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Thermodynamic Stability of the Q-2 DEG at the Oxide/Oxide Interface under Extreme Thermomechanical Conditions

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Final Report**

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14. ABSTRACT This was a very successful project that culminated in important discoveries, supported seven Ph.D. students and resulted in over fifty publications. The main focus of the study was the two-dimensional electron gas (2DEG) at the interface of oxides with oxygen-deficient SrTiO ₃ (STO). We demonstrated that at elevated temperature in high vacuum many metals scavenge oxygen from STO. This led to the discovery of large magnetoresistance in the 2DEG at the STO/EuO interface with possible applications in spintronics. Of practical importance is our development of atomic layer deposition (ALD) of several transition metal oxides (TMOs) and their integration on semiconductors. The lower thermal budget of ALD opens a way of integrating functionality of TMOs in the back end process. We achieved control of the 2DEG in Ge by switching ferroelectric polarization in BaTiO ₃ (BTO). We extended our ability to manipulate the 2DEG at oxide interfaces to TMO quantum wells, and demonstrated absorption in the THz frequency range. We developed Si-integrated BTO structures that exploit the extreme optical nonlinearity of BTO, and explored the ability to control light propagation in integrated photonics. This approach offers an avenue of miniaturizing electro-optical components, reducing power consumption and lowering cost in multiple defense applications.			
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**Thermodynamic Stability of the Q-2 DEG at the Oxide/Oxide Interface
under Extreme Thermomechanical Conditions**

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David Smith, Arizona State University

Final Report

This was a very successful project that culminated in several important discoveries, supported seven Ph.D. students and resulted in over fifty peer reviewed publications. Below we briefly summarize the main findings of five principal research thrusts.

The main initial focus of the study was the two-dimensional electron gas (2DEG) at the interface of oxides with oxygen deficient SrTiO₃ (STO). Oxygen deficiency results in conductivity in STO, as the oxygen vacancy is a donor impurity. Typically, oxygen deficiency is reported as a parasitic effect in oxide heterostructures involving STO, when the deposition used atomic sources, such as during molecular beam epitaxy (MBE). Our approach was to understand and control oxygen evolution as means to create a conductive layer below the interface. We have performed a fundamental study of γ -Al₂O₃ grown on STO by MBE and atomic layer deposition (ALD). The interface and the oxygen deficient layer of STO were investigated and understood with the help of electron microscopy, in particular atomic resolution scanning transmission electron microscopy (STEM). We have discovered that at elevated temperature Al scavenges oxygen from STO and this additional flux of oxygen needs to be taken into account when optimizing the oxygen supply during growth. We extended the investigation of this oxygen scavenging mechanism to other metals. This led to the discovery of EuO epitaxy without oxygen on STO and large magnetoresistance in the 2DEG at the STO/EuO interface. EuO is a prototypical Heisenberg magnet and at low temperature shows the largest known magnetic moments per Eu atom. It is actively studied for applications in spintronics.

Of great practical importance is our development of ALD of several oxides and their integration on Si and Ge. ALD is a lower temperature chemical deposition process. Commercial applications of ALD shifted from display technology to electronic devices in the late 90's, coinciding with the transition to high-k dielectrics (many of which are transition metal oxides (TMOs)) in CMOS technology. The lower thermal budget of ALD potentially opens a way of integrating additional functionality afforded by TMOs in the back end process as the thermal budget is quite low (controlled by the presence of 8-10 levels of metal (Cu)).

Integration of TMOs with conventional semiconductors enables exploitation of many emergent phenomena coming from a combination of well controlled carriers in a semiconductor and various ferroic orders (ferroelectricity, ferromagnetism, orbital ordering, etc.) in the oxide. We achieved control of the 2DEG in Ge by ferroelectric polarization in a heterostructure comprised of semiconducting Ge and ferroelectric BaTiO₃ (BTO). We first explored and understood critical differences in the surface electronic structure between Si and Ge (001). We then developed techniques to clean Ge without the need for sputtering and regrowth. We developed epitaxial integration of BTO on Ge using both MBE and ALD. We understood the atomic structure of the interface using a combination of density functional theory (DFT) and atomically-resolved STEM. We demonstrated the field effect using microwave impedance microscopy (MIM). The methodological aspect of this work that is worth mentioning is that the field effect (manipulation of charge by ferroelectric polarization) was clearly demonstrated without the need to build the actual transistor.

