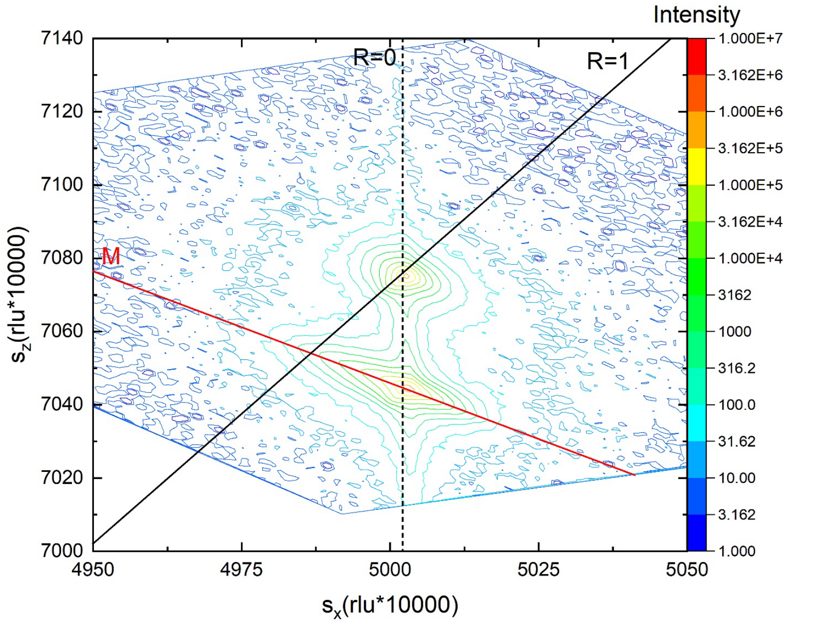
Bulk GaAs



Bulk Ge



GeSn on GaAs



W-Wavelength Streak

M-Mosaic Spread (Relaxation Line)

Black line drawn from origin (Relaxed)

Dashed line drawn through substrate peak (Pseudomorphic)

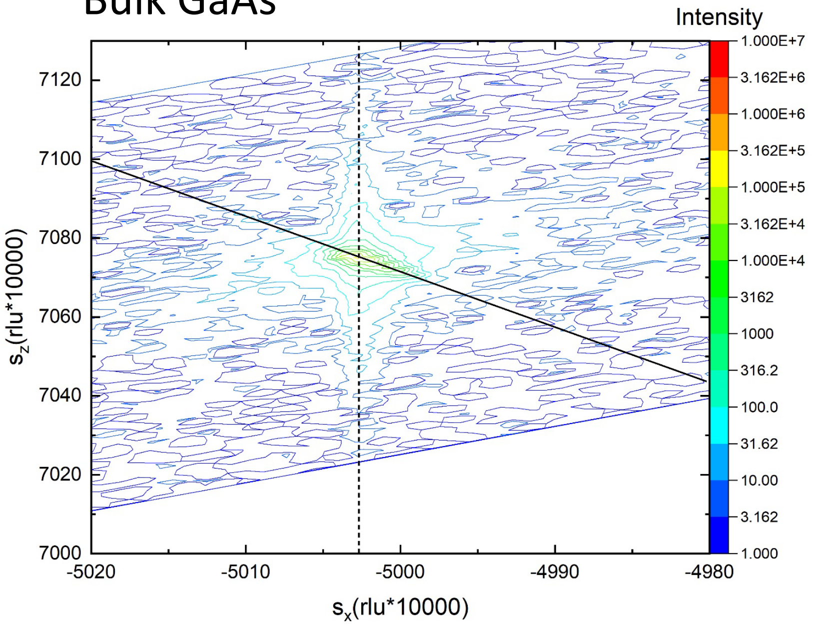
$$s_x = \frac{q_x}{2\pi} = \frac{1}{\lambda}[\cos(\omega) - \cos(2\theta - \omega)]$$

$$s_z = \frac{q_z}{2\pi} = \frac{1}{\lambda}[\sin(\omega) + \sin(2\theta - \omega)]$$

