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# The strain-stress relationships for band gap, phonon and plasmon energies in monoclinic Ga2O3 and related materials

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**14. ABSTRACT**
The objectives of this proposal are to map the strain-stress relationships for eigenenergies in semiconductor materials with monoclinic symmetry. The eigenenergies of interest in this proposal are phonon mode energies, coupled phonon and free charge carrier mode energies, and band-to-band transition energies. Specifically, this proposal aims (1) to perform strain analysis in homo- and heteroepitaxial monoclinic gallium oxide and related materials, (2) to perform experimental determination of phonons, band-to-band transitions, and free charge carrier eigenmodes as a function of strain, and (3) to determine the pressure and deformation potential relationship for phonon and phonon-plasmon coupled modes, and for the band-toband transitions in monoclinic semiconductors in gallium oxide and related materials. The approaches include the application of the generalized spectroscopic ellipsometry method from the Terahertz to the vacuum-ultraviolet spectral range, and the optical Hall effect in the THz to the Nearinfrared spectral range. The approaches further include the exploitation of epitaxial strain inherent to epitaxial layer growth. Crystal growth experts and collaborators provide large sets of samples with different states of strain.


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  - Mathias Schubert
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- Report Due Date
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- Report Period Start Date
  - 7/01/2018
- Report Period End Date
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- Current Program Officer
  - Dr. Ali Sayir

Please list any other Co-Program Officers (if applicable)

# Publications

Our servers will be contacting the Cross Reference open source database (https://www.crossref.org/) to find any publications related to your award number. These publications will automatically populate to your report page and you will be able to select the reports that you would like to submit for the reporting period. Note: for annual/interim reports, you should only report publications that were completed in the current reporting period. For final reports, you should report all publications throughout the entire lifecycle of the grant.

If a publication does not show up in the initial publication search, you will also be able to manually enter publications using the publication's DOI number. Our servers will then contact Cross Reference to see if they can verify your publication information. Lastly, if your publication does not contain a DOI number, you can simply enter the bibliographic information into the text field.

All publications are listed in the online questionnaire.

The following manuscripts are either under review or in preparation:

The influence of strain and composition on the infrared active phonons in epitaxial β-(AlxGa1-x)2O3 deposited onto (010) β-Ga2O3, M. Stokey, R. Korlacki, S. Knight, M. Hilfiker, V. Darakchieva, A. Mauze, Y. Zhang, J. Speck, and M. Schubert, Phys. Rev. B, (2022).

Electron Spin Resonance of cerium-II and cerium-III site-induced defect signatures in monoclinic symmetry lutetium silicate measured by THz generalized magnetooptic ellipsometry, S. Knight, S. Richter, M. Stokey, P. Kuehne, V. Darakchieva, and M. Schubert, Appl. Phys. Lett. (2022).

Strain and stress relationships for longitudinal optical phonon modes in β-Ga2O3, R. Korlacki, J. Knudtson, M. Stokey, A. Mock, S. Knight, A. Papamichail, V. Darakchieva, and M. Schubert, Appl. Phys. Lett. (2022).

Terahertz-EPR Ellipsometry identification of Fe3+ in monoclinic gallium oxide, S. Richter, S. Knight, M. Stokey, P. Kuehne, A. Ruder, V. Darakchieva, and M. Schubert, Nature group (2022).

Strain and composition dependencies of the near bandgap optical transitions in monoclinic (AlxGa1-x)2O3 alloys with coherent biaxial in-plane strain on (010) Ga2O3, R. Korlacki, M. Hilfiker, J. Knudtson, M. Stokey, U. Kilic, A. Mauze, Y. Zhang, J. Speck, V. Darakchieva, and M. Schubert, Phys. Rev. Applied XX, XX (2022)

Quantum Composites – Disordered Materials Exhibiting Strongly-Correlated Phenomena, Z. Barani, T. Geremew, M. Stokey, E. Raymond, F. Kargar, M. Schubert, T. T. Salguero, and A. A. Balandin, nature materials XX, XX (2022).

A note is made for the following publication: Dugan, C., Wang, L., Zhang, K., Mann, J.M., Kimani, M.M., Mei, W., Dowben, P.A. and Petrosky, J. (2022), Interband Transitions and Critical Points of Single-Crystal Thoria Compared with Urania. Phys. Status Solidi B 2200238. https://doi.org/10.1002/pssb.202200238, currently also listed under this current award:

> The PI has opened a scientific misconduct investigation with UNL about this publication. The PI suspects that his former graduate student, Alyssa Mock, was deliberately denied co-authorship in this paper, while his present AFOSR award number was acknowledged due to an apparent “copy and paste” error by the current group of authors. A detailed investigation is to follow. Presently, while to content of this paper is indeed the result of a collaboration between the current authors and members of the PIs team (Alyssa Mock, Rafal Korlacki and Mathias Schubert), the collaboration was not honored when this paper was prepared, submitted, and published.

