

Tuesday Afternoon Poster Sessions

Energy Science and Technology Focus Topic

Room: Hall D - Session EN-TuP

Energy Focus Topic Poster Session

EN-TuP1 Resistive Oxygen Gas Sensor Using Pure and Doped CeO₂, S. Gupta, Portland State University, S.V.N.T. Kuchibhata, M.H. Engelhard, P. Nachimuthu, V. Shuthanandan, L.V. Saraf, S. Thevuthasan, Pacific Northwest National Laboratory, S. Prasad, Portland State University

Oxygen sensors have come into wide use in automotive and industrial applications as leak detectors, industrial process flow evaluators, as well as in life science industry in diagnostic applications such as respiratory vital signs monitoring, and metabolic rate monitoring. All these applications require the fast monitoring of the oxygen gas. Hence we have explored the possibilities to develop an oxygen sensor operating on the chemiresistive principle at aggressive environments with a reduced response time. Ceria is known for its unique ability to lose or gain oxygen based on the ambient environment. The doping of trivalent elements including Y, Sm and Gd in ceria is expected to create oxygen vacancies and eventually influence virtually all types of transport properties like ionic and electronic properties. The overarching objective of this project is to study the effects of changes in surrounding conditions such as temperature, pressure, dopant concentration on the transport properties of doped ceria films. High quality, epitaxial, pure and doped ceria thin films were grown on sapphire (0001) substrates using oxygen plasma assisted molecular beam epitaxy (OPA-MBE) and characterized them using several bulk and surface sensitive techniques. Conductivity in these films was measured as a function of temperature (room temperature to 700C) under various oxygen partial pressure (1 torr to 100 torr) and vacuum conditions. Preliminary results show that response of the doped ceria film is much faster than the pure ceria films under the same conditions of temperature and pressure. Moreover response time of these films is few milliseconds with the change in the oxygen partial pressure. It was observed that the samarium concentration of approximately 4-6 atom% is the optimum doping content.

EN-TuP2 A Closer Look at H-CO Interaction on the Platinum Surface, T. Roman, H. Nakanishi, H. Kasai, Osaka University, Japan

The system comprised of coadsorbed hydrogen and carbon monoxide on platinum has been the subject of a number of experimental work due to its high relevance in heterogeneous catalysis, particularly in relation with hydrogen fuel cells. Several studies have asserted the strong repulsion between these two species on the solid surface, especially in high pressures, wherein the formation of homogeneous islands of CO have been reported. On the other hand, theoretical work specifically addressing the H/CO coadsorption system on Pt is rather limited. To fully understand the physical mechanisms involved at the atomic scale, it would be beneficial for example to quantify the extent to which H and CO interaction on Pt is repulsive, knowing that H-CO interaction in the gas phase is actually partly attractive, and comment on possibilities for H and CO closely coexisting on Pt. It is in this light that we in this study describe the behavior of hydrogen near a Pt surface-adsorbed carbon monoxide molecule using a potential energy term constructed from ab initio calculations. The considerable asymmetry of the repulsion extent around CO suggests that while incoming hydrogen experiences strong obstacles to adsorption even before the Pt surface is reached, adsorbed H can remain stable even in relatively compact conditions. Inhibiting effects of CO greater than what is expected from simple adsorption site exclusion are discussed with regard to adsorption/desorption and mobility on platinum, as well as possibilities of COH and HCO formation on platinum. A quantum mechanical treatment of the H atom behavior similar to what we have used before¹ is also performed on the obtained potential term. Theoretical results are lastly discussed with available experimental data on the H-CO coadsorbate system on transition metal surfaces.

¹T. Roman, H. Nakanishi, W. A. Diño, H. Kasai, e-J. Surf. Sci. Nanotech. 4 (2006) 619.