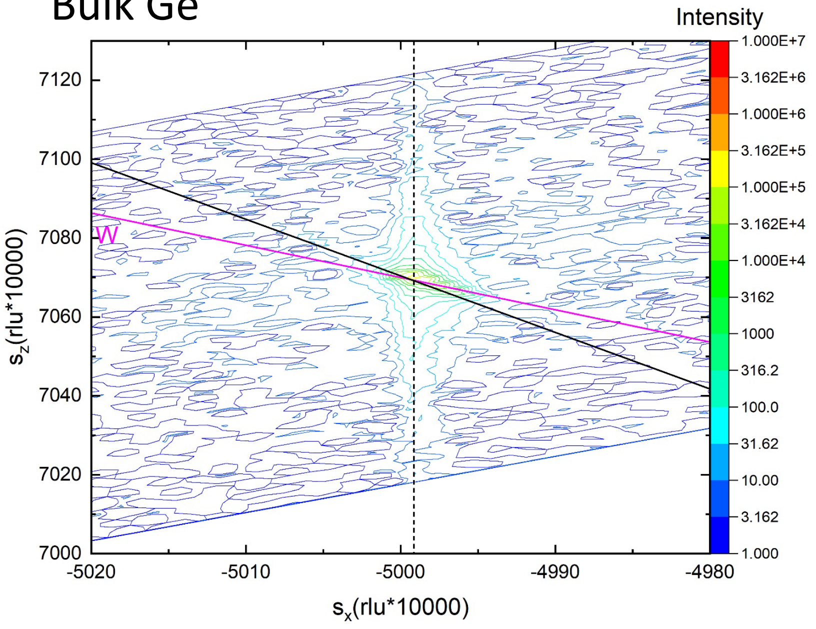
$$\lambda = 1.5406\ \text{Å}$$

$(\bar{2}\bar{2}4)$ Grazing Exit Reciprocal Space Map

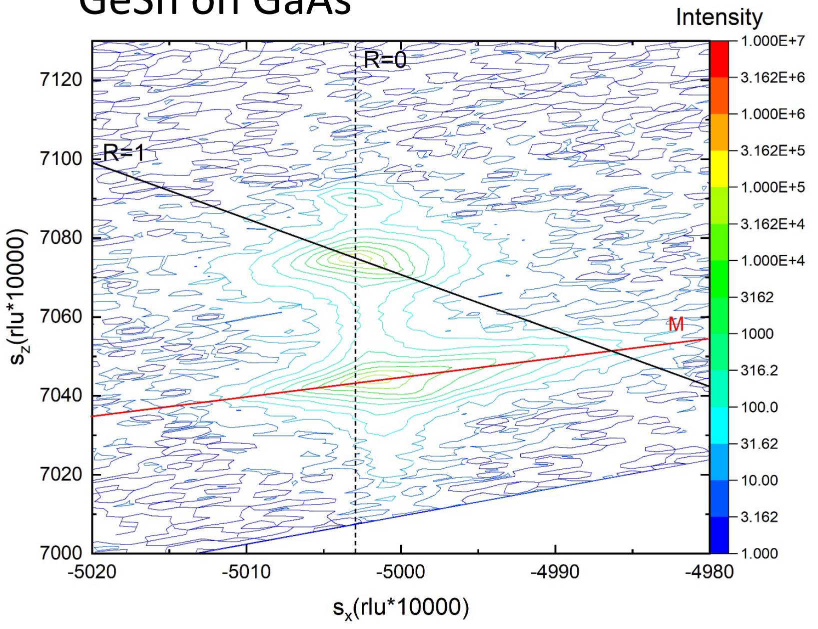
Bulk GaAs



Bulk Ge



GeSn on GaAs



W-Wavelength Streak

M-Mosaic Spread (Relaxation Line)

Black line drawn from origin (Relaxed)

Dashed line drawn through substrate peak (Pseudomorphic)

