1. DOE award # and name of the recipient (Institution)

DE-FG-02-06ER46328, University of Wisconsin Milwaukee

2. Project Title and name of the PI

Atomic and Electronic Structure of Polar Oxide Interfaces,
Marija Gajdardziska-Josifovska (PI), Michael Weinert (co-PI), Scott Chambers (co-PI)

3. Period covered by the report

August 14, 2006 – August 13, 2010

4. A brief description of accomplishments.

In this project we developed fundamental understanding of atomic and electronic mechanisms for stabilization of polar oxide interfaces. An integrated experimental and theoretical methodology was used to develop knowledge on this important new class of ionic materials with limited dimensionality, with implications for multiple branches of the basic and applied energy sciences. In the fist year of the project the focus was on growth of a comprehensive matrix of model iron oxide polar films on polar magnesia and alumina substrates, and on characterization of their average crystal structure and magnetic properties. In the second year the main effort was to obtain atomic level structure information from localized microscopy, diffraction and spectroscopy experiments. We also started to develop fundamental understanding of the surface and interface stabilization mechanisms through *ab-initio* modeling of their atomic and electronic structures. In the third year of the project we focused on density functional theoretical studies and on advanced electron microscopy studies of several important effects uncovered in the initial work. We also performed strategic growth of new samples to go beyond the initial matrix and fill gaps needed to answer our open questions for our model systems. A no cost extension period was used to delve into the complexities uncovered by experiment and theory and to make progress with publication of the major results.

The main findings are that polar oxide interfaces can be formed by epitaxial growth of oxide and nitride films on polar surfaces of oxide crystals. In difference with interface faceting that had been predicted by the "electrostatic catastrophe" models, it was found that planar polar interfaces are possible. Both hetero-epitaxial and homo-epitaxial growth modes are affected by the polarity of the substrate and film in ways that are fundamentally different for growth on neutral oxide surfaces. The stabilization mechanism for the polar surface has a strong effect on the resulting structure of the film. A new iron oxide structure was predicted and produced at the polar hematite/magnesia interface, which does not exist in nature and has novel properties. These findings were published in the peer review literature in four journal articles and four conference proceedings.

One PhD student (female) and one Masters student (male) earned their degrees under this project, and one postdoctoral scholar (female) received advanced research training.

5. A list of published papers in which DOE support is acknowledged.

Four journal papers and four conference papers have been published from this project, as follows:

1. "Atomic and Electronic Structure of Polar Fe_2O_3(0001)/MgO(111) Interfaces" K. Pande, M. Gajdardziska-Josifovska and M. Weinert, *Physical Review B* 86 (2012) 035431 (1-11). DOI: 10.1103/PhysRevB.86.035431 *[Journal]*
2. "Structural and Magnetic Properties of MBE-grown $GeMnN_2$ Thin Films" Y. Liu, V.K. Lazarov, S.H. Cheung, D.J. Keavney, M. Gajdardziska-Josifovska, M. Weinert and L. Li, *Physical Review B* 85 (2012) 144113 (1-8). DOI: 10.1103/PhysRevB.85.144113 *[Journal]*
3. "Effects of Unreconstructed and Reconstructed Polar Surface Terminations on Growth, Structure, and Magnetic Properties of Hematite Films" S. H. Cheung, A. Celik-Aktas, P. Dey, M. Weinert, B. Kabius, D. J. Keavney, V. K. Lazarov, S. A. Chambers and M. Gajdardziska-Josifovska, *Physical Review B* 85 (2012) 045405 (1-11). DOI: 10.1103/PhysRevB.85.045405 *[Journal]*
4. "Role of Mn and H in formation of cubic and hexagonal GaMnN" V. K. Lazarov, S. H. Cheung, Y. Cui, L. Li and M. Gajdardziska-Josifovska, *Applied Physics Letters*, 92 (2008) 101914(1-3). *[Journal]*
5. "Atomic and Electronic Structure of Polar Fe_2O_3/MgO Interface", K. Pande, V.K. Lazarov, M. Weinert and M. Gajdardziska-Josifovska, *Microscopy and Microanalysis* 16 (2010) 1474-1475. DOI: 10.1017/S143192761006215X *[Conference]* Proceedings of Microscopy Society of America Annual Conference, Portland, Oregon, August 2010
6. "The Role of Polar Oxide Surface Reconstruction on the Atomic Structure of Polar Oxide Films: HRTEM and SAD Study of Hematite Growth on Magnesia", S. H. Cheung, A. Celik-Aktas, M. Weinert, S. A. Chambers and M. Gajdardziska-Josifovska, *Microscopy and Microanalysis* 13 (2007) 814-815. *[Conference]* Proceedings of Microscopy Society of America Annual Conference, Fort Lauderdale, Florida, August 2007.
7. "Dopant Ordering in Antiferromagnetic Semiconducting Ti Doped Alpha-Fe_2O_3 Revealed by Electron Diffraction", A. Celik-Aktas, T. Droubay, S.A. Chambers and M. Gajdardziska-Josifovska, *Microscopy and Microanalysis* 13 (2007) 820-821. *[Conference]* Proceedings of Microscopy Society of America Annual Conference, Fort Lauderdale, Florida, August 2007.
8. "The structure and magnetic properties of Fe thin films grown on (1×1) and ($\sqrt{3}\times\sqrt{3}$)R30^o reconstructed MgO(111)", V.K. Lazarov, A. Kohn, S.H. Cheung, S.A. Chambers and M. Gajdardziska-Josifovska, *Microscopy and Microanalysis* 13 (2007) 1044-45. *[Conference]* Proceedings of Microscopy Society of America Annual Conference, Fort Lauderdale, Florida, August 2007.