2015

7th CCAC

Student Conference

COLORADO CENTER FOR ADVANCED CERAMICS

PROCEEDINGS

Yachao Chen

Debora Barcellos

Chuancheng Duan

Adam Stokes

Welcome to the meeting

We are very pleased to welcome all of you to the 7th Annual CCAC Student Conference. I hope you will enjoy the variety of scientific research and speakers.

We would like to begin by thanking Dr. Anthony Dean and Jean Yeager from the office of Research and Technology Transfer at Colorado School of Mines, Prof. Craig Taylor from REMRSEC (Renewable Energy Materials Research Science and Engineering Center), and Prof. Ivar Reimanis, Herman F. Coors distinguished professor of ceramic engineering for their generous sponsorship of this event. We sincerely hope research collaborations will continue to grow from these promising relationships.

We would also like to thank our keynote speakers: Dr. Andriy Zakutayev from NREL and Dr. Geoff Brennecka from CCAC. We are grateful to them for accepting our invitation in spite of their very busy schedule.

Additionally, we would like to give our deepest gratitude to our center director Prof. Ivar Reimanis for his guidance and mentoring throughout this process. Please join us in thanking and congratulating him on being elected as a Fellow of the American Ceramic Society. We are also very thankful to Elaine Wolfschlag for her great help in all the financial associated with the conference.

Last but not least, thanks to all of you for your hard work and active contribution to the conference.

Best Regards,

2015 CCAC Committee Members
Yachao Chen (Chair)
Debora Barcellos
Chuancheng Duan
Adam Stokes

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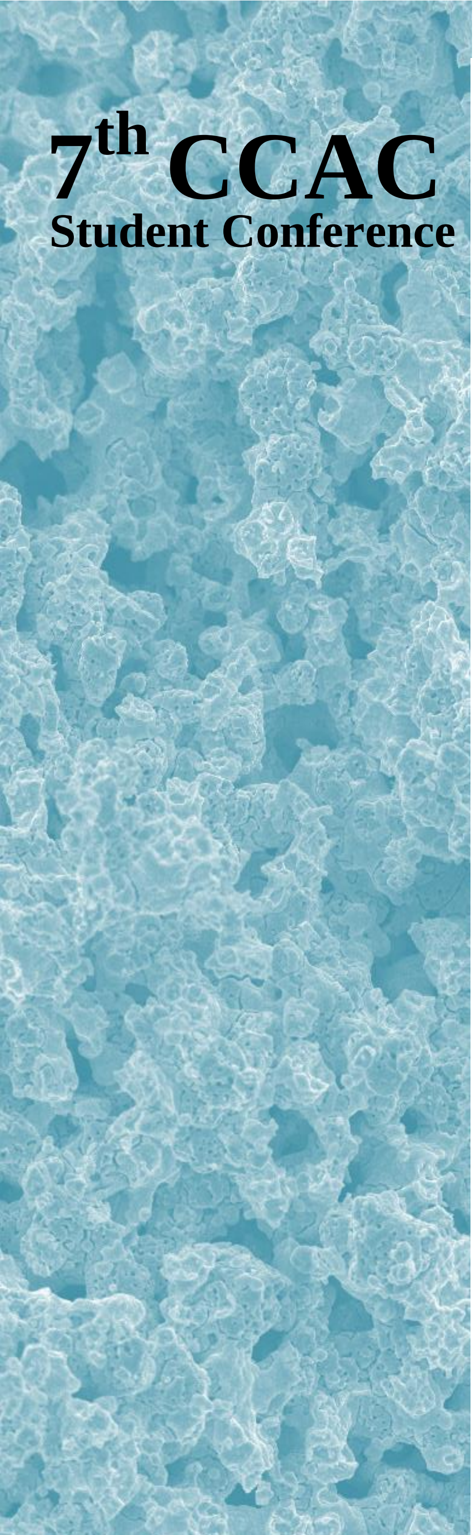

7th CCAC
Student Conference

Conference Schedule

Friday, August 21st, 2015

9:00-9:15 AM	Check in
9:15-9:30 AM	Introduction, welcome, and instructions by Prof. Ivar Reimanis
Invited Presentation	
9:30-10:10 AM	Keynote Speaker: Dr. Andriy Zakutayev – NREL
10:10-10:30 AM	Coffee Break
10:30-11:10 AM	Keynote Speaker: Dr. Geoff Brennecka – CCAC
11:10-11:30 AM	Group photo
Oral Session 1	
11:30-11:50 AM	“$ZnSiP_2$ as a potential monolithic top cell material on crystalline silicon photovoltaics” by Aaron D. Martinez
11:50AM-1:30PM	Lunch
Oral Session 2	
1:30-1:50 PM	“Synthesis and characterization of rare earth orthophosphates” by Matt Musselman
1:50-2:10 PM	“Effects of heat treatments on optical and mechanical properties of alumina-rich spinel” by Aaron Miller
2:10-2:30 PM	“Reversible protonic ceramic electrochemical cell technology for green fuel and power production” by Chuancheng Duan
2:30-4:30 PM	Poster Session
4:30-4:45 PM	Closing Remarks & Awards