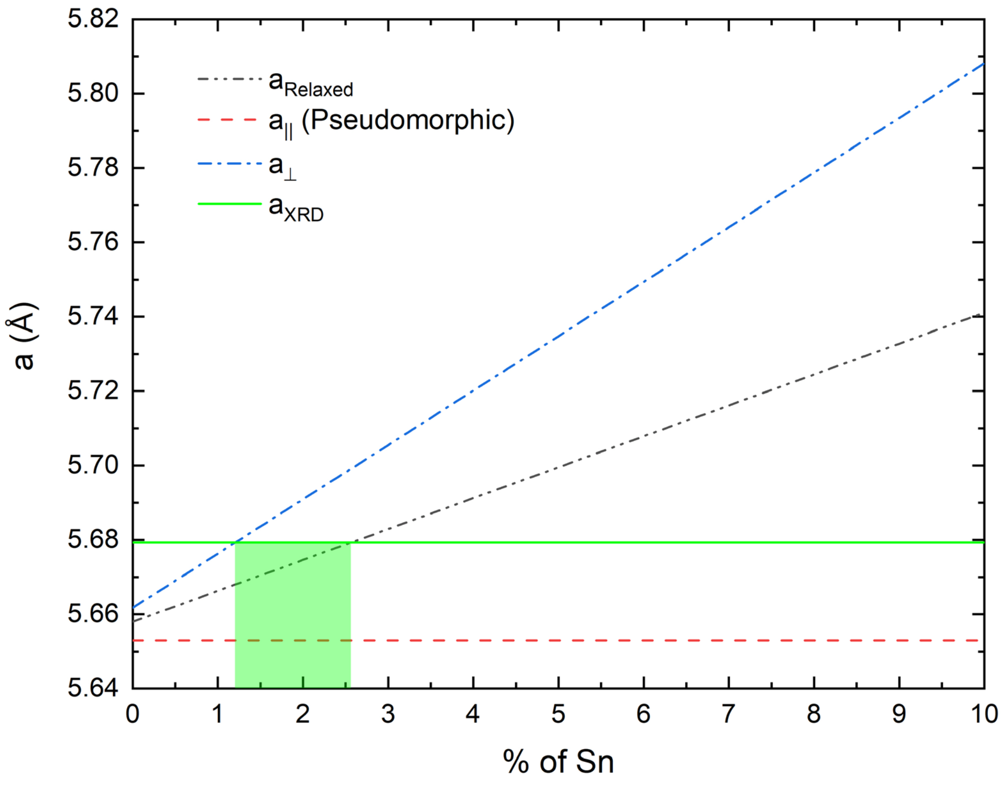
$$s_x = \frac{q_x}{2\pi} = \frac{1}{\lambda}[\cos(\omega) - \cos(2\theta - \omega)]$$

$$s_z = \frac{q_z}{2\pi} = \frac{1}{\lambda}[\sin(\omega) + \sin(2\theta - \omega)]$$

$$\lambda = 1.5406\ \text{Å}$$

NM STATE BE BOLD. Shape the Future.®

Lattice Constants



If layer is fully *relaxed*, the % Sn is 2.6%
If layer is fully *strained*, the % Sn is 1.2%

Bragg's Law:

$$n\lambda = 2d \sin\theta \qquad a_{GeSn} = 4d$$

a_{GeSn}= 5.679 Å

Vegard's Law:

$$\boldsymbol{a_{Relaxed}(y) = a_{Sn}y + a_{Ge}(1-y)}$$

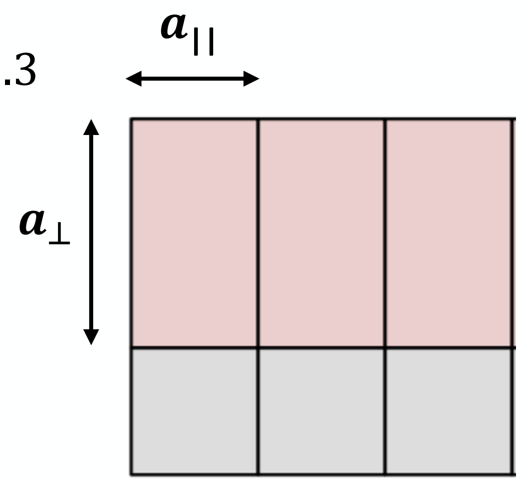
$\boldsymbol{a_{||} = a_{substrate}}$ **= 5.653 Å** *Pseudomorphic Condition*