EN-TuP3 Electronic Energy Level Alignment in Dye Sensitized Oxide Substrates, J.P. Theisen, S. Rangan, E. Bersch, R.A. Bartynski, J.D. Sorge, D.P. Birnie, Z. Duan, Y. Lu, Rutgers University

In dye-sensitized solar cell applications, the HOMO-LUMO gap of dye molecules determines the useful portion of the solar spectrum, and charge transfer of photoexcited electrons to the substrate depends on the alignment of the LUMO to the substrate conduction band edge. We have used direct and inverse photoemission to measure the occupied and unoccupied electronic states of several dye-related molecules and determine their alignment with the band edges of single crystal and nanostructured TiO₂ and ZnO substrates. On well characterized rutile TiO₂(110) and wurtzite

ZnO(11-20) single crystal surfaces, we have compared the position of the HOMO and LUMO levels of the N3 Ruthenium based-dye, of isonicotinic acid and catechol molecules. Isonicotinic acid, as a simpler form of the linker that binds the N3-dye on TiO₂, is found to have a very similar electronic structure as the N3-dye in the unoccupied states. This is consistent with the electronic transfer scheme where N3 excitation occurs from the HOMO localized on its Ruthenium center, to the LUMO delocalized on the dye linker to the surface. Catechol on TiO₂(110) however has no electronic states degenerated with the bottom of the conduction band edge. As a consequence the lower energy excitation process occurs via a HOMO to conduction band process. We have also measured the electronic structure of N3 adsorbed on more technologically relevant TiO₂ anatase nanoparticle and ZnO nanorod substrates.

EN-TuP4 High Efficiency Down Converting Powder Phosphors for Solid State Lighting Applications, S. Maslov, D. Bera, L. Qian, P.H. Holloway, University of Florida

High performance blue and white organic light emitting diodes (OLED) offer improved efficiencies for solid state lighting. A down converting phosphor layer allows color tuning capabilities when coupled with a blue emitting OLED, and leads to improved efficacies approaching 80 lm/watt. The efficacy, CIE color coordinates, color rendering index, and angle resolved photoluminescence intensity were characterized versus film thickness and phosphor weight fraction. Due to scattering by phosphor particles, the initially forward focused light is converted to a Lambertian distribution of intensity. The method for applying powder thin films will be illustrated and discussed. The advantages and disadvantages of PMMA versus silicones for the dispersion matrix will be reported. Optimum phosphor layers were those with high quantum yield and maximum light out coupling.

EN-TuP5 Ionic Conductivity of Scandia Doped Zirconia Thin Films by Oxygen-Plasma-Assisted Molecular Beam Epitaxy, M.H. Engelhard, Pacific Northwest National Laboratory, Z.Q. Yu, Nanjing Normal University, China, S.V.N.T. Kuchibhatla, C.M. Wang, O. Marina, W. Jiang, V. Shuthanandan, P. Nachimuthu, R. Devanathan, L.V. Saraf, S. Thevuthasan, Pacific Northwest National Laboratory

The development of electrolyte materials with high oxygen ion conductance at relatively low temperatures is essential to increase the efficiency and lifetime of electrochemical devices, such as solid oxide fuel cells (SOFC). Recently, there has been considerable interest in scandia stabilized zirconia (SSZ) since it shows high oxygen ionic conductance in comparison to commonly used yttria stabilized zirconia (YSZ) in SOFCs. We have used oxygen plasma assisted molecular beam epitaxy (OPA-MBE) to synthesize high quality SSZ thin films on sapphire (0001) substrates and systematically investigated the conductivity as a function of temperature and Sc concentration. The epitaxial films have been characterized using various surface and bulk sensitive capabilities to determine their structure and composition. The ionic conductivity of SSZ depends not only on the dopant concentration, but also on the crystalline structure of the thin films. The optimum Sc dopant concentration for the highest conductivity was observed as 18 cation % in the temperature range of 500-900 °C. Conductivity appears to be significantly high in high quality cubic SSZ films in comparison to mixed phases of cubic and monoclinic. Molecular dynamics simulations of oxygen diffusion in cubic SSZ between 1125 and 2500 K show that the oxygen vacancy has no preference between Sc and Zr first neighbors, but the activation energy for O diffusion changes with Sc dopant concentration. Insights into the role of Sc dopant concentration on conductivity of SSZ obtained from experiments and simulations will be presented