# Participants

You will be asked to provide the information below for: (1) PIs; and (2) each person who worked on and was funded by this grant during the current reporting period. Please include all participants including yourself.

- Provide the name and identify the role the person played in this project.
- Indicate the total number of months (including partial months) that the individual worked on this project.
- If applicable, the participant's ORCID.
- Project role, select the most senior role in which the person worked on the project for any significant length of time.
    - For example, if an undergraduate student graduated, entered graduate school, and continued to work on the project, report that person as a graduate student, preferably explaining the change in involvement.
- Contribution to the project (text field).
- If international business was accomplished during this reporting period
    - Did the individual collaborate with individuals located in a foreign country?
    - Did this individual travel to a foreign country as part of the collaboration?

    **If the answer to either question above is yes, you will be expected to report the country that business was conducted in, and the amount of days spent in that country.

1. Matthew Hilfiker 48 months graduate student 0000-0002-7015-5484
Matthew performed near-infrared to vacuum ultra violet ellipsometry investigations of ultra wide band gap metal oxide semiconductor bulk crystals and epitaxial layers such as Gallium Oxide, Aluminum Gallium Oxide, Indium Oxide, Zinc Gallate, Neodymium Gallium Oxide, Lutetium Silicon Oxide, Yttrium Silicon Oxide, and more. He also performed elevated temperature ellipsometry investigations. Matthew performed model data analyses of the ellipsmetric measurements and determined band to band transition including exciton properties, their anisotropy and direction dependencies, temperature dependencies and strain and composition dependencies where accessible.

Travel to Germany for one month. Collaborated with researchers at the Leibniz Institute for polymer research in Dresden. Author and co-author of 15 publications.
Graduated May 2022

2. Megan Stokey 48 months graduate student 0000-0003-0701-2218
Megan performed far-infrared and mid-infrared ellipsometry characterization of ultra wide band gap metal oxide semiconductor bulk crystals and epitaxial layers including Gallium Oxide, Aluminum Gallium Oxide, Indium Oxide, Zinc Gallate, Neodymium Gallium Oxide, Lutetium Silicon Oxide, Yttrium Silicon Oxide, and more. Megan determined phonon, plasmon, and free charge carrier properties, their composition, strain, and doping dependencies where accessible.

Author and co-author of 15 publications.

Will graduate in May 2023

3. Alexander Ruder 24 months graduate student 0000-0001-8023-8374

Alexander developed Terahertz ellipsometry and visible light imaging ellipsometry instrumentations. Alexander participated in the model analysis and investigations of the ultra wide band gap metal oxides investigated in this project. Alexander developed instrumentation and help performed temperature dependent ellipsometry measurements on ultra wide band gap metal oxide semiconductor materials.

Travel to Germany for one month. Collaborated with researchers at the Leibniz Institute for polymer research in Dresden. Travel to Sweden for one month. Collaborated with researchers at the physics department at Linkoping University. Author and co-author of 5 publications. Will graduate in December 2023

4. Shawn Wimer 24 months graduate student 0000-0001-8917-3351

Shawn performed structural investigations using high resolution transmission electron microscopy of selected samples and materials.

5. Korlacki, Rafal Research Engineer, 0000-0003-3989-2731

Rafal performed first principles calculations for strain and composition dependencies of band structure properties in Gallium Oxide, Aluminum Gallium Oxide, Indium Oxide, Zinc Gallate, Neodymium Gallium Oxide, Lutetium Silicon Oxide, Yttrium Silicon Oxide, and more. Bandstructure and electronic properties results were critical for correct interpretation of experimental data obtained with spectroscopic ellipsometry, to identify correct band to band transition energies, exciton contributions, effective mass parameters and phonon modes including their lattice direction dependencies. Rafal also supervised undergraduate students Jenna Knudtson and Teresa Gramer. Jenna performed first principles calculations for the strain dependencies of longitudinal phonon modes in the Aluminum Gallium Oxide system. Teresa performed phonon mode analysis for low symmetry lithium gallate.

6. Knudtson, Jenna 0000-0001-5338-3963

Jenna performed first principle calculations for the phonon mode properties in monoclinic and rhombohedral Gallium Oxide under strain, and provided detailed analyses for the deformation potentials. Jenna was trained by Rafal Korlacki in density functional theory and density functional perturbation theory approaches.

7. Gramer, Teresa 0000-0002-4499-5754

Teresa performed infrared measurements of anisotropic phonon mode properties in orthorhombic lithium gallate ($LiGaO_2$). She was trained by graduate student Megan Stokey in operation of ellipsometry instrumentation and present knowledge of data analyses for low symmetry metal oxides and other ultrawide band gap materials. Teresa has started to work as graduate student in our group at the end of this award period.