$$\boldsymbol{a_{\perp} = (1+\varepsilon_{\perp})a_{Relaxed}(y)}$$

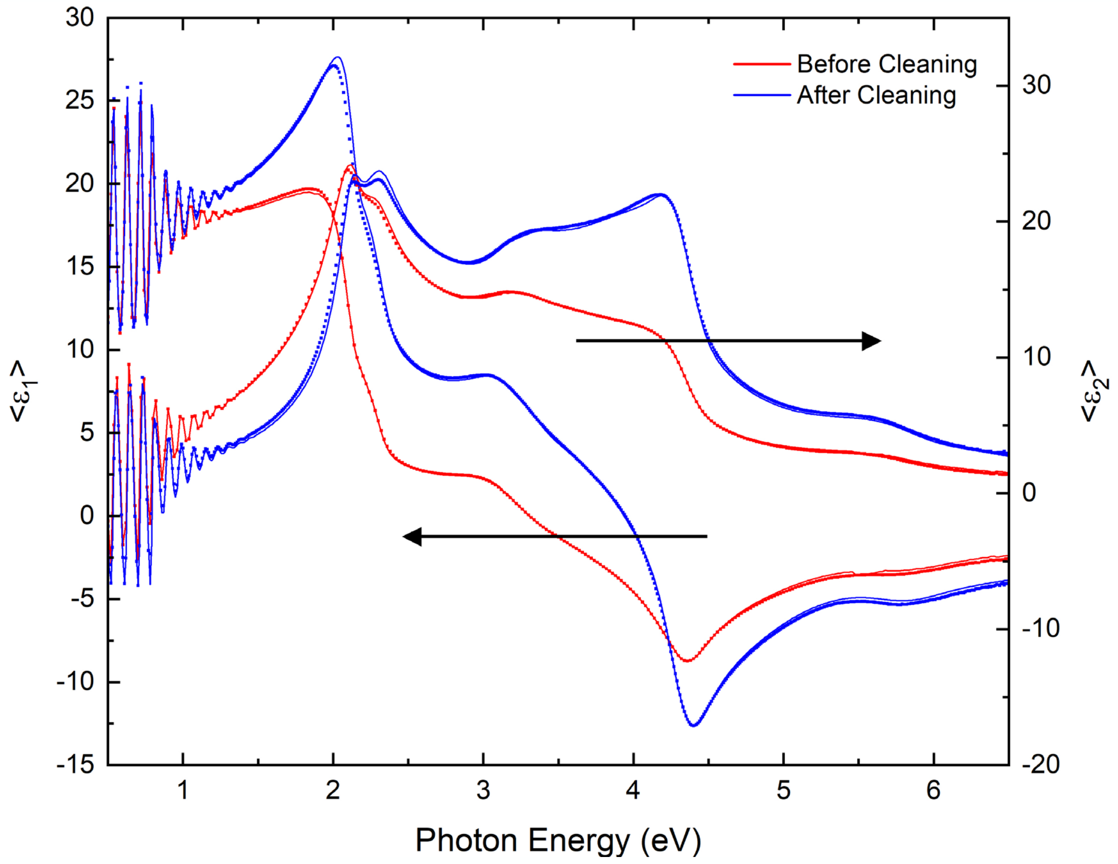
$$\varepsilon_{\perp} = -\frac{2v}{1-v}\varepsilon_{||}$$ Poisson Ratio: $v = 0.3$