We extended our ability to create and manipulate the 2DEG at oxide interfaces to TMO quantum wells (QW). In a pioneering study we have created a doped STO/LaAlO₃ superlattice comprised of up to 80 QWs and demonstrated intersubband absorption in the THz frequency range. In the course of the project we have developed in-situ doping techniques, and resolved multiple deposition problems such as amplification of the interfacial roughness with increasing superlattice thickness. Quantum mechanical theory of the intersubband absorption in the STO quantum wells was also developed. Development of the growth procedures, materials characterization and device testing were intimately linked with theory and STEM microscopy in a seamless learning cycle.

Towards the end of the project an opportunity arose to make a major impact on Si photonics. Si photonics is the information technology exploiting the outstanding ability of Si to guide IR light in micromachined waveguides, specifically at the telecom 1.55 μm wavelength. The most efficient way to control such light would be through the electro-optical or Pockels effect. Unfortunately, Si due to it having inversion symmetry doesn't exhibit the Pockels effect. The traditional material for this is LiNbO_3 , but its integration on Si is cumbersome. We have developed Si-integrated BTO structures that exploit the extreme optical nonlinearity of BTO, and explored the ability to control light propagation as a function of BTO microstructure. Functional electro-optical devices have been built by our collaborators, and promising results in terms of efficiency, loss, etc. have been demonstrated. This approach offers an avenue of miniaturizing electro-optical components, reducing power consumption and lowering cost in multiple defense applications. The work will be continued under the new program.

PhD's granted

- 2015 Ajit Dhamdhere (PhD), "Characterization of Oxide Thin Films and Interfaces Using Transmission Electron Microscopy"
- 2015 Kurt D. Fredrickson (PhD), "Effects of Film and Atomic Growth on Material Properties of Transition Metal Oxides"
- 2015 Thong Q. Ngo (PhD), "Atomic Layer Deposition of Functional Materials"
- 2017 Kristy J. Kormondy (PhD), "Oxide Materials at the Two-Dimensional Limit"
- 2017 Patrick Ponath (PhD), "Epitaxial Functional Oxide Integration on Germanium"
- 2018 Bryce Edmondson (PhD expected), "Epitaxial nonlinear oxides"
- 2018 Sirong Lu(PhD), "Transmission Electron Microscopy Study of the Two-Dimensional Electron Gas at STO-Based Oxide Interfaces"

Books:

- A. A. Demkov and A.B. Posadas, *Integration of Functional Oxides with Semiconductors*, (Springer, 2014).
- *Thin Films on Si: Electronic and Photonic Applications*, M. Frank, V. Narayanan and A. A. Demkov, Editors, (World Scientific, Singapore, 2016).

Book Chapters:

A. A. Demkov and A.B. Posadas, "Ferroelectric oxides on Silicon," in *Thin Films on Si: Electronic and Photonic Applications*, M. Frank, V. Narayanan and A. A. Demkov, Editors, p. 403 (World Scientific, 2016)

A. A. Demkov, K. J. Kormondy and K. D. Frederickson, "Two-dimensional electron gas at oxide interfaces," in *Oxide Materials at the Two-dimensional Limit*, Alessandro Fortunelli and Falko Netzer, Editors, p. 335 (Springer, 2016)

A. A. Demkov, K. D. Fredrickson, H. Seo and A. O'Hara, "First-principles Modeling of Interface Effects in Oxides," to appear in *Handbook of Materials Modeling, Vol. 1, Methods: Theory and Modeling*, Wanda Andreoni and Sidney Yip, Editors (Springer, 2018)

Other recognition:

- J. G. Ekerdt elected Fellow of the American Association for the Advancement of Science
- D. J. Smith elected Fellow, Microscopy Society of America
- D. J. Smith, recipient of 2014 Distinguished Physical Scientist Award, Microscopy Society of America.
- D. J. Smith, recipient of 2014 Helmholtz International Fellowship Award, Helmholtz Foundation, Germany.
- A. A. Demkov was the President du Jury at the Ph.D. defense for Hicham Zaid (advisor M.-H. Berger), University PSI, France in December 2016.