8. Williams, Emma 0000-0003-4154-7275

Emma performed temperature dependent measurements of the optical properties of Zinc Gallate, Neodymium Gallium Oxide, Lutetium Silicon Oxide, Yttrium Silicon Oxide, and more. She was trained by Matthew Hilfiker in instrumentation operation and ellipsometry data analysis. Emma analyzed temperature dependencies of band to band transitions and exciton properties in Zinc Gallate.

9. Kilic, Ufuk 0000-0002-4235-3002

Ufuk performed ultraviolet to vacuum ultraviolet spectroscopic ellipsometry investigations on Gallium Oxide, Aluminum Gallium Oxide, Indium Oxide, Zinc Gallate, Neodymium Gallium Oxide, Lutetium Silicon Oxide, Yttrium Silicon Oxide, and more. Ufuk supported model analysis of ellipsometry data performed by Matthew Hilfiker and Megan Stokey.

10. Traouli, Yusra 0000-0002-8566-8856

Yusra participated and supported temperature dependent nearinfrared to ultraviolet spectroscopic ellipsometry measurements of Neodymium Gallium Oxide. She performed model data analysis and was trained and supervised by Matthew Hilfiker.

11. Koeppe, Nate

Nate participated in THz ellipsometry instrumentation development. He performed data acquisition and supported model data analysis. Nate participated in development of new software routines for calibration of arbitrarily anisotropic waveplates for use in Mueller matrix ellipsometry at THz wavelengths.

12. Rivera-Castro, Jose 0000-0002-8241-5407

Jose was trained in in-situ ellipsometry measurement and data analysis. He participated in Development of remote controlled temperature control for ultra-high vacuum sample chamber used in elevated temperature ellipsometry measurements of ultra wide band gap metal oxides.

13. Abakar Choukou, assay 0000-0003-4068-1683

Assay participated in building the ultra high vacuum chamber with optical access for measurement of ellipsometric parameters from anisotropic samples placed at elevated temperatures.

14. Schubert, Mathias 0000-0001-6238-663X

Mathias led all activities and provided supervision for all graduate and undergraduate students. He trained or supervised training for all participants. Mathias initiated all activities, and organized and led group meetings with all members of the team as well as with outside collaborators. Mathias also organized all outside collaboration with teams at University Linkoping Sweden, Institute for Crystal Growth in Berlin, the Max Planck Society in Berlin (Fritz Haber Institute), and groups within the US at UCSB, Ohio State, Utah, Cornell, UC Riverside and others. Mathias oversaw organization of manuscript preparations by all participants. He also prepared all reports.

# Other Partners or Collaborators

This section will ask you to describe partner organization or collaborators who worked on this grant – academic institutions, other nonprofits, industrial or commercial firms, state or local governments, schools or school systems, or other organizations (foreign or domestic) – that were involved with the project. Partner organizations may have provided financial or in-kind support, supplied facilities or equipment, collaborated in the project, exchanged personnel, or otherwise contributed.

If you do not have any additional partners to report, please leave this section blank.

1. University of Linkoping

Department of Physics, Chemistry and Biology, Linköping University, 58183 Linköping, Sweden

The UNLincoln team collaborated with the team of Professor Dr. Vanya Darakchieva on ellipsometry characterization and data interpretation on ultra wide band gap metal oxide semiconductors. The teams collaborate on THz instrumentation development. The teams collaborate on development of advanced model approaches for analysis of low symmetry semiconductor materials. The Linkoping team provided in kind support, supplied facilities (THz and farinfrared ellipsometry), and provided materials. The Linkoping team also grows Gallium Oxide and related materials in heteroepitaxial form using hot wall metal organic vapor epitaxy. The Linkoping team provided support for visiting students (Alexander Ruder) and for visiting guest professors (Mathias Schubert).

Linkoping
Sweden

2. Leibniz-Institut für Kristallzüchtung, Berlin 12489, Germany

Zbigniew Galazka provided single crystals of Gallium Oxide with different doping (Sn, Al, Cr, Cu,

Fe) and of Zing Gallate. Guenther Wagner and Andreas Popp provided epitaxial Gallium Oxide samples grown on sapphire and Gallium Oxide. Klaus Irmscher and Andreas Fielder provided information and critical discussion on defect characteristics in Gallium Oxide using electron paramagnetic resonance spectroscopy techniques.

3. United States Naval Research Laboratory, Washington, DC 20375, USA

Virginia Wheeler provided epitaxial samples of Gallium Oxide with different phase compositions. Marko Tadjer provided epitaxial Gallium Oxide samples with different levels of Sn doping grown on sapphire and Gallium Oxide.

4. Materials Department, University of California Santa Barbara, Santa Barbara, California 93106, USA

James Speck provided epitaxial samples of beta-phase Aluminum Gallium Oxide grown pseudomorphic onto (010) Gallium Oxide.

5. Air Force Institute of Technology, Wright-Patterson Air Force Base, Ohio 45433-7765, USA

James Petrosky provided samples of Uranium Oxide and Thorium Oxide.