$$\varepsilon_{||} = \frac{a_{||}}{a_{Relaxed}(y)} - 1$$

a_{GeSn}= 5.679 Å
a_{GaAs} = 5.653 Å
a_{Ge} = 5.658 Å
a_{Sn} = 6.489 Å



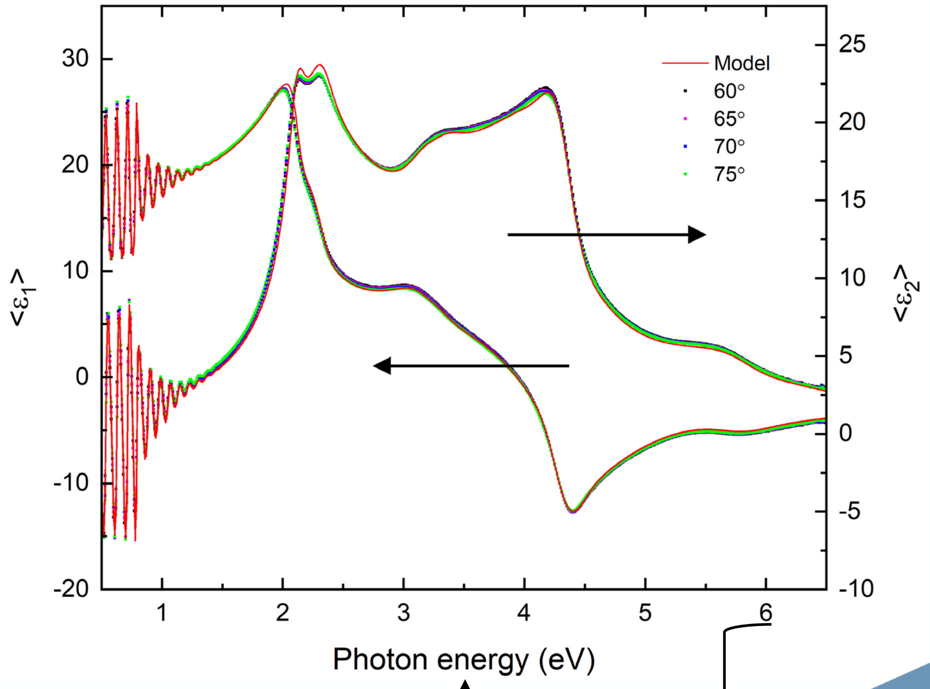
Pseudodielectric Function Before/After Cleaning



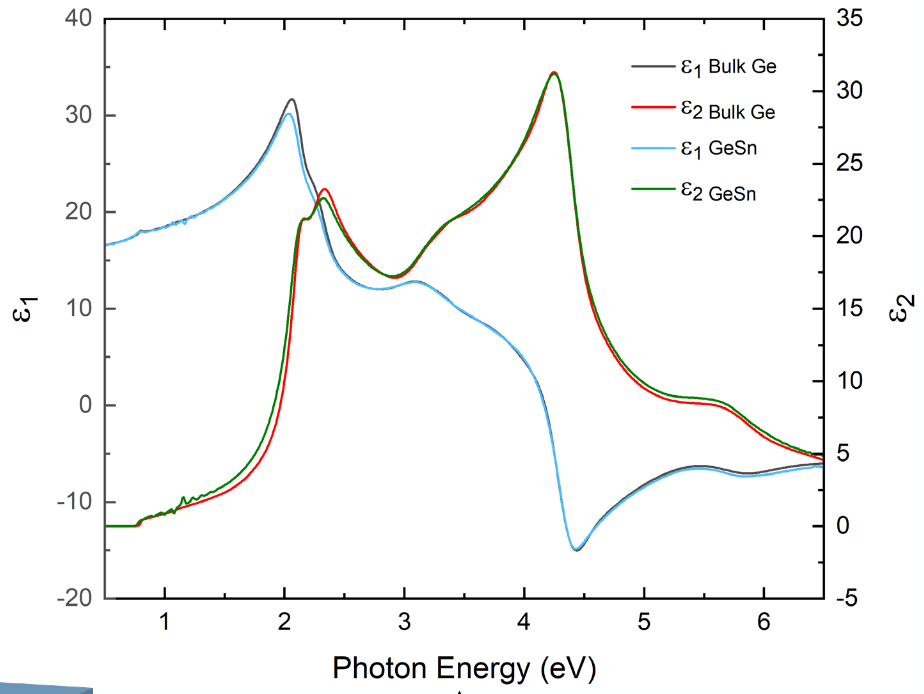
	Oxide Thickness
As Received (May 20th):	43.66 Å
Before Cleaning (June 14th):	72.07 Å
After Cleaning (June 14th):	26.50 Å
After 2nd Cleaning (June 15th):	25.90 Å