Presentations:

- John G. Ekerdt, "A chemical route to epitaxial oxides on semiconductors: Crystalline SrTiO_3 and SrHfO_3 grown directly on Ge (001) by ALD," 14th International Conference on ALD, Koyoto, Japan, June 2014.

- John G. Ekerdt, “Growth of Crystalline Perovskites on Si(001) and Ge(001) via Atomic Layer Deposition”, Telluride Research Conference on Semiconductor Surface Chemistry, Telluride, CO, July 2014.
- John G. Ekerdt, *Integration of a Conductive Perovskite [La-doped SrTiO₃] on Si (001) by ALD Using a Thin SrTiO₃ Buffer Layer*; Materials Research Society (MRS) Fall 2013 Meeting & Exhibit; Boston, Massachusetts; December 5, 2013.
- John G. Ekerdt, *Two-dimensional electron gas at the γ -Al₂O₃/SrTiO₃ heterostructures grown by ALD*, 2014 Materials Research Society (MRS) Fall meeting, Boston, Massachusetts, December 03, 2014.
- Sirong Lu, Martha R. McCartney, David J. Smith, Kristy J. Kormondy, Thong Q. Ngo, Agham Posadas, John G. Ekerdt, Alexander A. Demkov, “Characterization of the two-dimensional electron gas at the γ -Al₂O₃/SrTiO₃ interface”, presented at PICO 2015, held April 19-23, 2015 in Kasteel Valsbroek, The Netherlands.
- Sirong Lu, Kristy J. Kormondy, Thong Q. Ngo, Toshihiro Aoki, Agham Posadas, John G. Ekerdt, Alexander A. Demkov, Martha R. McCartney, and David J. Smith, “Characterization of the two-dimensional electron gas at the γ -Al₂O₃/SrTiO₃ interface”, presented at Microscopy and Microanalysis 2015, held August 2-6, 2015, in Portland, OR.
- Kristy J. Kormondy, Stefan Abel, Florian Fallegger, Youri Popoff, Patrick Ponath, Agham B. Posadas, Marilyne Sousa, Daniele Caimi, Heinz Siegwart, Emanuele Uccelli, Lukas Czornomaz, Chiara Marchiori, Jean Fompeyrine, and Alexander A. Demkov, “Ferroelectric BaTiO₃ thin films on silicon: crystalline structure and electro-optic response,” E-MRS Spring 2015, Lille, France, May 2015
- Kristy J. Kormondy, Stefan Abel, Florian Fallegger, Youri Popoff, Patrick Ponath, Agham B. Posadas, Marilyne Sousa, Daniele Caimi, Heinz Siegwart, Emanuele Uccelli, Lukas Czornomaz, Chiara Marchiori, Jean Fompeyrine, and Alexander A. Demkov, “Analysis of the Pockels effect in ferroelectric barium titanate thin films on Si(001),” INFOS 2015, Udine, Italy, June 2015
