Optical and X-ray Characterization of $Ge_{1-y}Sn_y$ Alloy on GaAs

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

1. Department of Physics, New Mexico State University, Las Cruces, NM

2. QuantTera, Scottsdale, AZ

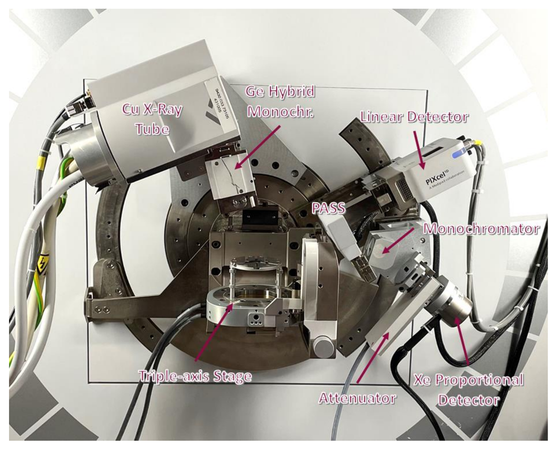
NM STATE

Abstract:

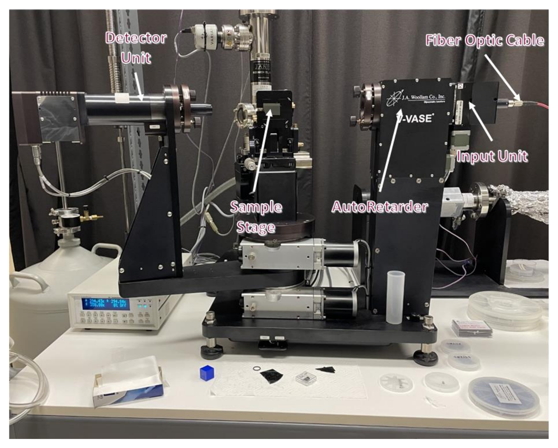
- A $Ge_{1-y}Sn_y$ alloy layer with 1600 nm thickness grown on GaAs by chemical vapor epitaxy.
- (004) reciprocal space maps and rocking curves: lattice constants.
- (224) reciprocal space maps: strain and relaxation.
- Ellipsometry spectra (ψ, Δ) were modeled to determine the dielectric function of the $Ge_{1-y}Sn_y$ layer.
- The optical constants for the layer was compared to bulk Ge.
- The second derivative of the dielectric function of $Ge_{1-y}Sn_y$ was fitted with analytical line shapes to determine the critical point parameters.

Methods:

- The sample was cleaned ultrasonically with water and isopropanol to remove organic layers and most of the native oxide before performing ellipsometry measurements.
- Using high resolution X-ray diffraction, we were able to obtain (004) and (224) rocking curves, ω-2θ scans, and (004), (224) grazing exit, and $(\bar{2}\bar{2}4)$ grazing incidence reciprocal space maps of $Ge_{1-y}Sn_y$ alloy on GaAs, bulk Ge, and bulk GaAs for comparison. Below is the configuration for the x-ray diffraction for (224) grazing exit geometry
- Using a vertical variable angle of incidence ellipsometer equipped with a Berek wave plate compensator, we obtained the ellipsometric angles of ψ and Δ from 0.5 eV to 6.5 eV and 60 to 75° incidence angles.
- The pseudodielectric function was fitted using a four-layer model consisting of a GaAs substrate, a pure Ge layer, a GeO_2 oxide, and air as the ambient.



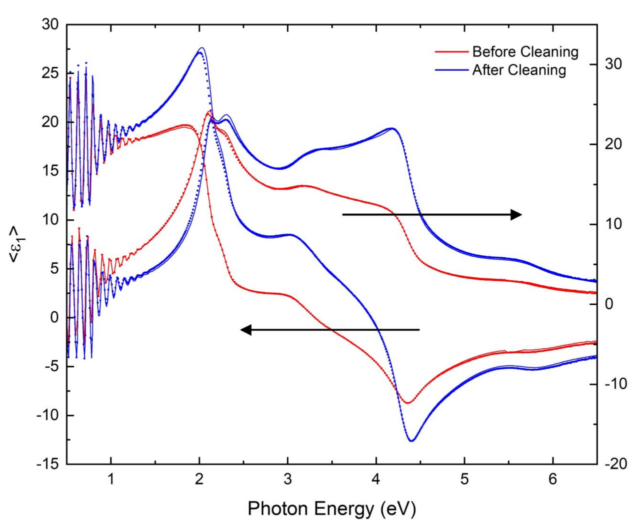
Malvern Panalytical Empyrean



J.A. Woollam WVASE

Sample Thickness and Cleaning:

PseudoDielectric Function:



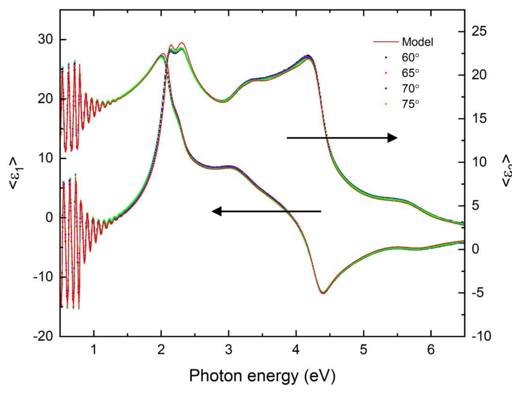
Ultrasonic cleaning, first with water then with isopropyl alcohol.

- Added water and sample into beaker. Placed beaker into ultrasonic cleaner for 15 mins. Remove sample from beaker.
- Added isopropyl alcohol and the sample to another beaker. Placed new beaker into ultrasonic cleaner for 15 mins.
- Remove sample and dried sample with compressed air.

	Oxide Thickness (Å):
As Received (May 20th):	43.6
Before Cleaning (June 14th):	72.1
After Cleaning (June 14th):	26.5
After 2nd Cleaning (June 15th):	25.9

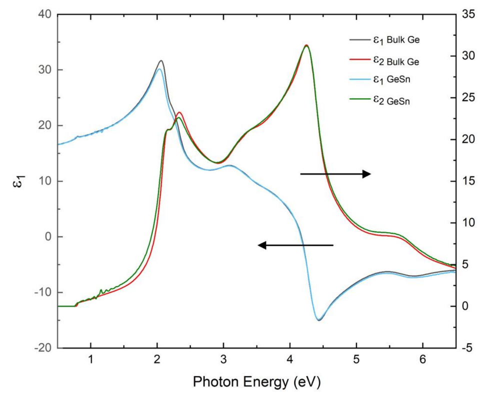
UV Ellipsometry Data:

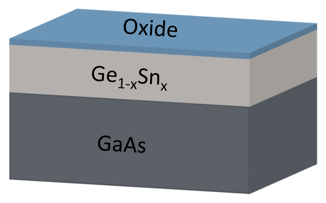
Pseudodielectric Function:



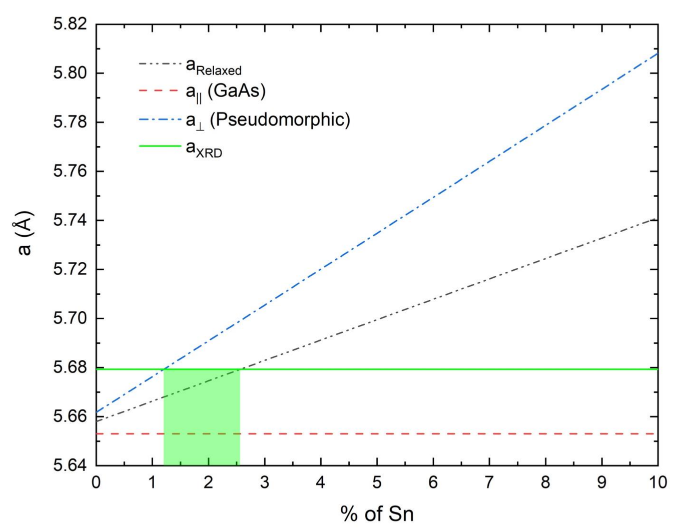
MODEL

Optical Constants:





Lattice Parameters:



Bragg's Law: $\lambda = 2d\sin\theta \qquad a_{GeSn} = 4d$

$a^{\perp}_{GeSn}$= 5.679 Å $\qquad a_{Ge}$= 5.658 Å

a_{GaAs}= 5.653 Å $\qquad a_{Sn}$= 6.489 Å

Vegard's Law: $a_{\text{Relaxed}}(y) = aSny + aGe(1-y)$

$a^{||}_{GeSn} = a_{\text{substrate}}$= 5.653 Å *Pseudomorphic Condition*

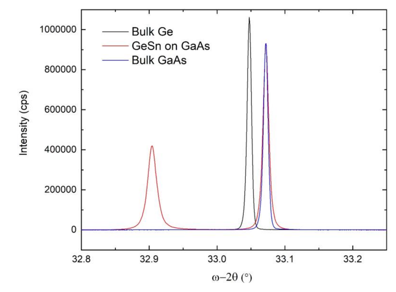
$$a_{\perp} = (1+\varepsilon_{\perp})a_{\text{Relaxed}}(y) \qquad \varepsilon_{\perp} = -\frac{2v}{1-v}\varepsilon_{||} \qquad \varepsilon_{||} = \frac{a^{||}_{GeSn}}{a_{\text{Relaxed}}(y)} - 1$$

Poisson Ratio: $v = 0.3$

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

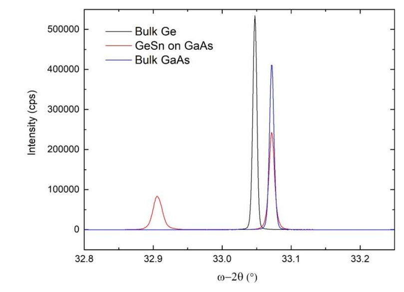
(004) Rocking Curve and Omega-2Theta Scans:

Omega-2Theta Open Detector:



FWHM
Bulk Ge 0.0075°
GaAs 0.0100°
GeSn 0.0156°
Bulk GaAs 0.0078°

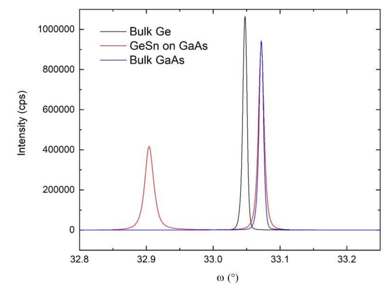
Omega-2Theta Receiving Slit:



FWHM
Bulk Ge 0.0069°
GaAs 0.0091°
GeSn 0.0154°
Bulk GaAs 0.0074°

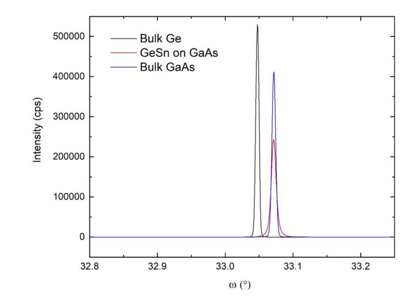
d-spacing:
Bulk Ge: 1.414 Å
GaAs: 1.413 Å
GeSn: 1.419 Å
Bulk GaAs: 1.413 Å

Rocking Curve Open Detector:



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

Rocking Curve Receiving Slit:



FWHM
Bulk Ge 0.0057°
GaAs 0.0084°
Bulk GaAs 0.0065°
Layer peak is missing (slit)

Reciprocal Space Maps:

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

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

$$\lambda = 1.5406 \text{ Å}$$

W-Wavelength Streak

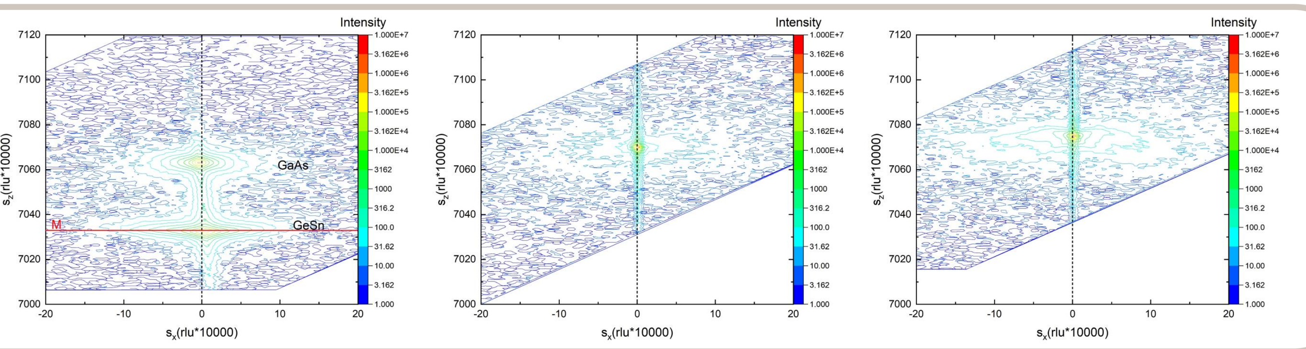
M-Mosaic Spread (Relaxation Line)