6. Air Force Research Laboratory, Sensors Directorate, Wright Patterson AFB, Ohio 45433, USA

Matthew Mann provided information on Uranium Oxide and Thorium Oxide for phonon and band structure analyses using ellipsometry.

7. Department of Electrical and Computer Engineering, The University of Utah, Salt Lake City, Utah 84112, USA

Berardi Sensale-Rodriguez and Michael A. Scarpulla provided single crystal Gallium Oxide samples and collaboration on THz characteristics of Gallium Oxide.

8. Electrical and Computer Engineering, Florida International University, University Park Campus, Miami, Florida 33199

Frank Urban III provided results from computational methods in search for time and cost reduction during spectroscopic analyses of monoclinic Gallium Oxide and heteroepitaxial systems.

9. J.A. Woollam Co. Inc., Lincoln, Nebraska 68508, USA

Craig Herzinger provided software support for operation and calibration of THz instrumentation.

10. Department of Material Science and Engineering, Cornell University

Huili Grace Xing and DebDeep Jena provided alpha-phase Aluminum Gallium Oxide samples and information about structural and electronic properties.

Note: All subsequent collaborators are not listed in online questionnaire since there seems to be a limit of 10.

11. Department of Electrical and Computer Engineering and Department of Materials Science and Engineering, The Ohio State University, Columbus, Ohio 43210, USA

Hongping Zhao provided epitaxial samples for Indium Oxide and monoclinic phase Aluminum Gallium Oxide.

12. CEITEC-Central European Institute of Technology, Brno University of Technology, Brno, Czech Republic

Petr Neugebauer provided critical discussions and insights into existing instrumentation and measurement approaches in high field electron paramagnetic resonance spectroscopy.

13. Electrical Engineering and Computer Science Department, University of Michigan, Ann Arbor, Michigan 48109, USA

Elaheh Ahmadi provided epitaxial alpha phase Aluminum Gallium Oxide samples.

14. Fritz Haber Institute of the Max Planck Society, Berlin, Germany

Alexander Paarman provided access to measurement facilities at the free electron laser source in Berlin, Germany, and collaborated by providing expertise and data analysis for infrared reflectance and prism configuration measurements.

15. Vanderbilt University, Nashville, TN, USA

Joshua Caldwell provided information and critical discussions about infrared vibration properties of materials.

16. Photonics Initiative, Advanced Science Research Center, City University of New York, New York, NY, USA

Andrea Alu provided critical expertise and computational results for correct interpretation of surface and bulk electromagnetic excitations in monoclinic Gallium Oxide.

# Section 2: Technical Report PDF Upload

You will be asked to complete the following questions as part of the report documentation section:

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# Accomplishments

The information provided in this section allows AFOSR to assess whether satisfactory progress has been made during this reporting period. The PI is reminded that the recipient organization is required to obtain prior written approval from the awarding agency grants official whenever there are significant changes in the project or its direction. See agency specific instructions for submission of these requests.

- Research Objectives: Please list the main research objectives of this project
  - List the major goals of the project including the scientific or technological objectives of this effort. Describe the proposed technical approach to obtain those goals. If the application listed milestones/target dates for important activities or phases of the project, identify these dates and show actual completion dates or the percentage of completion.
  - The objectives of this proposal are to map the strain-stress relationships for eigenenergies in semiconductor materials with monoclinic symmetry. The eigenenergies of interest in this proposal are phonon mode energies, coupled phonon and free charge carrier mode energies, and band-to-band transition energies. Specifically, this proposal aims (1) to perform strain analysis in homo- and heteroepitaxial monoclinic gallium oxide and related materials, (2) to perform experimental determination of phonons, band-to-band transitions, and free charge carrier eigenmodes as a function of strain, and (3) to determine the pressure and deformation potential relationship for phonon and phonon-plasmon coupled modes, and for the band-to-band transitions in monoclinic semiconductors in gallium oxide and related materials. The approaches include the application of the generalized spectroscopic ellipsometry method from the Terahertz to the vacuum-ultraviolet spectral range, and the optical Hall effect in the THz to the

Nearinfrared spectral range. The approaches further include the exploitation of epitaxial strain inherent to epitaxial layer growth. Crystal growth experts and collaborators provide large sets of samples with different states of strain. The approaches include further the determination of the monoclinic symmetry perturbation theory parameters for eigenenergies. The goal is to find deformation potential and pressure coefficient parameters for the eigenenergies (phonon modes, free charge carrier modes, band-to-band transitions) as a function of the strain variables determined from structural investigations. The approaches further include to explore the effects of strain onto new physical properties.