$ZnSiP_2$ as a potential monolithic top cell material on crystalline silicon photovoltaics

Authors: Aaron D. Martinez* [1], Emily L. Warren[2], Prashun Gorai[1,2] , Kasper A. Borup[1,3], Sukgeun Choi[2], Darius Kuciauskas[2], Patricia C. Dippo[2], Brenden R. Ortiz[1], Andrew G. Norman[2], Paul Stradins[2], Vladan Stevanovic[1,2], Eric S. Toberer[1,2], and Adele C. Tamboli[1,2]

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[2]National Renewable Energy Laboratory, 15013 Denver W Pkwy Golden, CO 80401, USA [3]Department of Chemistry, Aarhus University, Langelandsgade 140, DK-8000 Aarhus C, Denmark

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Abstract: For tandem photovoltaics using a silicon bottom cell, as well as for other optoelectronic applications, there has been a longstanding need for optically active, wide band gap materials that can be integrated with silicon. $ZnSiP_2$ is a wide band gap (2.1 eV) material that is lattice matched with silicon and comprised of inexpensive elements. Here, we examine photovoltaic-relevant properties of $ZnSiP_2$ to evaluate its use as a monolithic top cell on silicon. We have found this material to be stable at temperatures up to 800 ℃. Its index of refraction is matched with silicon such that reflection at a $ZnSiP_2$/Si interface is less than 1% in the spectral region.

Synthesis and characterization of rare earth orthophosphates

Authors: M. A. Musselman[1*], T. M. Wilkinson[1], Z. D. McMullen[1], C. E. Packard[1]

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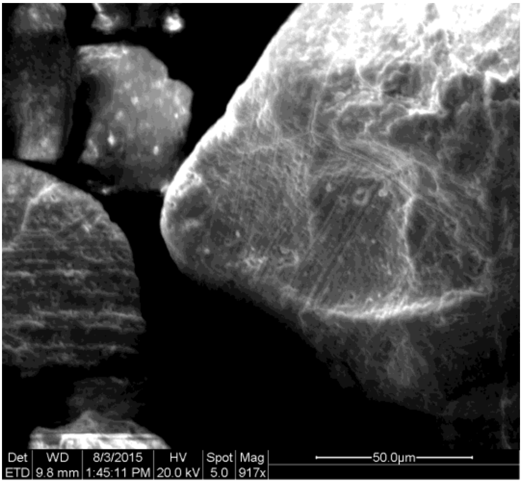
Abstract: Rare-earth (RE) orthophosphates ($REPO_4$) comprised of rare-earth lanthanide cations and can take on a tetragonal (xenotime) or monoclinic (monazite) structure. Some compounds in the xenotime phase can undergo a pressure-induced phase transformation to monazite. There is interest in applying this characteristic to fiber coatings in ceramic-matrix-composites (CMC's) to engineer fiber pullout stresses for increased fracture toughness. Solid solutions of rare earth phosphates may yield tunable transformation pressures to allow precise engineering of the transition. These materials are synthesized by precipitation from a mixture of rare-earth nitrates and phosphoric acid. Particle size and morphology were characterized by scanning electron microscopy (SEM). Temperature dependent phase presence was determined through simultaneous thermal analysis (STA) and X-ray diffraction. Material composition was determined by electron dispersive X-ray spectroscopy (EDS). The pure rare-earth phosphates that have been synthesized include Er, Dy, Tb, Gd, Eu, and La-based phosphates and solid solutions of Gd and Dy ($Gd_xDy_{(1-x)}PO_4$).



$Gd_{0.5}Dy_{0.5}PO_4$ powder after calcination

Effects of heat treatments on optical and mechanical properties of alumina-rich spinel

Authors: J. A. Miller[1*], I. E. Reimanis[1], W. Miao[2]

[1]Colorado Center for Advanced Ceramics, Colorado School of Mines, Golden, CO, USA
[2]Corning Incorporated, Corning, NY, USA

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Abstract: Certain ceramics show potential for use in transparent armor applications because of their unique combination of optical and mechanical properties. In particular, magnesium aluminate spinel exhibits Knoop hardness values of 160 GPa and in-line transmission as high as 85% in the visible through mid-infrared portion of the electromagnetic spectrum. However, spinel has fracture toughness of 1.5-1.9 $MPa*m^{0.5}$, which must be improved upon for armor applications. In this study, $MgO \bullet nAl_2O_3$ spinel where n=1.00 and n=2.00 was hot pressed, then hot isostatic pressed to form fully dense compacts. Specimens were then heat treated at 1300°C for 1, 10, and 20 hours in air and under vacuum to examine precipitation of second phase Al_2O_3 and its effects on the optical and mechanical properties of the material. Hardness, fracture toughness, and transmission results are presented. Energy Dispersive X-ray Spectroscopy and Scanning Electron Microscopy are used to characterize the microstructure and explain these results.