Black line drawn from origin (Relaxed)

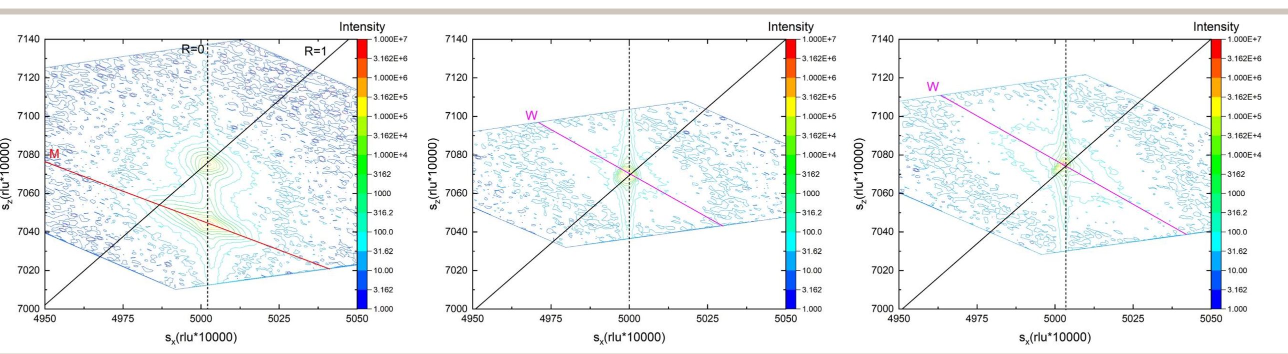
Dashed line drawn through substrate peak (Pseudomorphic)

GeSn on GaAs: **Bulk Ge:** **Bulk GaAs:**

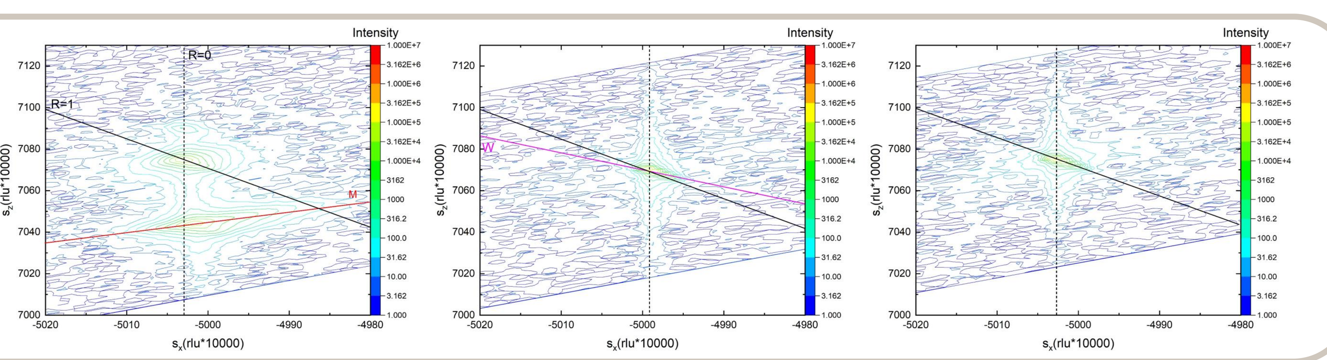
(004):



(224) Grazing Incidence:

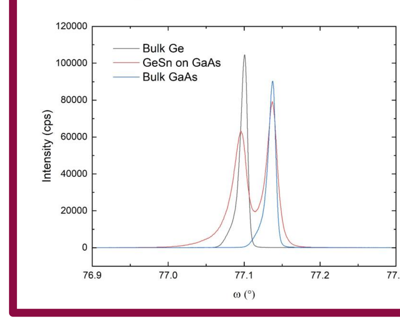


$(\bar{2}\bar{2}4)$ Grazing Exit:



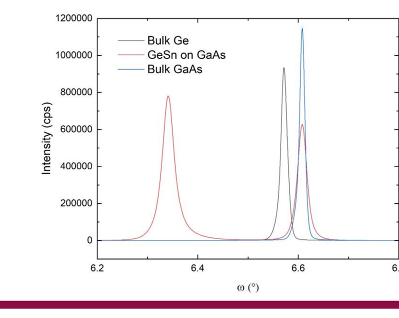
(224) and $(\bar{2}\bar{2}4)$ Rocking Curve (Open Detector):

Grazing Exit:



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

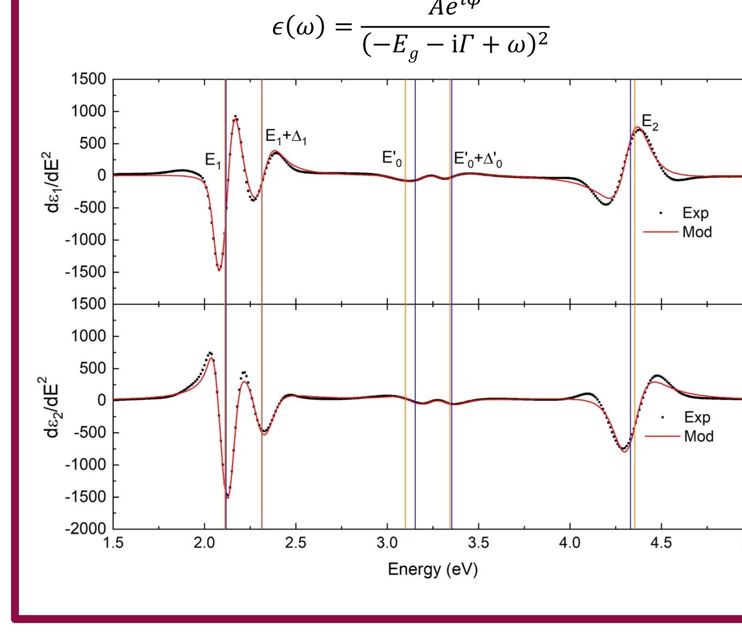
Grazing Incidence:



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

2nd Derivative of Dielectric Function of $Ge_{1-y}Sn_y$:

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



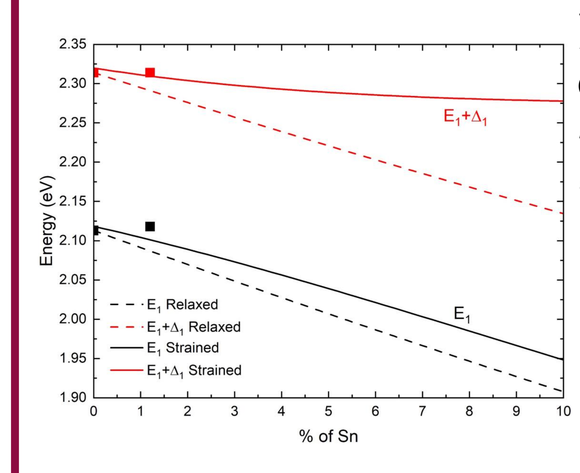
Critical Points of GeSn (Blue)

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

E_1 and $E_1+\Delta_1$ Tin Content:



Relaxed:

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

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

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

Strained:

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

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

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:

- Using Vegard's Law, continuum elasticity theory, and the (004) reciprocal space map, we determine that the tin content is y=0.012.
- The (224) reciprocal space maps allow us to find that the alloy layer was grown pseudomorphically on the GaAs substrate despite the large thickness.
- After modeling the ellipsometry data, we found that the oxide thickness is 2.6 nm and the epilayer thickness is 1600 nm.
- The point-by-point fit of the $Ge_{1-y}Sn_y$ dielectric function was very similar to bulk Ge.
- Using the second derivative, we found the critical point parameters, including amplitude, energy, broadening, and phase angle.
- E_1 is found to have a slightly higher energy in $Ge_{1-y}Sn_y$ than in bulk Ge. That is puzzling, even with the phase angle fixed to be the same.

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).

NM STATE **BE BOLD.** Shape the Future.

FA9550-20-1-0135

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