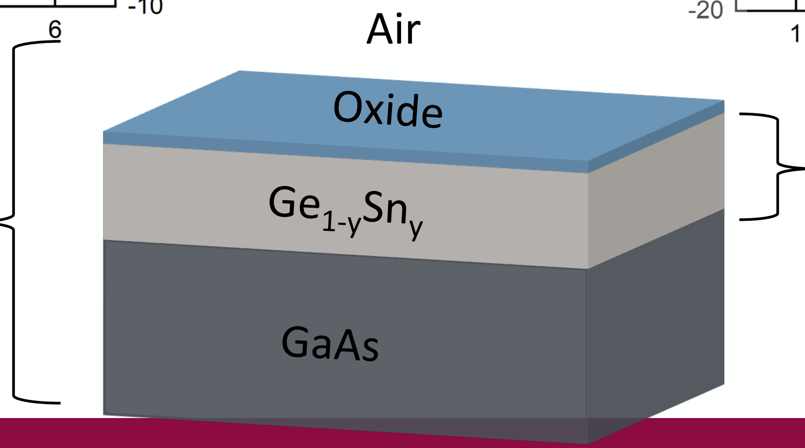
The $Ge_{1-y}Sn_y$ on GaAs sample was cleaned ultrasonically with water and then isopropanol to remove organic layers and most of the native oxide.

Pseudodielectric Function and Optical Constants

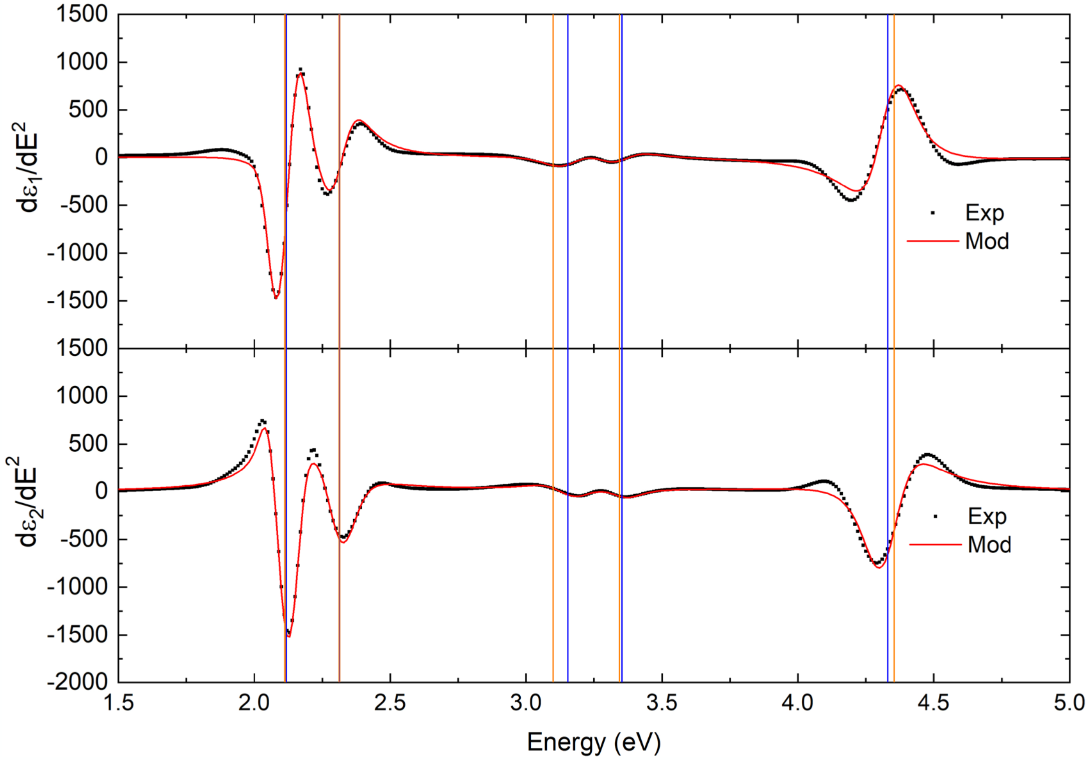


MODEL





2nd Derivative of the Dielectric Function



$$\varepsilon(\omega) = \frac{Ae^{i\phi}}{(-E_g - i\Gamma + \omega)^2}$$

Critical Points of GeSn (Blue)