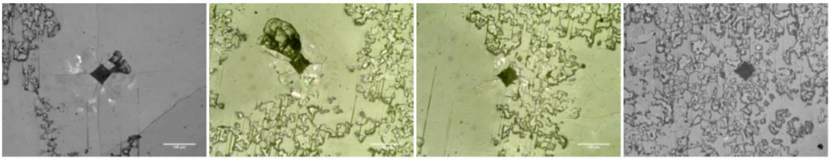


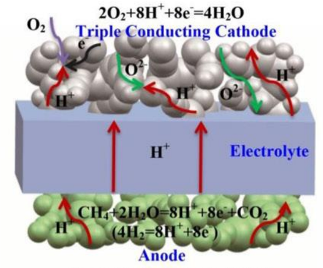
Figure 1: Vickers Hardness indents in various regions of alumina-rich spinel showing crack behavior around alumina precipitates.

Reversible protonic ceramic electrochemical cell technology for green fuel and power production

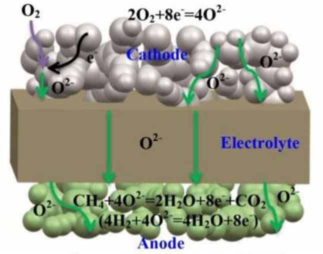
Authors: Chuancheng Duan[1], Jianhua Tong[1], David Shnaider[1], Ryan O'Hayre[1]

[1]Colorado Center for Advanced Ceramics, Colorado School of Mines, Golden, CO, USA

Abstract: Because of the generally lower activation energy associated with proton conduction in oxides compared to oxygen ion conduction, protonic ceramic electrochemical cells (PCECs) should be able to operate at lower temperatures than solid oxide fuel cells (250 °-550 ℃ vs. ≥600°C) on hydrogen, hydrocarbon fuels and other green fuels if fabrication challenges and suitable cathodes can be developed. We fabricated the complete sandwich structure of PCECs directly from raw precursor oxides with only one moderate-temperature processing step through the use of sintering agents such as copper oxide. We also developed a proton, oxygen-ion, and electron-hole conducting PCEC-compatible cathode material, $BaCo_{0.4}Fe_{0.4}Zr_{0.1}Y_{0.1}O_{3-\delta}$ (BCFZY0.1) that greatly improved oxygen reduction reaction kinetics at intermediate to low temperature. We demonstrated high performance of PCEC button cells on Hydrogen, Methane and Ammonia. PCECs also have potential to produce Hydrogen, Methane and Ammonia.



Protonic Ceramic Fuel Cell



Oxygen-ion Conductor SOFC

Engineering controlled spalling in (100)-oriented GaAs for wafer reuse

Authors: Cassi A. Sweet[1]*, Joshua E. McNeely[1], Brian P. Gorman[1], David L. Young[2], Aaron J. Ptak[2], Corinne E. Packard[1,2]

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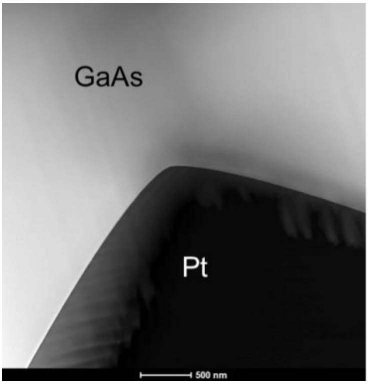
Abstract: Controlled spalling offers a way to cleave thin, single-crystal films or devices from wafers, particularly if the fracture planes in the material are oriented parallel to the wafer surface. Unfortunately, misalignment between the favored fracture planes and the wafer surface preferred for photovoltaic growth in (100)-oriented GaAs produces a highly faceted surface when subject to controlled spalling. This highly faceted cleavage surface is problematic in several ways: (1) it can result in large variations of spall depth due to unstable crack propagation; (2) it may introduce defects into the device zone or underlying substrate; and (3) it consumes many micrometers of material outside of the device zone. We present the ways in which we have engineered controlled spalling for (100)-oriented GaAs to minimize these effects. We expand the operational window for controlled spalling to avoid spontaneous spalling, find no evidence of dislocation activity in the spalled film or the parent wafer, and reduce facet height and facet height irregularity. Resolving these issues provides a viable path forward for reducing III-V device cost through the controlled spalling of (100)-oriented GaAs devices and subsequent wafer reuse when these processes are combined with a high-throughput growth method such as Hydride Vapor Phase Epitaxy.



Scanning transmission electron micrograph of a facet in GaAs. The lighter portion of the image is GaAs. No dislocations are present in the vicinity of the facet.

Investigating Pressure-Induced Phase Transformations in Rare-Earth Orthophosphates

Authors: Taylor M. Wilkinson[1*], Matthew A. Musselman[1], Zachary D. McMullen[1], Corinne E. Packard[1]

