PUBLICATIONS

Driscoll, D. R.; McIntyre, M. D.; Welander, M. M.; Sofie, S. W.; Walker, R. A. Studies of Aluminum Oxide and Nickel Aluminate Distributions in Alumina Doped Ni-YSZ Anodes. In preparation.

McIntyre, M. D.; Neuburger, D. M.; Walker, R. A. *In Operando* Raman Spectroscopy Studies of Temperature Dependent Carbon Accumulation on SOFCs Operating with Syngas. Submitted to the *Journal of Electrochemical Society*.

McIntyre, M. D.; Driscoll, D. R.; Welander, M. M.; Sofie, S. W.; Walker, R. A. *In Situ* Formation of Multifunctional Ceramics: Mixed Ion-Electron Conducting Properties of Zirconium Titanium Oxides. Submitted to the *Journal of Materials Chemistry A*.

Traulsen, M. L.; McIntyre, M. D.; Norrman, K.; Sanna, S.; Mogensen, M.; Walker, R. A. Reversible Decomposition of Secondary Phases in BaO Infiltrated LSM Electrodes – Polarization Effects. Submitted to *Advanced Material Interfaces*.

Driscoll, D. R.; McIntyre, M. D.; Welander, M. M.; Sofie, S. W.; Walker, R. A. Enhancement of High Temperature Metallic Catalysts: Aluminum Titanate Nickel-Zirconia System. *Applied Catalysis A: General,* 2016, *527*, 36-44.

McIntyre, M. D.; Neuburger, D. M.; Walker, R. A. In Situ Optical Studies of Carbon Accumulation with Different Molecular Weight Alkanes on SOFC Ni Anodes. *Electrochemical Society Transactions,* 2015, *66(32)*, 11-19.

McIntyre, M. D.; Traulsen, M. L.; Norrman, K.; Sanna, S.; Walker, R. A. Polarization Induced Changes in LSM Thin Film Electrode Composition by In Operando Raman Spectroscopy and TOF-SIMS. *Electrochemical Society Transactions,* 2015, *66(2)*, 47-59.

McIntyre, M. D.; Kirtley, J. D.; Singh, A.; Islam, S.; Hill, J. M.; Walker, R. A. Comparing In Situ Carbon Tolerances of Sn-Infiltrated and BaO-infiltrated Ni-YSZ Cermet Anodes in Solid Oxide Fuel Cells Exposed to Methane. *Journal of Physical Chemistry C,* 2015, *119(14)*, 7637-7647.

Reeping, K. W.; Halat, D. M.; Kirtley, J. D.; McIntyre, M. D.; Walker, R. A. In Situ Optical and Electrochemical Studies of SOFC Carbon Tolerance. *Electrochemical Society Transactions,* 2014, *61(1),* 57-63.

McIntyre, M. D.; Kirtley, J. D.; Halat, D. M.; Reeping, K. W.; Walker, R. A. In Situ Spectroscopic Studies of Carbon Formation in SOFCs Operating with Syn-gas. *Electrochemical Society Transactions,* 2013, *57(1),* 1267-1275.

Kirtley, J. D.; McIntyre, M. D.; Halat, D. M.; Walker, R. A. Insights into SOFC Ni/YSZ Anode Degradation Using In-Situ Spectrochronopotentiometrys. *Electrochemical Society Transactions,* 2013, *50(44),* 3-15.

Kirtley, J. D.; Halat, D. M.; McIntyre, M. D.; Eigenbrodt, B. C.; Walker, R. A. High-Temperature "Spectrochronopotentiometry": Correlating Electrochemical Performance with In Situ Raman Spectroscopy in Solid Oxide Fuel Cells. *Analytical Chemistry,* 2012, *84(22)*, 9745−9753.

Chu, X.; McIntyre M. Comparison of the strong-field ionization of N_2 and F_2: A time-dependent density-functional-theory study. *Phys. Rev. A*, 2011, *83(1)*, 013409.