- Please provide details of accomplishments during this reporting period.
  - For this reporting period describe: 1) major activities; 2) specific objectives; 3) significant results or key outcomes, including major findings, developments, or conclusions (both positive and negative); and/or 4) other achievements. Include a discussion of stated goals not met.
  - 1) major activities;
    - We investigated strain and composition dependencies of the near bandgap optical transitions in monoclinic $(Al_xGa_{1-x})_2O_3$ alloys with coherent biaxial in-plane strain grown on (010) $Ga_2O_3$.
      - Measured phonon modes and band to band transitions in monoclinic $(Al_xGa_{1-x})_2O_3$ alloys with coherent biaxial in-plane strain grown on (010) $Ga_2O_3$.
      - Calculated band structures for band to band transitions and phonon modes in monoclinic structure $Al_2O_3$.
      - Calculated the effects of strain onto band structure properties of monoclinic $Ga_2O_3$ and monoclinic $Al_2O_3$.
    - We also investigated the composition dependencies of the near bandgap optical transitions in rhombohedral $(Al_xGa_{1-x})_2O_3$ alloys with incoherent zero in-plane strain grown on sapphire (rhombohedral $Al_2O_3$).
      - Measured phonon modes and band to band transitions in monoclinic $(Al_xGa_{1-x})_2O_3$ alloys with coherent biaxial in-plane strain grown on (010) $Ga_2O_3$.
      - Calculated band structures to obtain band to band transitions and phonon modes in rhombohedral structure $Ga_2O_3$ and $Al_2O_3$.
      - Calculated the effects of strain onto band structure properties of rhombohedral $Ga_2O_3$ and $Al_2O_3$.
    - The PI with a group of external collaborators collected, categorized, and reviewed existing band structure and material properties of transparent conducting and semiconducting oxides $Ga_2O_3$, $Al_2O_3$, $In_2O_3$, ZnO, $SnO_2$, CdO, NiO, CuO, and $Sc_2O_3$, and development perspectives on future uses of such materials in high power devices.
    - The PI had predicted the existence of shear polaritons in monoclinic lattice, and during this cycle a collaborative effort completed investigation of shear polariton phonon modes in monoclinic $Ga_2O_3$ by augmenting free electron laser facility measurements of the polarization dependence of the evanescent wave character of polarized reflected infrared light under

prism excitation conditions.

- We completed investigations of the dependencies of bandgap energy and associated exciton properties in spinel structure zing gallate, a potential alternative to gallium oxide with simpler crystal structure.
- We performed optical Hall investigations on high electron mobility structures based on aluminum gallium nitride with high aluminum content barrier layers, which were grown by the Linkoping collaborator group.
- We investigated epitaxial monoclinic gallium oxide material grown by hot-wall metal organic chemical vapor deposition grown by the Linkoping collaborator group.

- 2) specific objectives;
  - We aimed at mapping the strain and composition dependencies of the near bandgap optical transitions and phonon modes in monoclinic $(Al_xGa_{1-x})_2O_3$ alloys with coherent biaxial in-plane strain grown on (010) $Ga_2O_3$ using simple functional relationships.
    - To differentiate between the effects of strain and composition.
    - To find relationships that predict strain evolution for band to band transitions for any coherent in-plane strain different than (010).
    - To find relationships predicting the band gap offsets within the monoclinic $(Al_xGa_{1-x})_2O_3$ alloy system with and without strain.
  - We aimed at mapping the composition dependencies of the near bandgap optical transitions and phonon modes in rhombohedral $(Al_xGa_{1-x})_2O_3$ alloys with and without strain.
    - To differentiate between the effects of strain and composition.
    - To find relationships that predict strain evolution for band to band transitions for any coherent in-plane strain in the rhombohedral crystal system.
    - To find relationships predicting the band gap offsets within the monoclinic $(Al_xGa_{1-x})_2O_3$ alloy system with and without strain.
  - We aimed at developing perspectives on future uses of transparent conducting and semiconducting oxides $Ga_2O_3$, $Al_2O_3$, $In_2O_3$, ZnO, $SnO_2$, CdO, NiO, CuO, and $Sc_2O_3$in high power devices.
  - We aimed at demonstrating unequivocally the existence, and potential use of shear polariton modes in structures with monoclinic symmetry.
  - We aimed at demonstrating unequivocally the existence of excitons and their mechanisms to apparently reduce the energy of absorption onset in ultrawide bandgap metal oxide semiconductors.
  - We aimed at achieving better confinement of the electron channel in high electron mobility structures based on aluminum gallium nitride with high aluminum content barrier layers.
  - We aimed at evaluating the hot-wall metal organic chemical vapor deposition as a potential tool for cost reduced production of highest quality epitaxial monoclinic gallium oxide material.