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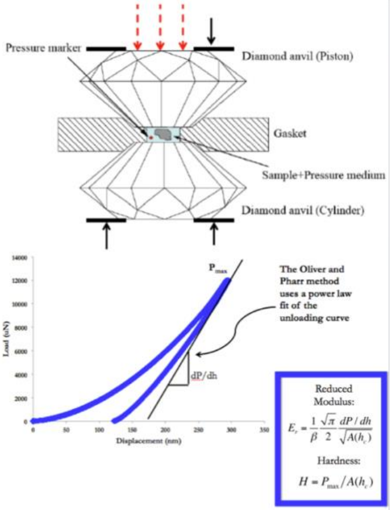
Abstract: Some rare-earth orthophosphates ($REPO_4$) in the xenotime crystal structure have been observed to undergo a pressure-induced phase transformation to the monazite crystal structure. This phenomenon has briefly been investigated using Diamond Anvil Cell (DAC) and nanoindentation (NI). DAC (Figure 1 – Top) applies hydrostatic pressure to the material of interest and a reference (ruby) located between two diamond cutlets. Raman spectra are collected *in situ* and analyzed to determine the onset pressure for the xenotime-to-monazite phase transformation. NI (Figure 1 – Bottom) uses a diamond probe to apply small loads to a material while simultaneously measuring the displacement of the probe into the material over a large range of strain rates. Unlike DAC, NI offers an understanding of the dynamic behavior of the phase transformation of $REPO_4$s, with the challenge that the data is derived from a more complex stress state. This research combines both techniques in order to understand the kinetics of the transformation under different stress states and as a function of chemistry. DAC and NI data will be further analyzed to determine the reversibility of the phase transformation and its associated hysteresis solutions of Gd and Dy ($Gd_xDy_{(1-x)}PO_4$).



Diamond Anvil Cell (DAC) schematic (Top)
Normal quasistatic nanoindentation curve (Bottom)

Surface Analysis of Templated Palladium-Platinum Nanostructured Hydrogenation Catalysts

Authors: T. Nitka and S. Pylypenko[1]
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[2] Applied Chemical and Materials Division, National Institute of Standards and Technology
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Y. Reng, S. Lee, B. Reinhart5
[5]X-Ray Sciences Division, Argonne National Laboratory

Abstract: Bimetallic catalysts are used for various applications, but are more complicated than monometallic catalysts and require surface tuning for optimal performance. This work focuses on palladium-platinum nanostructured catalysts for hydrogenation of allyl alcohol. A series of palladium-platinum nanostructures were synthesized using the R5 peptide template with the following sequence: SSKKSGSYSGSKGSKRRIL. These materials were investigated with x-ray photoelectron spectroscopy (XPS), identifying the elemental composition and surface functionality of the catalysts. The catalysts were also analyzed using extended X-ray absorption fine-structure spectroscopy (EXAFS)), transmission electron microscopy (TEM), and energy dispersion x-ray spectroscopy (EDS). Due to the presence of the template XPS signals of palladium and platinum are relatively low, nevertheless, two major trends were identified. First, the surface of the catalysts was found to be rich in platinum. Second, significant oxidation was observed for all catalysts, with less oxidation observed in the catalysts with higher ratios of palladium to platinum. XPS data supports the observations made by other spectroscopic techniques, confirming similar trends between the bulk and surface composition.

Rapid prediction of oxygen vacancy formation energies in metal oxides

Authors: Ann M. Deml,[1,2] Aaron M. Holder,[2] Ryan P. O'Hayre,[1] Charles B. Musgrave,[3] and Vladan Stevanović[1,2]

[1] Colorado School of Mines, Golden, CO, USA

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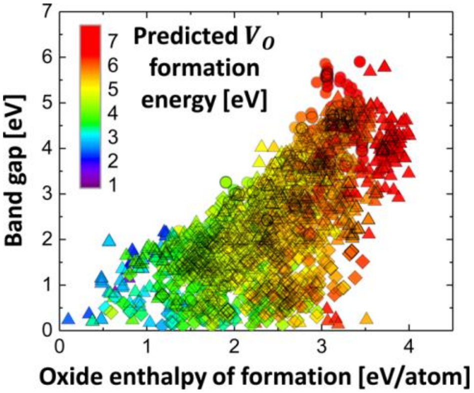
[3] University of Colorado Boulder, Boulder, CO, USA

Abstract: Point defects such as oxygen vacancies in metal oxides are extensively used to manipulate vital material properties. While methods to predict such defect formation energies have advanced significantly, high throughput calculations of defective systems remain a challenge largely due to prohibitive computational costs. We demonstrate an approach to move beyond the current high throughput calculations of perfect materials to rapid predictions of defect systems, a key for enabling materials genome inspired design and discovery of materials. We use first principles calculations to study the connection between intrinsic (bulk) material properties and the energy to form a single, charge neutral oxygen vacancy (E_V). We investigate 45 binary and ternary oxides and find that a simple model which combines (*i*) the oxide enthalpy of formation, (*ii*) the mid-gap energy relative to the O-2p band center, and (*iii*) atomic electronegativities reproduces calculated E_V within ~0.2 eV. This result provides both a direct method to predict E_V and valuable insights into the key properties influencing E_V. We predict the E_V of ~1800 oxides and validate the predictive nature of our approach against direct defect calculations for a subset of 18 randomly selected materials. We advocate use of this direct and simple method to predict E_V at significantly reduced computational cost in order to identify candidate materials for applications where oxygen vacancies (or lack thereof) are of critical significance.



Predicted oxygen vacancy formation energies (E_V) for ~1800 oxide materials calculated from intrinsic, bulk material properties.

Dopant and Interfacial Analysis of Epitaxial CdTe Using Atom Probe Tomography

Authors: George L. Burton[1]*, David R. Diercks[1], Brian P. Gorman[1]

[1]Metallurgical and Materials Engineering, Colorado School of Mines, Golden, CO.