MONTANA STATE UNIVERSITY
Mountains & Minds

Department of Chemistry and Biochemistry

Doctor of Philosophy in Chemistry

D I S S E R T A T I O N D E F E N S E

Ms. Melissa D. McIntyre

B.Sc. Montana State University, Bozeman, MT (2007)

Wednesday, November 2, 2016 – 11:30 pm
Byker Auditorium
Department of Chemistry and Biochemistry

"*In Operando* Spectroscopic Studies of High Temperature Electrocatalysts Used For Energy Conversion"

Graduate Committee

Dr. Robert Walker (Research Advisor)
Dr. Paul Gannon (Chemical Engineering)
Dr. Tim Minton (Chemistry)
Dr. Stephen Sofie (Mechanical Engineering)

ABSTRACT

Solid-state electrochemical cells are efficient energy conversion devices that can be used for clean energy production or for removing air pollutants from exhaust gas emitted by combustion processes. For example, solid oxide fuel cells generate electricity with low emissions from a variety of fuel sources; solid oxide electrolysis cells produce zero-emission H_2 fuel; and solid-state DeNO_x cells remove regulated NO_x gases from diesel exhaust. In order to maintain high conversion efficiencies, these systems typically operate at temperatures ≥ 500˚C. The high operating temperatures, however, accelerate chemical and mechanical cell degradation. To improve device durability, a mechanistic understanding of the surface chemistry occurring at the cell electrodes (anode and cathode) is critical in terms of refining cell design, material selection and operation protocols. The studies presented herein utilized *in operando* Raman spectroscopy coupled with electrochemical measurements to directly correlate molecular/material changes with device performance in solid oxide cells under various operating conditions. Because excessive carbon accumulation with carbon-based fuels destroys anodes, the first three studies investigated strategies for mitigating carbon accumulation on Ni-based cermet anodes. Results from the first two studies showed that low amounts of solid carbon actually stabilized the electrical output and improved performance of solid oxide fuel cells operating with *syn-gas* (H_2/CO fuel mixture). The third study revealed that infiltrating anodes with Sn or BaO suppressed carbon accumulation with CH_4 fuel and that H_2O was the most effective reforming agent facilitating carbon removal. The last two studies explored how secondary phases formed in traditional solid oxide cell materials doped with metal oxides improve electrochemical performance. Results from the fourth study suggest that the mixed ion-electron conducting $Zr_5Ti_7O_{24}$ secondary phase can expand the electrochemically active region and increase electrochemical activity in cermet electrodes. The final study of lanthanum strontium manganite cathodes infiltrated with BaO revealed the reversible decomposition/formation of a $Ba_3Mn_2O_8$ secondary phase under applied potentials and proposed mechanisms for the enhanced electrocatalytic oxygen reduction associated with this compound under polarizing conditions. Collectively, these studies demonstrate that mechanistic information obtained from molecular/material specific techniques coupled with electrochemical measurements can be used to help optimize materials and operating conditions in solid-state electrochemical cells.

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BIOGRAPHICAL NOTES

Academic Preparation:

2003-2007 Montana State University, Bozeman, MT (May 2007)
Bachelor of Science in Physics
Bachelor of Science in Applied Mathematics
Thesis: Solid Oxide Fuel Cell Conductivity Research
Advisor: Dr. Hugo V. Schmidt

2005-2007 AdvR, Inc. (Jan. 2005–May 2007)
Undergraduate Research Intern
Research: Development and Characterization of Potassium Titanyl Phosphate Optical Waveguides
Advisor: Dr. Phillip Battle

2006 Montana State University, Bozeman, MT (March-July)
NSF Small Business Innovation Research, Department of Chemistry
Research: Development of Analog Fractional Order Controllers
Advisor: Dr. Gary W. Bohannan

2003-2006 Montana State University, Bozeman, MT (July 2003-May 2006)
Electro-Active Materials Laboratory, Department of Physics
Research: Development of High Temperature Electrical Conductivity Cell for Solid Oxide Fuel Cell Research
Advisor: Dr. Hugo V. Schmidt

Graduate Studies

Field of Study: Physical Chemistry

Courses

Teaching and Outreach Activities

2013 Physical Chemistry Lecture TA, Montana State University (Jan.-May)
2012 General Chemistry Lab TA, Montana State University (Jan.-May, Sep.-Dec.)
2011 General Chemistry Lab TA, Montana State University (Sep.-Dec.)

Awards

2006 Sisters of Charity Vincent de Paul Scholarship
2005 MSU Undergraduate Scholars
2004 MSU Undergraduate Scholars