Feasibility of a Stack Integrated SOFC Optical Chemical Sensor

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Objectives

We propose to further investigate the feasibility of an innovative chemical sensor based on monitoring the surface plasmon resonance (SPR) bands of metal and bimetallic nanoparticle doped Y_2O_3 stabilized ZrO_2 (YSZ nano-cermets), as a function of fuel concentrations, impurities(CO and H_2S) and temperature(500-900°C). Since the SPRs of nano-cermets are directly correlated to the composition and shape of the metal particles,[1] along with the composition of the surrounding matrix[2], the nano-cermets will be tested and designed to provide real time sensory outputs for the chemicals of interest. The proposed sensor has a YSZ matrix, which is commonly used as both an electrolyte and, when doped with nickel, as an anode in SOFC[3,4], thus upon feasibility demonstration, integration directly into the SOFC will be possible. The development of an integrated SOFC chemical sensor will provide the following benefits: 1)In situ monitoring of the fuel cell chemical composition, linked to a feedback loop, will allow smart control of the SOFC, 2)Monitoring the chemical composition of a low temperature SOFC in real time will enable a more complete understanding of the catalytic and reaction mechanisms and thus lead to more efficient stack designs, 3)The development of sensors for operation within a simulated SOFC environment will at the same time be satisfying the need for chemical sensors for the Department of Energy Vision 21 Initiative.

Accomplishments to Date

Nanocomposite films deposited using dual target confocal physical vapor deposition have been deposited and analyzed using x-ray diffraction, Auger spectroscopy, Rutherford backscattering spectroscopy, spectroscopic ellipsometery and scanning electron microscopy. We used in-situ uv-vis absorption spectroscopy to evaluate the surface plasmon resonance bands of embedded Au nanoparticles in a YSZ matrix as a function of CO or NO_2 exposure at operating temperatures up to 800°C. We are currently able to detect CO at concentrations between 0.1 and 1% in an air carrier gas and NO_2 at concentrations ranging from 5ppm to 1% in an air carrier gas. Studies have also been completed for the titration reaction of hydrogen with varying levels of oxygen at an operating temperature of 500°C. The reaction mechanism behind the sensing response is under investigation, but appears to be dependent on a charge transfer reaction between surface bound oxygen anions and the gold nanoparticles, which in turn causes changes in the surface plasmon resonance band of the Au nanoparticles. Recent measurements have also displayed the CO reaction dependence on Au nanoparticle diameter which may provide the ability to develop tailored nanocomposite films to form a sensor array and thereby enhance the selective detection of CO, H_2 and NO_2 with this technique.

Future Work

Perform extensive experiments on both the Au-YSZ and Pd/PdO-YSZ nanocomposite systems as a function of target gas concentration, temperature, Au particle diameter and matrix chemistry for the development of optimized sensing materials. Further development and optimization of the materials set using the parallel testing capabilities will be pursued to obtain a sensitive and reliable sensing material for harsh environment applications.

Publications

1. G. Sirinakis, R. Siddique, I. Manning, P. H. Rogers and M. A. Carpenter, "High Temperature Detection of CO: Development of Au-YSZ Surface Plasmon Resonance Based Chemical Sensors", J. Phys. Chem. B, **110**, 13508 (2006)
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3. G. Sirinakis, R. Siddique, M. A. Carpenter, A. E. Kaloyeros, "Microstructure and optical properties of Y_2O_3-stabilized ZrO_2-Au nanocomposite films", Journal of Materials Research, **20**, 2516 (2005)

Patent Applications

N/A

Conference Presentations

1. G. Sirinakis, R. Siddique, I. Manning, P.H. Rogers, M. A. Carpenter, "All-Optical Detection of CO and NO_2 at High Temperatures by Au-YSZ Nanocomposites", Materials Research Society Spring 2006)
2. G. Sirinakis, R. Siddique, Z. Zhao, M. A. Carpenter, "All-Optical Chemical Gas Sensors for Harsh Environments Based on Au-YSZ Nanocomposite Films", Materials Research Society (Spring 2005)
3. G. Sirinakis, L. Sun, R. Siddique, H. Efstathiadis, M. A. Carpenter, A. E. Kaloyeros, "Synthesis and Spectroellipsometric Characterization of Y_2O_3-stabilized ZrO_2-Au Nanocomposite Films for Smart Sensor Applications", Materials Research Society (Fall 2004)

Awards Received as a Result of Supported Research

N/A

Students Supported

George Sirinakis, Ph.D. – graduated January 2007
Phillip H. Rogers, Ph.D.

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[1] R. Jin, Y. Cao, C. Mirkin, K. L. Kelly, G. C. Schatz, J. G. Zheng, "Photoinduced conversion of silver nanospheres to nanoprisms", *Science*, **294**, 1901 (2001).
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[3] S. C. Singhal, "Advances in solid oxide fuel cell technology", *Solid State Ionics*, **135**, 305 (2000).
[4] O. Yamamoto, "Solid oxide fuel cells: Fundamental aspects and prospects", *Elect. Act.*, **45**, 2423 (2000).