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Abstract: In this study, the growth parameters of epitaxially-grown Cadmium Telluride (CdTe) are optimized by examining impurities within the material using high throughput, high resolution microscopy. CdTe has a high absorption coefficient, a direct band gap and can be produced easily from raw materials, and as a result has shown exceptional promise in the field of photovoltaics, with polycrystalline devices reaching efficiencies of over 20%. However, to approach the theoretical efficiency of ~30%, CdTe can be grown as a single crystal with meticulous control over chemical purity and dopant concentration by molecular beam epitaxy (MBE). This approach allows for a fundamental study of the material, since grain boundaries, which give rise to high recombination rates, current leakage, device shunting, and enhanced migration of dopants, are eliminated. With its unparalleled three-dimensional atomic spatial resolution, laser-pulsed atom probe tomography (APT) is used to identify the concentration, uniformity, and location of impurity species, whether for dopants or unwanted contaminants. Transmission Electron Microscope (TEM) images of specimens taken prior to and following APT are used to produce an accurate analysis volume for APT 3D reconstructions. A number of samples with a variety of dopants and device geometries were analyzed. At high dopant concentrations, clustering, particularly of arsenic, was discovered with local segregation of over 40 atomic % throughout the sample. Samples grown on CdTe substrates showed carbon contamination at the homojunction interface, helping to explain the higher defect densities measured previously. APT analysis also showed a slight increase in oxygen and other contaminants at the bottom interface between cadmium magnesium telluride and CdTe layers. Interfacial contamination and dopant clustering discussed here are detrimental to defect densities and carrier lifetimes, and therefore the potential device efficiency. The correlation between growth conditions and APT findings, as well as their influence on material performance will be presented.

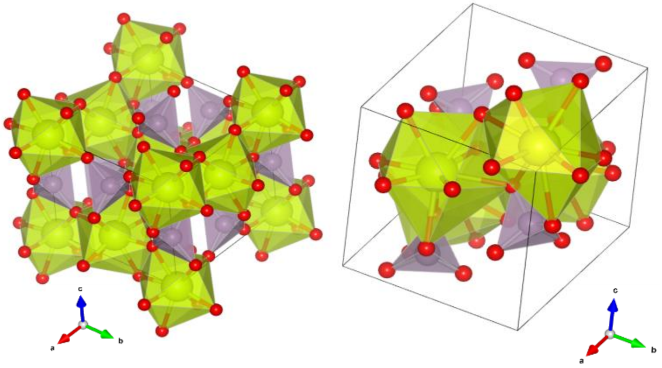
Rare Earth Orthophosphates and their Applications

Authors: Zachary McMullen[1], Matthew Musselman[1], Taylor Wilkinson[1], Corinne E. Packard[1*]

[1]Metallurgical and Materials Engineering, Colorado School of Mines, Golden, CO.

*Correspondence to: **cpackard@mines.edu**

Abstract: Rare-earth orthophosphates ($REPO_4$) are materials of interest for a multitude of applications, specifically for their ability to host a range of different RE cations in their crystal structure, their mechanical properties and their thermochemical stability. RE ions from the lanthanide series are located at the center of polyhedra with 8- or 9-fold coordination with oxygen, depending on whether the $REPO_4$ forms in the tetragonal xenotime or monoclinic monazite crystal structure. The atmospheric equilibrium crystal structure is a function of ionic radius and changes from monoclinic monazite to tetragonal xenotime on the lanthanide series between gadolinium and terbium. This research deals specifically with $REPO_4$'s based on gadolinium (Gd) and dysprosium (Dy) to tailor the structural transition and properties of the materials. These materials have been found to be very machinable, thermally and electrically insulating, and highly resistant to thermal, chemical, and radiological attack. Potential applications for these materials have not been fully developed, but include things such as fiber coatings for ceramic matric composites to permit fiber pull-out, proton conductors for fuel cells, and emissive hosts for lasers and phosphors. Historically, the most studied application of rare-earth orthophosphates was for their potential to host nuclear waste. Rare-earth orthophosphates make up a classification of materials that with their varying crystal structure and properties provide both intriguing science and a wide range of applications.



VESTA generated crystal structure model for xenotime (left) and monazite (right).
Red atoms=O, purple=P and yellow=RE

Investigation on Nonstoichiometric Perovskite Oxides of $Sr_{1-x}La_xMn_{1-y}Al_yO_{3-\delta}$ for Solar Thermochemical Hydrogen Production

Authors: D. R. Barcellos[1*], M. Sanders[1], J. Tong[1], A. McDaniel[2], R. O'Hayre[1]

[1]Metallurgical and Materials Engineering, Colorado School of Mines, Golden, CO, USA