- Kristy J. Kormondy, Stefan Abel, Florian Fallegger, Youri Popoff, Agham B. Posadas, Steffen Reidt, Daniele Caimi, Marilyne Sousa, Marta D. Rossell, Chiara Marchiori, Jean Fompeyrine, and Alexander A. Demkov, “A hybrid approach to integration of electro-optically active barium titanate thin films on Si (001),” E-MRS Fall 2015, Warsaw, Poland, September 2015
- Kristy J. Kormondy, Agham B. Posadas, Thong Q. Ngo, Sirong Lu, Nicholas Goble, Jean Jordan-Sweet, Xuan P. A. Gao, David J. Smith, Martha R. McCartney, John G. Ekerdt, and Alexander A. Demkov, “Quasi-two-dimensional electron gas at the epitaxial alumina/SrTiO₃ interface: Control of oxygen vacancies,” Fall EMRS, Warsaw, Poland, Sept 2015.
- Kristy J. Kormondy, Stefan Abel, Florian Fallegger, Youri Popoff, Agham B. Posadas, Steffen Reidt, Daniele Caimi, Chiara Marchiori, Marilyne Sousa, Marta D. Rossell, Gabriele De Luca, Morgan Trassin, Manfred Fiebig, Alexander A. Demkov, and Jean Fompeyrine, “Electro-Optically Active Barium Titanate Thin Films on Si: A Hybrid Approach,” 2015 Fall MRS, Boston, December 2015
- Kristy J. Kormondy, Stefan Abel, Florian Fallegger, Youri Popoff, Thilo Stöferle, Agham B. Posadas, Marilyne Sousa, Daniele Caimi, Heinz Siegwart, Lukas Czornomaz, Chiara Marchiori, Marta D. Rossell, Bert J. Offrein, Alexander A. Demkov, and Jean Fompeyrine, “Influence of Tetragonal Structure on the Electro-Optic Response of BaTiO₃/Silicon Photonic Structure”, 2015 Fall MRS, Boston, December 2015
- Kristy J. Kormondy, Stefan Abel, Youri Popoff, Daniele Caimi, Chiara Marchiori, Marilyne Sousa, Marta D. Rossell, Alexander A. Demkov, and Jean Fompeyrine, “Electro-optically active barium titanate thin films on Si”, “Electro-optically active barium titanate thin films on Si”, 2015 SISC, Washington DC, December 2015
- K. D. Fredrickson and A. A. Demkov, “Two-dimensional electron gas at the interface of two nonpolar oxides: BaTiO₃ and SrTiO₃,” E-MRS Spring 2015, Lille, France, May 2015
- K. D. Fredrickson, M. McDaniel, J. Ekerdt and A.A. Demkov, “Theoretical modeling and experimental observations of the atomic layer deposition of SrO using a cyclopentadienyl Sr precursor,” E-MRS Spring 2015, Lille, France, May 2015