- 3) significant results or key outcomes, including major findings, developments, or conclusions (both positive and negative); and/or

- We derived a set of deformation potential parameters and bowing parameters which correctly describe the observed near bandgap optical transitions in monoclinic $(Al_xGa_{1-x})_2O_3$ alloys with coherent biaxial in-plane strain grown on (010) $Ga_2O_3$. We also described the same for all optical phonon modes.
    - These functions treat the effects of strain and composition separately.
    - These functions permit to predict the in-plane strain induced band to band transition shifts for epitaxial strain that arises on any surface template, for example on monoclinic gallium oxide with (-201) orientation.
    - We found that the band offsets between monoclinic $Ga_2O_3$ and $(Al_xGa_{1-x})_2O_3$ with coherent biaxial in-plane strain grown on (010) $Ga_2O_3$ is much less than previously thought.
- We derived a set of linear and bowing parameters which correctly describe the composition dependencies of the near bandgap optical transitions and phonon modes in monoclinic $(Al_xGa_{1-x})_2O_3$ alloys.
    - We found a transition from indirect to direct characteristics between $Ga_2O_3$ and $Al_2O_3$, respectively, and we identified a switch in band order where the lowest band-to-band transition occurs with polarization perpendicular to c in $Ga_2O_3$ whereas for $Al_2O_3$ the lowest transition occurs with polarization parallel to c. We estimate that the change in band order occurs at approximately 40% Al content. Additionally, the characteristic of the lowest energy critical point transition for polarization parallel to c changes from M1 (quasi-2D) type in α-$Ga_2O_3$ to M0 (3D) type van Hove singularity in $Al_2O_3$.
- In our literature review we provided a critical discussion of experimentally determined bandgap energies available in the literature for monoclinic $Ga_2O_3$ potentially ending a long standing controversy about the bandgap energy. We derived the need for studies of metastable phases due to their potential use in device architectures for $Ga_2O_3$ and related alloys. Also, prospects for $Ga_2O_3$ alloys incorporating scandium became evident for possible use in high power devices.
- Our demonstration of the existence of shear polariton modes in monoclinic symmetry adds an interesting phenomenon into the tool box of the emerging field of phononics, where lattice vibrations are thought to be used for data storage, transport, and possibly also computation.
- In all linear optical absorption spectra of ultrawide bandgap metal oxides one must consider the existence of excitons prior to concluding the bandgap energy from the onset of absorption.
- An increase of the effective mass in the electron channel under the the aluminum gallium nitride barrier layer with 78% aluminum content was found (0.63 free electron mass versus 0.33 in bulk aluminum gallium nitride barrier layer with 78% aluminum content) and the physical origin

of this phenomenon remains unsolved so far.

- It was found that hot-wall metal organic chemical vapor deposition can produce high quality epitaxial monoclinic gallium oxide material. Further studies are warranted to expand understanding and controls to improve the technique.

- 4) other achievements
    - In a collaboration with the Leibniz Institute for Polymer Research the PI published a paper on Stretchable Thin Film Mechanical-Strain-Gated Switches and Logic Gate Functions Based on a Soft Tunneling Barrier in Advanced Materials (https://onlinelibrary.wiley.com/doi/10.1002/adma.202104769).

- How were the results disseminated to communities of interest? If there is nothing significant to report during this reporting period, state "Nothing to Report."
    - Describe how the results were disseminated to communities of interest for this reporting period. Include any outreach activities that were undertaken to reach members of communities who are not usually aware of these project activities, for the purpose of enhancing public understanding and increasing interest in learning and careers in science, technology, and the humanities.
        - PI Schubert presented a talk on Defect Characterization in Gallium Oxide and Related Materials Using Terahertz Electron Paramagnetic Resonance Ellipsometry: Fe in $Ga_2O_3$ during the 5th U.S. Gallium Oxide Workshop (GOX 2022) in Washington, D.C. in person in August 2022. He also presented an Invited Tutorial on Generalized Ellipsometry analysis of low-symmetry materials using a generalized polarizability model: A tutorial during the International Conference on Spectroscopic Ellipsometry 9, Beijing, China, online in May 2022. He also presented a colloquium on Exploring extreme wide bandgap metal-oxides for a carbon-emission-free power infrastructure: Strain, stress, alloying and defects in monoclinic gallium oxide and related compounds: Determination of phonon, free charge carrier, band gap and defect properties with THz Electron Paramagnetic Resonance, Optical Hall effect and ultra-wideband generalized ellipsometry at the Leibniz Institute for Surface Modification Leipzig e.V., Leipzig, Germany, online in January 2022. He also presented an invited talk on Ellipsometry and density functional theory characterization of gallium aluminum oxide: Effects of strain and alloying onto band gaps, excitons and phonons, and the $Fe^{3+}$ defect at the University of Utah, Salt Lake City, UT, online in April 2022. He also presented an invited talk on Defect Characterization in Gallium Oxide and Related Materials Using Terahertz Electron Paramagnetic Resonance Ellipsometry: Fe in $Ga_2O_3$ at the SiC 2022 Workshop in Cleveland, OH in person in August 2022. He also gave a talk on Oxide based high power electronic materials research for the future of green energy during the The 4th Conference on Advanced Functional Materials in Kolmarden, Sweden, in person in August 2022.
        - Graduate student Megan Stokey presented a poster on the Evolution of

Anisotropy and Order of Band-to-Band Transitions, Excitons, Phonons, Static and High Frequency Dielectric Constants Including Strain Dependencies in Alpha and Beta Phase (AlxGa1-x)2O3 during the 5th U.S. Gallium Oxide Workshop (GOX 2022) in Washington, D.C., in person in August 2022. She also presented a talk on Far-infrared and mid-infrared analysis of the dielectric function tensor of alpha and beta phase (AlxGa1-x)2O3 by combined density functional theory and generalized spectroscopic ellipsometry during the International Conference on Spectroscopic Ellipsometry 9, Beijing, China, online in May 2022.