EN-TuP6 Chemical Mechanical Polishing Characteristics of CdS for CdS/CdTe Thin Film Solar Cell Applications, H.-Y. Na, J.-S. Park, P.-J. Ko, Chosun University, Korea, N.-H. Kim, Chonnam National University, Korea, J.-T. Yang, Gwangju College of Korea Polytechnic V, W.-S. Lee, Chosun University, Korea

CdS is widely used for the window layer material for the various thin film solar cells including CdS/CdTe, CdS/Cu₂S, and CdS/CuInSe₂ due to its excellent permeability with band gap of 2.42 eV while CdTe is one of the most promising photovoltaic materials with a direct band gap of about 1.45 eV, high optical absorption coefficients, the low cost, high efficiency and stable performance. The surface morphology of window layer materials was well known to affect the performances including the gain in photocurrent by increase of light scattering.¹ Therefore the surface morphology of CdS thin film as an window layer must be enhanced by the improved processes. Sputtering method was employed for preparation of CdS thin film, but it showed the rough surface morphology. Chemical mechanical polishing

(CMP) processing was firstly proposed for improving the surface morphology of CdS thin film on behalf of the plasma treatment reported in some researches. Removal rate was estimated by the obtained results through the application to Hernandez power law as a generalization version of Preston's equation for a better description of removal rate. Surface roughness and within-wafer non-uniformity (WIWNU%) of the sputtered CdS thin film was also examined with a change of CMP process parameters including table speed and down force. The optimized process condition was selected considering to both the surface roughness and the hillock-free surface with the good uniformity.

¹M. Phytton et al., J. Non-Cryst. Solids 2008.

EN-TuP7 High Quality TCO Deposition using New DC Power Supplies. *D. Ochs*, HUETTINGER Elektronik GmbH + Co KG, Germany, *P. Ozimek*, HUETTINGER Electronic Sp z o. o., Poland

The main application of magnetron sputter processes for thin film solar cell production is the deposition of transparent conductive oxides (TCO). The most significant example for this TCO material class is ZnO:Al (AZO) which is of great importance as a transparent conductive layer for photovoltaic applications. Since this material has an especially high arcing rate, pulsed DC power processes have been used for deposition in the past. A new DC power supply family has been developed with the goal of replacing these pulsed DC processes with economic standard DC processes. The most important feature of this power supply is an extremely fast and advanced arc management with the capability to run stable processes with high arcing rates. The arc management has three different detection criteria: a voltage, a current and a combined voltage/current criteria. After detecting an arc, a positive voltage is applied to the cable between the power supply and cathode. This so-called Cable Length Compensation compensates the stored energy of the cable and reduces the energy supplied into the arc after power shut off. In this way residual arc energies of less than 0.5 mJ/kW, are achievable. Stable processes over a long time with arcing rates of up to 20,000 arcs/s become possible. The fast arc management with adaptable parameters results in superior film quality, and homogeneity of the deposited film. The new economic DC power supplies replace pulsed DC power without any disadvantages.

EN-TuP8 Vacuum Insulating Glass: Window of the Future. *P.J. Petit*, V-Glass LLC

This paper provides a brief summary of the past, present and potential near-term future of energy efficient windows, based on vacuum insulating glass, for residential buildings. It presents a brief history of window technology to the present day, summarizes known efforts around the world today to develop improved insulating window technology, and describes a "Window of the Future"¹ that might reasonably be assumed to be available in 2015. This "Window of the Future" consists of a Vacuum Insulating Glass (VIG) unit mounted in a low-heat-loss frame. Using a 3 ft by 5 ft window assembly as a representative "average" size for the purpose of this exercise, the overall U-value for a window of this design and size is estimated to be about 0.091 Btu/hr-sq ft-°F, which is equivalent to a wall rated at R11. Barriers which have prevented vacuum windows from being realized over the past two decades will be described, as well as the current strategies intended to overcome them.

