Oxide Heterostructures-Interface Form & Function
Focus Topic
Room: Central Hall - Session OX-TuP

Oxide Interfaces and Heterostructures Poster Session

OX-TuP1 A Kinetic Monte Carlo Study of Cu Cluster Formation on Cu and ZnO Surfaces using COMB Potentials, *Y.-T. Cheng, T. Liang,* University of Florida, *X.W. Nie,* The Ohio State University, *S.R. Phillpot,* University of Florida, *A. Asthagiri,* The Ohio State University, *S.B. Sinnott,* University of Florida

Heterogeneous systems of Cu clusters on ZnO surfaces are used as catalysts and it is a challenge to maintain the stability and activity of the catalyst under reaction conditions. Processes such as sintering, alloying, and encapsulation may play an important role in the activity of the catalyst but are difficult to model directly with electronic structure calculations. In this work, we will report on the development and use of charge-optimized many-body (COMB) potentials to model the Cu/ZnO system. In particular, the diffusion of Cu atoms and the ripening of Cu clusters on Cu and ZnO surfaces are modeled using kinetic Monte Carlo simulations, which is used in conjugation with the dimer method to find possible transition paths for Cu migration. Simulations allow for a comparison of transport mechanisms on the two different surfaces (Cu and ZnO) and the predictions are compared to the results of density functional theory calculations and published experimental data. This work was supported as part of the Center for Atomic Level Catalyst Design, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under award number DE-SC0001058.

OX-TuP3 Molecular Dynamics Simulation Studies of The Toughening Mechanisms of Bio-inspired Hybrid Ceramic-based Materials, *K. Yao, T. Liang, D.E. Yilmaz, S.R. Phillpot, S.B. Sinnott,* University of Florida

Bio-inspired hybrid ceramic-based materials have attracted attention due to their high yield strength and fracture toughness. In this work, the mechanisms associated with the mechanical responses of composites of poly(methyl methacrylate), or PMMA, and Al_2O_3 in two hierarchical configurations, lamellar and brick-and-mortar, are considered. In particular, classical molecular dynamics simulations using charge optimized many-body (COMB) potentials are carried out to identify these mechanisms. The influence of such factors as the arrangement of the phases in the two different configurations, interfacial composition, nanometer-scale structure, and polymer thickness are considered. The nanometer-scale responses of the composites nanoindentation, shearing, and bending are compared with experimental data. This work is supported by DARPA.

OX-TuP4 A Variable Charge Reactive Potential for Nitrogen based Hydride and Oxide Molecules to Simulate Oxide Growth on AlN and TiN, *J. Martinez, S.R. Phillpot, S.B. Sinnott,* University of Florida

An empirical, variable charge potential for Nitrogen hydride and Nitrogen oxide molecular systems based on the charge optimized many body (COMB) potential framework is proposed. The potential is fitted to structure and energetic properties of certain key molecules such as NH_3 and NO_2. This potential is used in conjunction with TiN/TiO_2 and the AlN/Al_2O_3 variable charge potentials based in the same COMB framework to study the structure, energetics, and mechanics of oxide growth on TiN and AlN under varying conditions.

OX-TuP5 Effects of Nonstoichiometry on the Structure and Electronic Properties of $LaCrO_3$ Thin Films on $SrTiO_3(001)$, *K.H.L. Zhang, Y.G. Du, L. Qiao, S.A. Chambers,* Pacific Northwest National Laboratory

The ability to precisely control the structure, stoichiometry and defect densities in epitaxial perovskite films is emerging as one of the major challenges for understanding the sometimes novel physical properties exhibited by interfaces and superlattices of these materials. Recently we have demonstrated that structurally excellent, stoichiometric $LaCrO_3$ thin films can be grown on $SrTiO_3(001)$ by molecular beam epitaxy. In this contribution, we further explore the effects of nonstoichiometry on the structure and electronic properties of $La_{1+x}Cr_{1-x}O_3$ thin films with -0.13<x<0.05. Interestingly, La-deficient films maintain high crystalline quality in spite of very large deviations from stoichiometry, while La-rich films exhibit significantly degraded crystalline quality. Ongoing studies of lattice parameters, film and interface microstructures, and electronic properties will be discussed in order to elucidate different mechanisms of accommodating A-site and B-site cation imbalances during the epitaxial growth of perovskites.

OX-TuP6 The Influence of Nano-Scale Interfaces and Co-Doping on the Oxygen Ionic Conductivity of Ceria and Zirconia Based Thin Film Electrolytes, *M.I. Nandasiri, Q. Langfitt, M. Quintero, T. Varga, A. Devaraj, S. Manandhar, P. Nachimuthu, V. Shutthanandan, S. Thevuthasan,* EMSL, Pacific Northwest National Laboratory, *A. Kayani,* Western Michigan University

The high temperature operation of solid oxide fuel cells (SOFC) is one of the main challenges we have to overcome, especially for commercializing SOFC for portable power generating applications. Solid state electrolytes with enhanced oxygen ionic conductivity at low and intermediate temperatures are needed to lower the operating temperature of SOFC. Thus, there is an ongoing need to develop new electrolytes or modify existing electrolytes to enhance the ionic conductivity. Co-doping can be used to modify existing ceria and zirconia based electrolytes. On the other hand, new electrolytes can be developed by utilizing the engineered interfaces in multi-layer thin films. Here, we investigate the influence of nano-scale interfaces and co-doping on the ionic conductivity of ceria and zirconia based electrolytes.

In this study, we have grown (i) multilayers of high quality samaria doped ceria (SDC) and scandia stabilized zirconia (ScSZ) epitaxial thin films, and (ii) samaria and gadolinia co-doped high quality ceria thin films using oxygen plasma-assisted molecular beam epitaxy and characterized using various capabilities. The number of layers in the SDC/ScSZ multi-layer thin films was varied from 2 to 20 by keeping the total film thickness constant at 140 nm to understand the effect of nano-scale interfaces on the ionic conductivity. To understand the effect of co-doping on the ionic conductivity of optimized SDC thin films, $Ce_{0.85}Sm_{0.15-x}Gd_xO_{2-\delta}$ (SGDC) thin films were deposited by varying the Gd concentration. The film growth was monitored using in-situ reflection high energy electron diffraction (RHEED). Structural properties of these films were studied using x-ray diffraction (XRD) and the XRD patterns confirmed the growth of epitaxial thin films. The film and layer thicknesses were determined by x-ray reflectivity. X-ray photoelectron spectroscopy was used to find the composition, depth profile and chemical state of elements of the films. The SDC/ScSZ multi-layer and SGDC thin films were carefully characterized using Rutherford backscattering spectrometry, coupled scanning transmission electron microscopy and atom probe tomography to study the oxygen vacancy and dopant distributions along with the inter-diffusion and dopant segregation at the interfaces. Oxygen ionic conductivity measurements were carried out as a function of temperature on well characterized samples using four probe surface impedance spectroscopy. Detailed analysis of oxygen ionic conductivity as a function of individual layer thickness, dopant concentration, and crystalline quality of the films will be discussed.

Authors Index
Bold page numbers indicate the presenter