- Graduate student Matthew Hilfiker presented a talk on Phonons and band-to-band transitions in zinc gallate - A combined density functional theory and ellipsometry approach during the International Conference on Spectroscopic Ellipsometry 9, Beijing, China, online in May 2022. He also presented a talk on The influence of strain and alloying onto the exciton and band-to-band transitions in (AlxGa1-x)2O3 at the International Conference on Spectroscopic Ellipsometry 9, Beijing, China, online in May 2022.
- Graduate student Alexander Ruder presented a talk on Mueller matrix imaging using slanted columnar thin film mirrors during the International Conference on Spectroscopic Ellipsometry 9, Beijing, China, online in May 2022.
- Undergraduate student Teresa Gramer presented on the Infrared-Active Phonon Modes and Static Dielectric Constants of Orthorhombic LiGaO2 at the 5th U.S. Gallium Oxide Workshop (GOX 2022) in Washington, D.C. in person in August 2022.
- Undergraduate student Emma Williams presented a poster on Spectroscopic Ellipsometry Optical Analysis of Zinc Gallate at Elevated Temperatures during the 5th U.S. Gallium Oxide Workshop (GOX 2022) in Washington, D.C. in person in August 2022.
- Summer REU student Jennifer Rittenhouse presented on the Extraction of Thin Film Dielectric Functions using Ex-situ Spectroscopic Ellipsometry based Multi-sample Analysis Approach at the UNL Summer Research Symposium in Lincoln in person in August 2021.
- Our group member Dr. Ufuk Kilic reported on Spatially coherent helical and non-helical nano-heterostructures with tuneable plasmonic response at the The European Optical Society Annual meeting (EOSAM) in Rome Italy online in September 2021. He also reported on Tunable broadband enhanced chirality with hybrid helical metamaterials at the International Congress on Artificial Materials for Novel Wave Phenomena and Metamaterials online in August 2021. He also presented a talk on the Dual Box model based In-situ Ellipsometry growth characterization: Oxygen Plasma Enhanced Atomic Layer Deposition of metal Oxide Ultra-thin Films at the 48th The International Conference on Metallurgical Coatings and Thin Films (ICMCTF), San Diego in person in May 2022. He also presented a talk on Unravelingthe Bisignate and Broadband Chiroptical Response from All-Dielectric Distorted L-Shape Metamaterials at the 48th

The International Conference on Metallurgical Coatings and Thin Films (ICMCTF), San Diego, in person in May 2022. He gave an invited talk on Design, fabrication and optical characterization of glancing angle deposited quantum metamaterials at The world networking event Humboldt meets Leibniz - Metamaterials, Hannover, Germany, in person in May 2022. He also gave an Invited talk on Extremely broadband plasmonic chiroptical activity revealed by heterostructure helical metamaterials at the International Conference on Spectroscopic Ellipsometry 9, Beijing, China, online in May 2022. He presented a poster on Mueller matrix generalized spectroscopic ellipsometry based chiroptical characterization of glancing angle deposited all-dielectric distorted L-shape metamaterials during the Nebraska EPSCoR NRIC workshop on Commercializing Quantum Technologies in Nebraska, Lincoln, NE, in person in March 2022. He also gave an invited talk on Engineering the broadband enhanced chirality revealed by glancing angle deposited metamaterial platforms at the UNL physics and astronomy department in Lincoln NE online in February 2022.

- Collaborator Dr. Steffen Richter presented a poster on The Electron Spin Hamiltonian for $Fe^{3+}$ in Monoclinic beta-$Ga_2O_3$ during the 5th U.S. Gallium Oxide Workshop (GOX 2022) in Washington D.C. (shown by PI Schubert) August 2022. He also presented a poster on The electron spin Hamiltonian for $Fe^{3+}$ in monoclinic beta-$Ga_2O_3$ at the Defects in solids for quantum technologies (CECAM 2022) conference in Stockholm Sweden in person in June 2022.
- Collaborator Dr. Vanya Darakchieva presented an invited talk Terahertz Electron Paramagnetic Resonance ellipsometry for interrogating point defects in ultrawide bandgap semiconductors at the Defects in solids for quantum technologies (CECAM 2022) conference in Stockholm Sweden in person in June 2022.
- Collaborator Dr. Philipp Kuehne presented a talk on A high frequency, high field, field and frequency domain, cavity-free, EPR ellipsometry instrument during the International Conference on Spectroscopic Ellipsometry 9, Beijing, China, online in May 2022.