- K. D. Fredrickson, H. Seo and A.A. Demkov, "Oxidation protection of the Si(001) surface due to adsorbed Sr," E-MRS Spring 2015, Lille, France, May 2015
- A. A. Demkov, "Integrated films of transition metal oxides with semiconductors," XXIV International Materials Research Congress," Cancun, Mexico, August 2015
- A. A. Demkov, "Designing transition metal oxide heterostructures," XXIV International Materials Research Congress, Cancun, Mexico, August 2015
- A. A. Demkov, "Integration of ferroelectric oxides on Si and Ge," Insulating Films on Semiconductors (INFOS), Udine, Italy, June 2015
- A. A. Demkov, "Integration of ferroelectric oxides on Si and Ge," European Materials Research Society Spring Meeting, Lille, France, May 2015
- J. G Ekerdt "Atomic Layer Deposition of Crystalline Perovskite Oxides on Si (001) and Ge (001)," 2015 MRS Fall meeting, Boston, MA, December 2015
- Patrick Ponath, A. B. Posadas, Y. Ren, X. Wu, R. K. Vasudevan, M. B. Okatan, S. Jesse, S. V. Kalinin, K. Lai, M. Schmidt, P. Hurley, R. Duffy and A. A. Demkov, "Advances towards the ferroelectric field-effect transistor - Epitaxial BaTiO₃ on Ge(001)," Fall MRS Meeting, Boston, MA, November 2015.
- P. Ponath, A. B. Posadas, M. Schmidt, P. H. Hurley, R. Duffy, A. A. Demkov, "Formation of nanoscale BaTiO₃ MOSCAPs without wet-etching," Semiconductor Interface Specialists Conference, Washington, DC, December 2015.
- Sirong Lu, Kristy J. Kormondy, Thong Q. Ngo, Elliott Ortmann, Toshihiro Aoki, Agham Posadas, John G. Ekerdt, Alexander A. Demkov, Martha R. McCartney, and David J. Smith, "ELNES analysis of gamma-Al₂O₃/SrTiO₃ and LaTiO₃/SrTiO₃ interfaces", *Microscopy and Microanalysis*, **22**(S3) 1660-1661 (2016)
- Sirong Lu, Kristy J. Kormondy, Thong Q. Ngo, Toshihiro Aoki, Agham Posadas, John G. Ekerdt, Alexander A. Demkov, Martha R. McCartney, and David J. Smith, "Characterizing the γ -Al₂O₃/SrTiO₃ interface", 2016 MRS Spring Meeting, Phoenix, April 2016.
- Sirong Lu, Kristy J. Kormondy, Thong Q. Ngo, Elliott Ortmann, Toshihiro Aoki, Agham Posadas, John G. Ekerdt, A. A. Demkov, Martha R. McCartney, and David J. Smith, "ELNES analysis of γ -Al₂O₃/ SrTiO₃ and LaTiO₃/ SrTiO₃ interfaces", 2016 Microscopy and Microanalysis Meeting, Columbus, July 2016.
- K. Kormondy, "Symmetry, strain, defects, and the nonlinear optical response of crystalline BaTiO₃/silicon," APS March, Baltimore, MD, March 2016.
- Ali Hamze, Kristy Kormondy, Agham Posadas, and Alex Demkov, "First principles study of γ -Al₂O₃/SrTiO₃ interface formation," APS March, Baltimore, MD, March 2016
- J. Elliott Ortmann, Nish Nookala, Qian He, Agham Posadas, Albina Borisevich, Mikhail Belkin, Alex Demkov, "Beyond GaAs: Room-temperature intersubband absorption in SrTiO₃/LaAlO₃ Multiple Quantum Wells", APS March, Baltimore, MD, March 2016
- J. Elliott Ortmann, Nish Nookala, Qian He, Agham Posadas, Albina Borisevich, Mikhail Belkin, A. A. Demkov, "Beyond GaAs: Room-temperature intersubband absorption in SrTiO₃/LaAlO₃ Multiple Quantum Wells", MRS Spring, Phoenix, AZ, March 2016
- Patrick Ponath, A. B. Posadas, Y. Ren, X. Wu, R. K. Vasudevan, M. B. Okatan, S. Jesse, S. V. Kalinin, K. Lai, M. Schmidt, P. Hurley, R. Duffy, J. Wang, C. Young, A. A. Demkov "Formation of Nanoscale BaTiO₃ MOSCAPs for Ferroelectric Field-Effect Transistor Application," CIMTEC, Perugia, Umbria, Italy, *June 2016*
- Patrick Ponath, A. O'Hara, H.-X. Cao, A. B. Posadas, R. Vasudevan, M. B. Okatan, S. Jesse, M. Berg, Z. Li, D. Zhang, A. J. Kellock, A. de Lozanne, J. Zhou, S. Kalinin, D. J. Smith, A. A. Demkov, "The nature of Co doped BaTiO₃," Material Research Society (MRS) meeting 2016, Phoenix, Arizona, USA, *March 2016*
- Patrick Ponath, A. B. Posadas, Y. Ren, X. Wu, R. K. Vasudevan, M. B. Okatan, S. Jesse, S. V. Kalinin, K. Lai, M. Schmidt, P. Hurley, R. Duffy, A. A. Demkov, "Nanoscale BaTiO₃ MOSCAP formation for