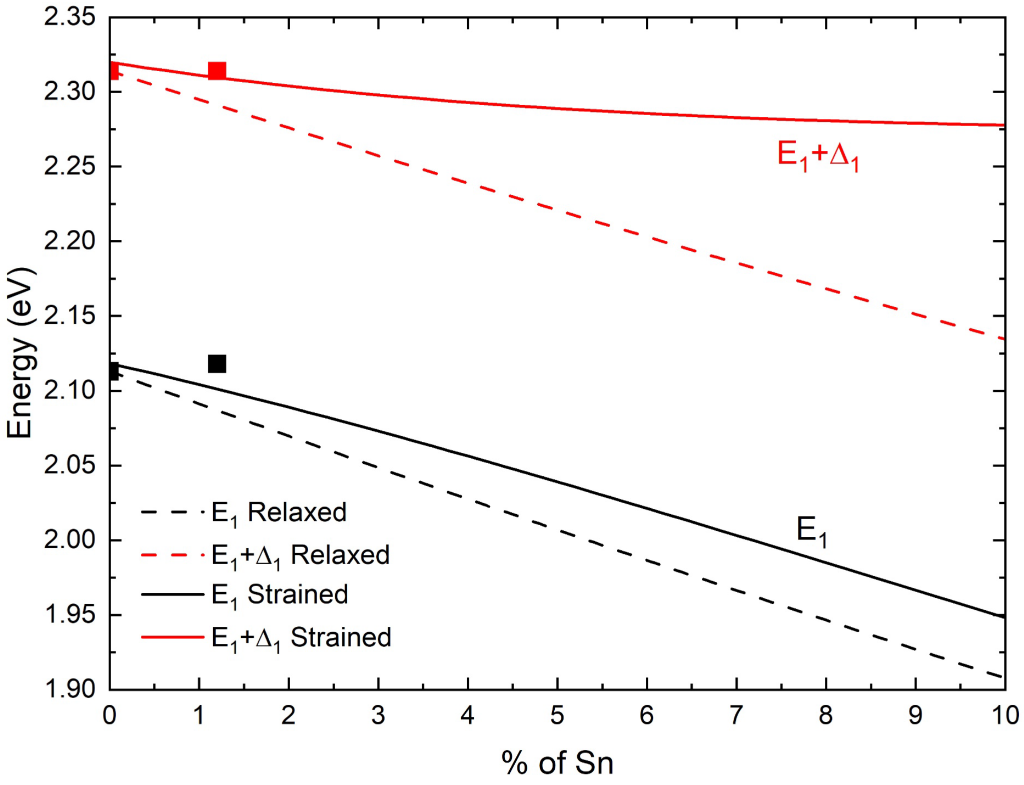
CP	*E* (eV)	*A*	Φ (deg)	Γ (meV)	*n*
E_1	2.118	5.73	248	0.048	0
$E_1+\Delta_1$	2.269	5.43	248	0.088	0
E'_0	3.155	1.32	224	0.115	0
$E'_0+\Delta'_0$	3.324	0.873	235	0.103	0
E_2	4.329	13.1	310	0.121	0

Critical Points of Ge (Orange)

CP	*E* (eV)	*A*	Φ (deg)	Γ (meV)	*n*
E_1	2.113	5.32	246	0.050	0
$E_1+\Delta_1$	2.314	3.53	246	0.066	0
E'_0	3.099	1.33	175	0.102	0
$E'_0+\Delta'_0$	3.344	0.486	266	0.139	0
E_2	4.354	11.2	318	0.097	0

By fitting the 2nd derivative of the dielectric function, the critical point parameters were found. This includes energy, amplitude, phase angle, broadening, and the line shape. The phase angle for E_1 and $E_1+\Delta_1$ were fixed to be the same.

Theoretical E_1 & $E_1+\Delta_1$ with Tin Content



The marked squares are the measured energies of bulk Ge and the $Ge_{1-y}Sn_y$ epitaxial layer. The $Ge_{1-y}Sn_y$ energy for the E_1 is slightly higher.