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Abstract: Solar thermochemical (STC) fuels production is seeing increased scientific interest because of its high theoretical efficiency (~60%). The nonstoichiometric perovskite oxides of $Sr_{1-x}La_xMn_{1-y}Al_yO_{3-\delta}$ (SLMA) were discovered in our recent work (*Energy & Environmental Science*, *2013, 6 (8), 2424-2428*) to be excellent STC materials for both water splitting and carbon dioxide decomposition, and demonstrated a hydrogen yield of 9 times higher than ceria, the state-of-the-art STC material. However the kinetics of the water splitting (reoxidation) step is much slower for SLMA than that for ceria. Furthermore, even small changes in SLMA stoichiometry are thought to significantly alter the reoxidation kinetics. Because Mn-containing materials frequently suffer from Mn-loss during calcination at high temperatures (e.g. 1300°C), we adopt a modified polymeric gelation synthesis method and calcination profile for the synthesis of SLMA, which allows precise control of the SLMA stoichiometry. Based on this process, rectangular bars of stoichiometric SLMA and Mn-deficient SLMA were fabricated for conductivity measurement. Steady-state and transient conductivities versus temperature, oxygen partial pressure, and water vapor pressure were measured by a four-probe DC method and used for deriving the diffusivities of oxygen vacancy and electron hole and the surface reaction constant. These measurements are used to provide insights into the reoxidation mechanism in SLMA, which involves the combination of surface reaction ($H_2O + V_O^{\cdot\cdot} = O_O^X + 2h^{\cdot} + H_2$) and bulk internal oxidation (ambipolar diffusion of oxygen vacancies and electron holes from the surface to the bulk).

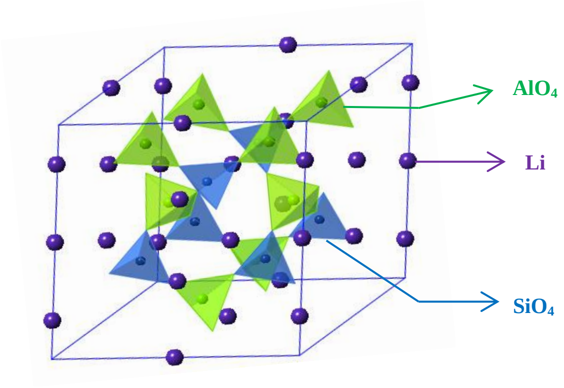
Ionic Conductivity of β-eucryptite Doped with Mg

Authors: Yachao Chen[1], Lei Cheng[2] and Ivar E. Reimanis[1]

[1]Colorado Center for Advanced Ceramics, Colorado School of Mines, Golden, CO, USA

[2]Lawrence Berkeley National Laboratory, Berkeley, CA, USA

Abstract: Lithium aluminum silicates such as β-eucryptite ($LiAlSiO_4$) are well-suited for thermal shock resistant structures, precision optics platforms, and various other applications where low or negative coefficient of thermal expansion (CTE) is required. Particularly, β-eucryptite has potential use in many of these applications because it exhibits an average negative CTE. When β-eucryptite is doped with small amounts of Zn (as low as 0.1 molar percent), the CTE increases significantly, and the tendency of microcracking decreases greatly compared with pure β-eucryptite. The present study explores the reasons Zn influences the CTE so dramatically and also extends the work to Mg doped β-eucryptite. In-situ high temperature X-ray diffraction tests were performed on pure and Mg doped β-eucryptite synthesized from chemical precursors. And the temperature dependence of ionic conductivity of β-eucryptite is measured for doped and un-doped samples to explain Mg occupation in the structure.



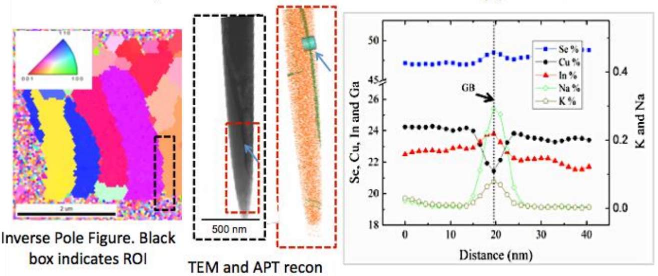
Alkali segregation related to matrix concentrations of thin film Cu (In,Ga)Se_2 at targeted grain boundaries characterized in 3-D at the nanoscale

Authors: Adam Stokes[1], Brian Gorman[1]

[1]Metallurgical and Materials Engineering, Colorado School of Mines, Golden, CO, USA

Abstract: Recently, the highest laboratory efficiencies of polycrystalline Cu(In,Ga)Se_2 thin film solar cells have been achieved by introducing alkali impurity atoms, namely K and Na. The role of K is believed to mimic the same role as Na, which has been long exploited for enhanced efficiencies, but we still do not know key details of where the K resides and what affect this has on the matrix elements. This contribution will discuss a novel technique used to target grain boundaries with known structure to relate quantified K and Na segregation to matrix elements concentrations. We used this technique to select from roughly 30 grain boundaries with known misorientations, extracted from electron backscattered diffraction (EBSD) micrographs, and then chemically analyzed them in 3-D using atom probe tomography (APT). The grain boundaries analyzed exhibited a correlation of K and Na segregation to matrix elements concentrations and grain boundary misorientations. We believe this is the first time such impurities have been characterized with such sensitivity (PPM) and nm spatial resolution.