ferroelectric field-effect transistor application,” American Physical Society (APS) March meeting, Baltimore, Maryland, USA, *March 2016*.

- Patrick Ponath, A. B. Posadas, Y. Ren, X. Wu, R. K. Vasudevan, M. B. Okatan, S. Jesse, S. V. Kalinin, K. Lai, M. Schmidt, P. Hurley, R. Duffy, J. Wang, C. Young, A. A. Demkov, “Formation of nanoscale BaTiO₃ MOSCAPS on Germanium without wet- etching,” MBE 2016, Montpellier, France, *September 2016*
- K. J. Kormondy, A. Posadas, and A. A. Demkov, “Oxygen removal from STO: Co₂O₄ and γ -Al₂O₃,” 19 European MBE Conference, Montpellier, France, *September 2016*.
- A. A. Demkov “Integrating films of functional in transition metal oxides on semiconductors,” Colloquium, Texas Tech University, Lubbock, TX, *October 2016*
- A. A. Demkov “Phase transformations in transition metal oxides for device applications,” Four Corners Meeting of the American Physical Society, Las Cruces, NM, *October 2016*
- K. J. Kormondy, A. Posadas, W. Guo, S. Shen, L. Gao, M. Tsoi, X. Li, J. Zhu, S. Lu, M. R. McCartney, D. J. Smith and A. A. Demkov, “Oxygen removal from STO and formation of interface 2DEGs,” Fall MRS Meeting, Boston, *November 2016*.
- Patrick Ponath, A. B. Posadas, M. Schmidt, P. Hurley, R. Duffy, J. Wang, C. Young, A. A. Demkov, “Selective area growth of BaTiO₃ for ferroelectric field-effect transistor application”, American Physical Society (APS), March meeting, New Orleans, Louisiana, USA, *March 2017*
- Patrick Ponath, A. B. Posadas, M. Schmidt, P. Hurley, R. Duffy, J. Wang, C. Young, A. A. Demkov, “Advances of the development of a ferroelectric field-effect transistor on Ge(001),” International Conference on IC design and Technology (ICICDT), Austin, Texas, USA, *May 2017*
- A. A. Demkov “Nonlinear Optics with fully integrated transition metal oxides,” International Conference on IC Design and Technology, Austin, TX, *May 2017*
- A. A. Demkov “Modelling for Integrated Oxide Electronics and Photonics,” March Meeting of the American Physical Society, New Orleans, LA, *March 2017*
- A. A. Demkov and J. G. Ekerdt “Integration of functional oxides on semiconductors,” AFRL Wright-Patterson AFB, Dayton, OH, *April 2017*
- A. A. Demkov “Nonlinear Optics with fully integrated transition metal oxides,” International Conference on IC Design and Technology, Austin, TX, *May 2017*
- A. A. Demkov “Non-linearity of ferroelectric oxides and possible applications in neuromorphic computing?” International Meeting on Ferroelectricity, San Antonio, TX, *September 2017*
- A. A. Demkov “Non-linearity of ferroelectric oxides and possible applications in neuromorphic computing?” Workshop on Innovative Nanoscale Devices and Systems, Kohala Coast, Hawaii, *November 2017*

Publications

2013

1. R. C. Hatch, M. Choi, K. Fredrickson, H. Seo, C. Lin, A. B. Posadas and A. A. Demkov, “Surface electronic structure for various surface preparations of Nb-doped SrTiO₃ (001),” *J. Appl. Phys.* **114**, 103710 (2013).
2. A. B. Posadas, C. Lin, A. A. Demkov and S. Zollner, “Band gap engineering in perovskite oxides: Al-doped SrTiO₃,” *Appl. Phys. Lett.* **103**, 142906 (2013).
3. A. A. Demkov, A. B. Posadas, H. Seo, M. Choi, K. J. Kormondy, P. Ponath, R. C. Hatch, M. D. McDaniel, T. Q. Ngo and J. G. Ekerdt, “Monolithic integration of oxides on semiconductors,” (invited) *ECS Transactions* **54**, 255 (2013).

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4. H. Seo, R. C. Hatch, P. Ponath, M. Choi, A. B. Posadas, and A. A. Demkov, “Critical differences in the surface electronic structure of Ge(001) and Si(001): ab-initio theory and angle-resolved photoemission spectroscopy,” *Phys. Rev. B* **89**, 115318 (2014).