Relaxed:

$$\boldsymbol{E_1^{GeSn} = yE_1^{Sn} + (1-y)E_1^{Ge} - b_{GeSn}y(1-y)}$$

$$\boldsymbol{(E_1+\Delta_1)^{GeSn} = y(E_1+\Delta_1)^{Sn} + (1-y)(E_1+\Delta_1)^{Ge} - b_{GeSn}y(1-y)}$$

$$b_{GeSn} = 1.350 \text{ eV}$$

Strained:

$$\boldsymbol{E_1^{GeSn} = E_1^{Relaxed} + \Delta E_H - \frac{\Delta E_s^2}{\Delta_1}}$$

$$\boldsymbol{(E_1+\Delta_1)^{GeSn} = (E_1+\Delta_1)^{Relaxed} + \Delta E_H + \frac{\Delta E_s^2}{\Delta_1}}$$

small shear approximation
$\Delta E_s \ll \Delta_1$

$$\Delta E_H = \sqrt{3}\left[yD_1^{1\,Sn} + (1-y)D_1^{1\,Ge}\right]\varepsilon_H$$

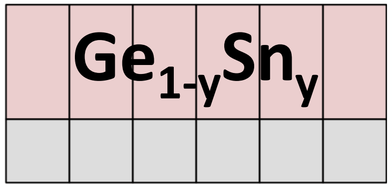
$$D_1^{1\,Sn} = -5.4 \text{ eV}, \quad D_1^{1\,Ge} = -8.7\text{eV}, \quad \varepsilon_H = \frac{\varepsilon_\perp + 2\varepsilon_{||}}{3}$$

$$\Delta E_S = \sqrt{6}\left[yD_3^{3\,Sn} + (1-y)D_3^{3\,Ge}\right]\varepsilon_S$$

$$D_3^{3\,Sn} = -3.8 \text{ eV}, \quad D_3^{3\,Ge} = -5.6 \text{ eV}, \quad \varepsilon_S = \frac{\varepsilon_\perp + \varepsilon_{||}}{3}$$

Conclusion

- The (224) reciprocal space maps showed that the GeSn epitaxial layer was grown pseudomorphically (fully strained).
- Using Vegard's Law, continuum elasticity theory, and the (004) reciprocal space map, the tin content is found to be y=0.012.
- After cleaning the sample, the thickness of the oxide was reduced to 26 Å
- Using the ellipsometry data, the fitted GeSn dielectric function was similar to bulk Ge most likely because of the low tin content.
- The fit second derivative of the dielectric function helped find the critical point parameters and compared to bulk Ge
- The energy for the E_1 is slightly higher in the GeSn layer despite theory.



Questions?

BE BOLD. Shape the Future.®

References

[1] P. F. Fewster, *X-ray scattering from semiconductors*. London: World Scientific (2016)

[2] N.S. Fernando, R.A. Carrasco, R. Hickey, J. Hart, R. Hazbun, S. Schoeche, J.N. Hilfiker, J. Kolodzey, and S. Zollner, Band gap and strain engineering of pseudomorphic $Ge_{1-x-y}Si_xSn_y$ alloys on Ge and GaAs for photonic applications, J. Vac. Sci. Technol. B **36,** Mar/Apr (2018).

[3] N.S. Fernando, T.N. Nunley, A. R. Ghosh, C.M. Nelson, J.A. Cooke, A.A. Medina, S. Zollner, C. Xu, J. Menendez, and J. Kouvetakis, Temperature dependence of the interband critical points of bulk Ge and strained Ge on Si, Applied Surface Science **421**, 905-912 (2017).

[4] T.N. Nunley, N.S. Fernando, N. Samarasingha, J.M. Moya, C.M. Nelson, A.A. Medina, and S. Zollner, Optical constants of germanium and thermally grown germanium dioxide from 0.5 to 6.6 eV via a multi-sample ellipsometry investigation, J. Vac. Sci. Technol. B **34,** 061205 (2016).

[5] H.G. Tompkins, and J.N. Hilfiker. *Spectroscopic Ellipsometry: Practical Application to Thin Film Characterization,* Momentum Press (2016).