¹ "Window of the Future", Swing Research LLC, April, 2008.

EN-TuP9 Characterization of the Photovoltaic Heterostructure CdS:F/CdSTe*, *F. de Moure-Flores*, *M. Meléndez-Lira*, *J.G. Quiñones-Galván*, *E. Mota-Pineda*, *S. Cerón-Gutiérrez*, CINVESTAV-IPN, México, *A. Hernández-Hernández*, Escuela Superior de Física Matemáticas-IPN, México, *M. González-Alcudia*, *M. Zapata-Torres*, CICATA-IPN Unidad Altamira, México, *C. Davet-Lazos*, *M.delaL. Olvera*, CINVESTAV-IPN, México

We present results of the characterization of the structural, electronic and electrical properties of the photovoltaic heterostructure: ITO / CdS:F / CdSTe. The ITO film was deposited by the technique of rf sputtering. The CdS layer was deposited employing chemical bath deposition adding fluorine to increase n-type doping. The top CdSTe layer was deposited by the modified laser ablation technique.¹ The motivation to deposit a CdSTe layer, instead just CdTe, is to limit the S interdiffusion at the CdS/CdTe interface in order to improve the characteristics of the interfacial electric field.² We report the characteristic I vs. V, the spectral response, as well as the efficiency of the photovoltaic heterostructure. These results are correlated with those obtained from the chemical, structural and electronic characterization obtained through EDX and X-ray diffraction and UV-Vis and Raman spectroscopies.

* This work is partially supported by CONACYT-Mexico

¹ M. González-Alcudia, A. Márquez-Herrera, M. Zapata-Torres, M. Meléndez-Lira and O. Calzadilla-Amaya, Adv. in Tech. of Mat. And Mat. Proc. J. 9, 81 (2007).

² M.A. Santana-Aranda, M. Meléndez-Lira, Applied Surface Science, 175-176 (2000) 538-542.

EN-TuP10 Photoconduction Properties of Titanium Dioxide Films Prepared by Reactive Magnetron Sputtering. *H.A. Shukur*, Kogakuin University, Japan, *H. Nagai*, *I. Takano*, *M. Sato*, Kogakuin University, Japan

Since TiO₂ has been used as one of lower cost materials and is harmless to the environment, it is expected to use as a material of a clean energy system in future. Furthermore its photocatalysis have antifouling and antibacterial properties. At the same time, the electric property shows n-type semiconductor characteristics and is classified as a high dielectric material. However, details of electric property for TiO₂ have not been researched on the relations between the oxygen deficit state and light. Generally the resistance of TiO₂ is decreases by the excitation of electrons due to the light irradiation. We anticipate that these properties are applied to a photo sensor of electronic parts. In this study the electrical property of TiO₂ thin film was investigated under irradiation with the ultraviolet or visible light. The formation conditions was changed the substrate temperature 100 and 200°C. Furthermore O₂ flow rate was changed from 0.1 to 1.7 sccm for each substrate temperature. I-V property of films on a slide glass was measured by using an unresisted current meter under fluorescence light (FL), a black light (BL) or a sterilizing light (SL). The measurement size of the film was 200nm in thickness, 10 mm in length and 8 mm in width. The resistivity of films depends on O₂ flow rate. On the other hand the films resistivities in both temperature conditions hadn't a large different property until 1.3 sccm, but the films formed under substrate temperature 200°C showed a large resistivity. The microstructure of these films investigated by X-ray diffraction showed clearly that the both of O₂ flow rate and substrate temperature affected films in crystalline structure. In case of high substrate temperature and large O₂ flow rate, the crystalline structure of films changed to an anatase type and films resistivity was raised. The measurement of photoconduction current under each light irradiation showed two important results. Firstly the TiO₂ thin films obtained a large effect of photoconduction current under BL irradiation in all formation conditions. The second point was that the photoconduction current reduced with increase of the film resistivity and the maximum photoconduction current was obtained at the film of 0.5 sccm with both of a substrate temperature.