5. M. Choi, A. B. Posadas, C. O. Rodriguez, A. O'Hara, H. Seinige, A. J. Kellock, M. M. Frank, M. Tsoi, S. Zollner, V. Narayanan and A. A. Demkov, "Structural, optical and electrical properties of strained La-doped SrTiO₃ films," *J. Appl. Phys.* **116**, 043705 (2014).
 6. K. D. Fredrickson, P. Ponath, A. B. Posadas, M. R. McCartney, T. Aoki, D. J. Smith, and A. A. Demkov, "Atomic and electronic structure of the ferroelectric BaTiO₃-Ge(001) interface," *Appl. Phys. Lett.* **104**, 242908 (2014).
 7. K. J. Kormondy, A. B. Posadas, A. Slepko, A. Dhamdhare, D. J. Smith, K. N. Mitchell, T. I. Willett-Gies, S. Zollner, L. G. Marshall, J. Zhou, and A. A. Demkov, "Epitaxy of polar semiconductor Co₃O₄: growth, structure, and characterization," *J. Appl. Phys.* **115**, 243708 (2014).
 8. M. Choi, C. Dubourdieu, A. J. Kellock, K. L. Lee, R. A. Haight, A. Pyzyna, M. M. Frank, A. A. Demkov and V. Narayanan, "Tunable electrical properties of TaN_x thin films grown by ionized physical vapor deposition," *J. Vac. Sci. Technol. B* **32**, 051202 (2014).
 9. T. Q. Ngo, M. D. McDaniel, A. Posadas, A. A. Demkov, J. G. Ekerdt, "Growth of crystalline LaAlO₃ by atomic layer deposition," in *Oxide-based Materials and Devices V*, Edited by F. H. Teherani, D. C. Look, D. J. Rodgers, *Proceedings of SPIE*, **8987**, 898712 (2014).
 10. M. D. McDaniel, T. Q. Ngo, A. B. Posadas, Chengqing Hu, S. Lu, D. J. Smith, E. T. Yu, A. A. Demkov, and J. G. Ekerdt, "A chemical route to monolithic integration of crystalline oxides on semiconductors, *Advanced Material Interfaces* (doi: 10.1002/admi.201400081) 1400081(1-8) (2014).
 11. M. D. McDaniel, A. Posadas, T. Q. Ngo, C. M. Karako, J. Bruley, M. M. Frank, V. Narayanan, A. A. Demkov, J. G. Ekerdt, "Incorporation of La in epitaxial SrTiO₃ thin films grown by atomic layer deposition on SrTiO₃-buffered Si (001) substrates," *J. Appl. Phys.* **115**, 224108-(1-8) (2014).
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12. P. Ponath, K. Fredrickson, A. B. Posadas, Y. Ren, X. Wu, R. K. Vasudevan, M. B. Okatan, S. Jesse, T. Aoki, M. R. McCartney, D. J. Smith, S. V. Kalinin, K. Lai, and A. A. Demkov, "Carrier Density Modulation in Ge Heterostructure by Ferroelectric Switching," *Nature Comm.* **6**, 6067 (2015).
 13. K. J. Kormondy, A. B. Posadas, T. Q. Ngo, S. Lu, N. Goble, J. Jordan-Sweet, X. P. A. Gao, D. J. Smith, M. R. McCartney, J. G. Ekerdt, and A. A. Demkov, "Quasi-two-dimensional electron gas at the epitaxial alumina/SrTiO₃ interface: control of oxygen vacancies," *J. Appl. Phys.* **117**, 095303 (2015).
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Abstract

This was a very successful project that culminated in important discoveries, supported seven Ph.D. students and resulted in over fifty publications. The main focus of the study was the two-dimensional electron gas (2DEG) at the interface of oxides with oxygen-deficient SrTiO₃ (STO). We demonstrated that at elevated temperature in high vacuum many metals scavenge oxygen from STO. This led to the discovery of large magnetoresistance in the 2DEG at the STO/EuO interface with possible applications in spintronics. Of practical importance is our development of atomic layer deposition (ALD) of several transition metal oxides (TMOs) and their integration on semiconductors. The lower thermal budget of ALD opens a way of integrating functionality of TMOs in the back end process. We achieved control of the 2DEG in Ge by switching ferroelectric polarization in BaTiO₃ (BTO). We extended our ability to manipulate the 2DEG at oxide interfaces to TMO quantum wells, and demonstrated absorption in the THz frequency range. We developed Si-integrated BTO structures that exploit the extreme optical nonlinearity of BTO, and explored the ability to control light propagation in integrated photonics. This approach offers an avenue of miniaturizing electro-optical components, reducing power consumption and lowering cost in multiple

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New discoveries, inventions, or patent disclosures:

Do you have any discoveries, inventions, or patent disclosures to report for this period?

No

Please describe and include any notable dates

Do you plan to pursue a claim for personal or organizational intellectual property?

Changes in research objectives (if any):

Change in AFOSR Program Officer, if any:

Extensions granted or milestones slipped, if any:

A six month no-cost extension was granted in October of 2017.

AFOSR LRIR Number

LRIR Title

Reporting Period

Laboratory Task Manager

Program Officer

Research Objectives

Technical Summary

Funding Summary by Cost Category (by FY, \$K)

	Starting FY	FY+1	FY+2
Salary			
Equipment/Facilities			
Supplies			
Total			

Report Document

Report Document - Text Analysis

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Appendix Documents

2. Thank You

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