EBSD, TEM and APT Correlative Microscopy



Inverse Pole Figure. Black box indicates ROI

TEM and APT recon showing same GB

GB Chemistry

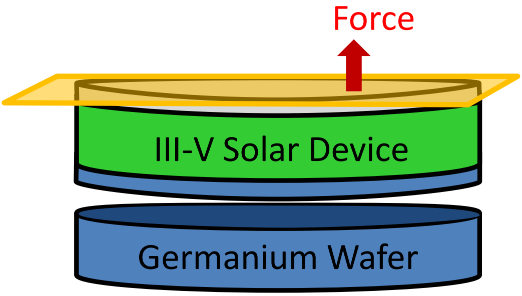
Controlled spalling of Ge for cost-effective III-V solar cell applications

Authors: D. Crouse[1]*, C. E. Packard[1,2], J. Simon[2], A. Ptak[2], D. Young[2], N. Jain[2]

[1]Colorado School of Mines

[2]National Renewable Energy Laboratory

Abstract: III-V solar cells grown on germanium (Ge) substrates face severe challenges meeting the Department of Energy's SunShot price goal to reach $1/W by the year 2017. III-V solar cells can achieve >30% efficiencies for one-sun applications, yet suffer from high material costs. Ge substrates represent a signification fraction of overall production costs. The goal of this project is to delaminate III-V devices grown on Ge substrates with attention toward device quality, substrate reuse, and manufacturability. Substrates will be reused via a recently developed controlled spalling technique. The spalling process is a substrate removal process that utilizes fracture to create wafer cleavage parallel to the surface as a result of the stress field generated by a residually stressed thin film. In this study, factors that influence the spall depth of germanium and spall uniformity were investigated in a series of experiments. The experimental process included a nickel (Ni) stressor layer electroplated onto an etched germanium substrate. The optimal processing window was determined for a Nickel-Watts plating bath. Electroplated Ni film thickness was calibrated to residual stress. Spalled film thickness was measured and compared to trends expected by fracture mechanics theory. Results suggest thinner Ni layers with higher internal stress leads to shallower spall depths of germanium. Controlled spalling has proven to be a simple and cost effective method for removing thin Ni stressor layers from brittle Ge substrates. Once residual stress within the stressor layer can be reliably predicted using finite element analysis software, controlled spalling may provide an economic means to produce commercial III-V solar cells.



Nanoscale Seed Layers for Enhanced Performance of Transparent Conducting Oxide Thin Films on Glass

Authors: Stefan Nikodemski[1*], Arrelaine Dameron[2], David Ginley[2], John Perkins[2], Joseph Berry[2] and Ryan O'Hayre[1]

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Abstract: Transparent conducting niobium doped TiO_2 films were deposited on amorphous substrates (glass) by sputtering. The deposition conditions to produce crystalline anatase films were first optimized and indicated that the substrate temperature and oxygen pressure are important parameters to produce the desired phase and high conductivity. To generate the anatase phase, films must be deposited in a high oxygen pressure environment with subsequent annealing/crystallization done in a reducing atmosphere (typically vacuum). The conductivity of these doped TiO_2 films were improved through the use of nanoscale seed layers deposited by atomic layer deposition (ALD). The bottom seed layer appears to behave as a nucleation center during crystallization to produce films with larger crystal domains at lower temperatures. A variety of ALD growth conditions including precursor chemistry, seed layer thickness, and temperature were examined. Design of experiments was subsequently used to identify the key parameters to produce the highest performing thin films. Results mapping out this complex deposition parameter space and the consequences to the obtained electrical transport properties will be presented along with an observed order of magnitude enhancement in the Nb-TiO_2 films using a nucleation/seed layer approach. Raman spectroscopy, X-ray diffraction, and transmission measurements used to assess the role of the seed layer in determining the performance of the oxide thin films will also be presented.

The Effect of Yttrium Source on the Microstructure and Hygroscopic Behavior of $BaCe_{0.8}Y_{0.2}O_{3-\delta}$ Using ZnO as Sintering Aid

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Abstract: Yttrium-doped barium cerate (BCY) is a well-known proton-conducting oxide with perovskite structure which has been extensively studied along the last 30 years mainly for uses such as solid electrolyte in SOFCs. In this work the influence of two different sources of Yttrium on the BCY microstructure was investigated. Two samples with similar composition $BaCe_{0.8}Y_{0.2}O_{3-\delta}$ + 1 wt% ZnO were obtained via the Solid-State Reactive Sintering method, developed by researchers from the Colorado School of Mines. The use of small amounts of ZnO as sintering aid is an efficient way to increase the BCY sinterability without compromising its proton conductivity. Stoichiometric amounts of comercial $BaCO_3$, CeO_2, ZnO and Y_2O_3 (YO-sample) or $Y(NO_3)_3\ 6H_2O$ (YN-sample) were all dispersed in isopropanol in a jar together with 1 wt% of PVB. The slurries were ball milled for about 60 h and then dried and sieved with a 300 µm mesh. The powders were pressed into pellets isostatically at 200 MPa and sintered at different temperatures ranging from 1000 to 1500 ℃ for 12 h, using a heating rate of 2 ℃/min. Both samples presented the highest densification at 1100 ℃ (YN-sample = 5.92 ± 0.03 g/cm^3 and YO-sample = 6.03 ± 0.03 g/cm^3). The fracture surface and the polished cross section of 1.28 mm thickness sintered pellets were analyzed by SEM. Both samples presented a visually distinguishable core region with smaller grain size and a shell region with larger ones. Z-contrast images and EDS maps also showed grains with different Y and Zn content. Comparing both samples sintered at 1100 C, the YN-sample presented larger grain size and more homogenous Y and Zn distribution than the YO-sample; however it was visually observed that the YN-sample presented a hygroscopic behavior starting to degrade after two weeks exposed to the environment, while the YO-sample stayed unchanged.