- (Interim Reports Only) What do you plan to do during the next reporting period to accomplish the goals and objectives? If there are no changes to the agency-approved application or plan for this project or if this is the final report, state “Nothing to Report.”
  - Describe briefly what you plan to do during the next reporting period to accomplish the goals and objectives.
  - N/A

# Impacts

This component is used to describe ways in which the work, findings, and specific products of the project have had an impact during this reporting period. Describe distinctive contributions, major accomplishments, innovations, successes, or any change in practice or behavior that has come about as a result of the project. You can report on the following impact categories, but you are not required to report on all categories. Please only report in the categories that are relevant to your project:

**Development of the principal discipline(s) of the project**
Describe how findings, results, techniques that were developed or extended, or other products from the project made an impact or are likely to make an impact on the base of knowledge, theory, and research in the principal disciplinary field(s) of the project. Summarize using language that a lay audience can understand (e.g., Scientific American style).

The deformation potential parameters provided for valence and conduction bands in monoclinic aluminum gallium oxide can be used to predict the band off sets between conduction and valence bands as a function of composition and strain, and for all lattice directions. This information will be crucial as it inform which growth direction of monoclinic aluminum gallium oxide on template gallium oxide substrate produces the optimum conduction band confinement. This information is currently missing.

The knowledge on how strain and composition affect Raman and Infrared phonon modes will permit to determine composition and strain in epitaxial heterostructures.

The knowledge that phonon plasmon coupled modes change their direction as a function of free carrier concentration is important for correct calculation of electron and thermal transport. The concepts to determine the properties of phonon plasmon coupled modes developed in this award can be easily transferred now to alloys as well. It is subject of future publications to report on phonon plasmon coupling in doped monoclinic aluminum gallium oxide.

**Other disciplines:**
Describe how the findings, results, or techniques that were developed or improved, or other products from the project made an impact or are likely to make an impact on other disciplines.

The concept of the eigendielectric polarization model for low symmetry materials will impact research in other disciplines which also begin to investigate low symmetry materials, such as in 2dimensional materials.

**Describe the impact in this reporting period on the development of human resources**
For example, how has the project provided opportunities for research and teaching in the relevant fields; improved the performance, skills, or attitudes of members of underrepresented groups that will improve their access to or retention in research, teaching, or other related professions; provided scholarships; provided exposure to science and technology for practitioners, teachers, young people, or other members of the public?

Graduate student Matthew Hilfiker graduated in May 2022. He is now employed with ONTO and continues to use spectroscopic ellipsometry in materials development and product quality assessment. Undergraduate student Jennifer Knudtson has graduated in May 2022 and will become graduate student within the PI's team. Jennifer was trained in first principles computational methods. Undergraduate student Emma Williams was trained in ellipsometry analysis techniques, vacuum equipment, and temperature control of optical experiments. Undergraduate student Teresa Gramer was trained in use of farinfrared and infrared ellipsometry equipment and analysis of phonon modes in multiple phonon mode materials with low symmetry structures. Teresa became graduate student in the PI's team summer 2022. Graduate student Megan Stokey will graduate in Spring 2023. Graduate student Alexander Ruder acquired knowledge in 3D printing of high precision parts for optical (THz) instrumentation, and in software programing for compex optical instrument calibrations. Graduate student Shawn Wimer was trained in xrd and electron microscopy techniques. Undergraduate student Yusra Traouli was trained in vacuum equipment and deposition systems. She also was trained in ellipsomerty instrumentation and data modeling aporaches. She will start as graduate student in the PI's group in January 2023.

**Describe the impact on teaching and educational experiences**
For example, has the project: Developed and disseminated new educational materials; led to ideas for new approaches to course design or pedagogical methods; or developed online resources that will be useful for teachers and students and other school staff?

The PI has incorporated the eigendielectric polarization model description for dielectric and magnetic responses of low symmetry materials into the class material for ELEC 408/808 Electrodynamics at the ECE department of UNL. The PI teaches this class every year.

**Describe the impact in this reporting period on physical, institutional, and information resources that form infrastructure.**
For example: Physical resources such as facilities, laboratories, or instruments; institutional resources (such as establishment or sustenance of societies or organizations); or information resources, electronic means for accessing such resources or for scientific communication, or the like.

Nothing to report.

**Impact on society beyond science and technology:**
Describe how results from the project made an impact, or are likely to make an impact, beyond the bounds of science, engineering, and the academic world on areas such as: improving public knowledge, attitudes, skills, and abilities; changing behavior, practices, decision making, policies (including regulatory policies), or social actions; or improving social, economic, civic, or environmental conditions.

A measurable immediate impact is not available presently. However, in a near future the knowledge created under this award will help to enable a new class of high-power electronic devices which will be critical to build the new electric and electronic infrastructure for a sustainable green energy future.