¹Akira Fujishima, Kazuhito Hashimoto and Toshiya Watanabe, "TiO₂ Photocatalysis Fundamental and Applications".

EN-TuP11 Effects of Pulse Sputtering Condition on Al: ZnO's Uniformities of TCO Properties for Solar Cell Application. *W.K. Yang*, *J.E. Jee*, *J.H. Joo*, Kunsan National University, Korea

Bipolar pulsed magnetron sputtering is used to deposit Al doped ZnO on a glass substrate for a TCO (transparent conducting oxide) in a solar cell structure. A 5"x25" AZO target was sputtered by 50 – 250 kHz bipolar pulsed dc power supply to deposit 400x400mm area by swinging back and forth. Sheet resistance, surface morphology and optical transmittance were measured at 16 slide glasses (1"x3") to evaluate uniformity. In the thickness of 800nm, the average value of sheet resistance was 37Ω/□ and uniformity was 21.4% in 400x400mm area. The thickness of AZO thin film was 800nm and the resistivity was 2.9×10⁻³ Ω•cm. Generally, magnetron sputtering plasma is thought to be well confined above a target's race track. As substrate carrier is swinging, plasma is observed to be severely disrupted to go around to the back side at 5cm of target-substrate distance. To fully address these phenomena, we must use self consistent plasma model incorporating pulsed dc not just a simple dc cathode. As a first approach, we analyzed gas flow using a 3D fluid model as a substrate carrier is moving around a target and a gas distribution pipe. In here, we found that the gas flow distribution affected the plasma. Also we thought that this plasma might affect the deposited thin film. So, we expected that the uniform gas flow distribution could improve the plasma uniformity and the characteristics of AZO thin film.

EN-TuP12 Germanium Nanowires: Applications in Photovoltaics and Electronics. *L.A. Klein*, *D.D.T. Mastrogiovanni*, *A. Du Pasquier*, *E. Garfunkel*, Rutgers University

Single crystal germanium nanowires are grown via vapor-liquid-solid methods in a hot-wall chemical vapor deposition reactor. We present the results of nanowire growth and discuss potential applications of nanowires grown on a variety of substrates. The relatively low growth temperature required for germanium nanowire formation combined with the enhanced semiconducting properties such as higher carrier mobility of germanium over silicon makes these wires an attractive building block in the rapidly expanding field of nanotechnology. In addition to our investigations into how growth conditions and substrates can affect the shape and orientation of the nanowires, we have investigated various chemical passivation methods, including chlorination, H-termination, and thiol and alkene passivation. Passivation becomes of utmost importance for germanium devices as germanium does not possess a stable native oxide as does silicon. These chemistries are also used to facilitate further surface functionalization

and ohmic formation, and to improve device electrical performance. Most recently, the germanium nanowires were also used to enhance the properties of organic photovoltaic devices through the creation of a bulk heterojunction solar cell with poly(3-hexylthiophene) (P3HT). This hybrid-inorganic/organic device exhibits a significant increase in exciton dissociation and photocurrent when compared to pure P3HT. The photoelectrical properties of this device are characterized by measuring absorbance and photoluminescence spectra, current-voltage curves, and AM 1.5 filtered external quantum efficiency. In addition to the aforementioned techniques, other studies utilizing x-ray diffraction, Rutherford backscattering spectroscopy, and inductively coupled plasma mass spectroscopy enable us to observe how variations in nanowire concentration can affect the relative crystallinity and crystallite orientation of P3HT. We conclude with a discussion of our plans to improve the performance of these devices through surface passivation and the controlled introduction of phosphine impurities.

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