CCAC News

- Dr. Ivar Reimanis was elected as a Fellow of the American Ceramic Society and the award was presented in October in Pittsburgh at the MS&T14 meeting.
- Dr. Geoff Brennecka joined the MME department as an Assistant Professor. He serves on the Board of Directors of the American Ceramics Society (ACerS). He has many other committee responsibility with ACerS, including chair of the Education Integration Committee and Vice Chair of the Electronics Division. Dr. Brennecka also has significant activity with the Institute of Electrical and Electronics Engineers (IEEE) Ultrasonics, Ferroelectrics, and Frequency Control Administrative Committe. This year he was recognized with the ACERS Du-CO Ceramics Young Professional Award, the Missouri S&T Distinguished Alumnus Award, and the IEEE Ferroelectrics Young Investigator Award. He will be teaching the Ceramics Engineering course this fall and will be an active member of Colorado Center for Advanced Ceramics (CCAC).
- Dr. Corinne Packard received the CAREER award from NSF's Ceramics Program. This prestigious award from the National Science Foundation is "to support junior faculty who exemplify the role of teacher scholars though outstanding research, excellent education, and the integration of education and research within the context of the mission of their organizations." This special award will allow Dr. Packard to extend and deepen her research over a longer period of time than a typical grant would allow.
- Dr. Corinne Packard's collaborative work with NREL on next generation solar PV technologies has been awarded $1.5 million by the US Department of Energy. The project aims to develop an InGaAsP/Si tandem photovoltaic technology that will yield low-cost, high-efficiency devices. The research conducts controlled liftoff of III-V devices grown on Ge substrates with attention toward device quality, substrate reuse, and manufacturability. Focus is also given to developing a low-cost, high-throughput growth of highly efficient III-V solar cells with the optimal bandgap to achieve the maximum efficiency from a two-junction structure. The Mines-NREL joint project is funded through SunShot's "Next Generation Photovoltaics Program" - a collective national effort put forth by the Department of Energy with the goal of making solar energy fully cost-competitive with traditional energy sources before the end of the decade.
- Dr. Ryan O'Hayre authored a first edition textbook titled, "Materials Kinetics Fundamentals: Principles, Processes, and Applications," published by Wiley in January 2015. MME Research Prof. Michael Sanders provided illustrations for the book.

- Dr. Brian Gorman is the 2014 recipient of the W. F. J. Heinrich Award from the Microscopy and Microanalysis Society. This award, given to one individual per year, is for the best scientific accomplishment by an individual under the age of 40.
- Dr. Brian Gorman is the recipient of a DOE/EFRC award with NREL and MIT for $3.5 M titled "Center for Next Generation of Materials by Design: Incorporating Metastability"
- Dr. Ryan O'Hayre's team (Ryan O'Hayre, Neal Sullivan, Robert Braun, Sandrine Ricote and Jianhua Tong) officially started a $1M, 2-year ARPA-E project on the Protonic Ceramic "Flex Fuel Cell". They are in the process of filing several patents through Will Vaughn's office to protect the IP that led to the successful ARPA-E grant award.
- Dr. Ryan O’Hayre received the CSM Excellence in Research Award for Junior Faculty, at the April 22nd Faculty Forum. Pictured right.
- Dr. Svitlana Pylypenko, previously a research professor in the Center, began in September as an assistant professor in the Chemistry and Geochemistry Department at Mines.
- Group of Dr. Ryan O’Hayre’s fuel cell breakthrough was reported by Science Magazine.
- Marc Rubat du Merac, Ann Deml, Kevin Wood, Jason Fish, Archana Subrimaniyan, Liangju Kuang, Wan Zheng, Dan Clark and Amy Leigh Morrissey earned their PhDs. Yunjiang Jiang earned his Master degree. Congratulations!
- Graduate student Yachao Chen received the Graduate Excellence in Materials Science (GEMS) award at the 2014 MS&T Conference. Yachao was one of only three students to receive the highest of nine awards - the Diamond Award - as a result of an open competition for all 887 graduate students at the conference.
- Adam Stokes received the best student presentation award at the IEEE Photovoltaic Specialists Conference in Denver last summer.

New researchers

- Meagan Papac will be joining Professor Ryan O’Hayre’s group as a graduate student.
- Elcio Liberato Pires is working on the role of purity in the sintering and microstructure of barium zirconate as a vising student with Prof. Reimanis.
- Jaya Dorsey is working on understanding abnormal grain growth in oxide ceramics with Prof. Reimanis.
- Tamoghna Chakrabarti will be working on the mechanical behavior of clays with Prof. Reimanis.

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