

Thin Film

Room 2022 - Session TF-WeA

Thin Films for Energy Applications in Photovoltaics, Fuel Cells, Hydrogen Storage & Batteries

Moderator: R. Carter, Advanced Micro Devices

2:00pm **TF-WeA1 Na Doped V₂O₅ Thin Films for the Thermoelectric Device Applications**, S. Iwanaga, M. Marciniak, R.B. Darling, F.S. Ohuchi, University of Washington

The thermoelectric properties of bronze-like V₂O₅ thin films were investigated above room temperatures. The potential utilization of these materials for thin film based thermoelectric devices were considered. The original motivation for this research came from the fact that V₂O₅ exhibits an unusually high Seebeck coefficient of about -550 $\mu\text{V/K}$; however, low electrical conductivity ($\sigma \sim 1\text{E-4 @OMEGA@cm}$) hinders its usage as a thermoelectric material in practical applications. Systematic doping of Na into the V₂O₅ host lattice was investigated in an attempt to find the conditions that maximize a power factor described by σS^2 , where σ and S are the electrical conductivity and Seebeck coefficient, respectively. The Na doped V₂O₅ solutions were made by the melt-quench method, which provides very stable solutions that lasts for months. The solution was then coated on quartz substrates. It was experimentally shown that proper annealing of Na doped V₂O₅ thin films dominantly produce $\beta\text{-Na}_x\text{V}_2\text{O}_5$. The electrical conductivity was increased by a factor of about 1000, while the Seebeck coefficient decreased to ~40% of the original value, resulting in an improvement of the power factor by a factor of about 160. These improved thermoelectric properties were further studied by current-voltage (I-V) measurements. The I-V measurements were performed while applying a temperature gradient to the film by applying a current source in such a way that the thermopower current was suppressed by applying the current in the opposite direction. The I-V characteristics at different applied ΔT were thus obtained, from which the output power was calculated from the I-V data. The $\beta\text{-Na}_x\text{V}_2\text{O}_5$ thin films were used in a sensor application and their performance was evaluated.

2:20pm **TF-WeA2 Effect of Na Quantity on the Morphology of the Absorber Layer in the CIGSS/CdS Thin Film Solar Cell**, V.V. Hadagali, S.A. Peth, N.G. Dhere, Florida Solar Energy Center, University of Central Florida

The highest efficiencies of CIGS thin-film solar cells have been obtained by using soda lime glass as substrate material. Soda lime glass contains significant amounts of sodium in the form of Na₂O. The presence of Na during growth of the CIGS absorber layer is beneficial. Na promotes increase in grain size and preferred (112) orientation of CIGS films. The overall effect of Na incorporation during grain growth is an increase in efficiency by enhancements of fill factor and open circuit voltage. This paper presents the effect of the Na quantity on the morphology of CIGSS thin film solar cells. Among the available sodium containing precursor, NaF is non-hygroscopic, stable in air and evaporates stoichiometrically. NaF of various thicknesses ranging from 30-120 Å is deposited by thermal evaporation on a Mo coated glass. The CIGSS is grown in a two stage process. The Cu-In and Ga are deposited by sputtering and the selenization / sulfurization process in a conventional furnace. The absorber layer was deposited on the substrates with various NaF quantities in the same process. Various morphological effects such as hillocks and valleys have been observed due to the presence of Na. The area density of hillocks and valleys varied with the quantity of NaF. Selenization of the film containing Na results in the formation of Na₂Se compounds. In some cases, absorber layer peeled immediately after deposition or during chemical bath deposition of CdS heterojunction layer. The peeling effect could be attributed to the non-optimum sodium and selenium contents. SEM, AES and Optical microscopy techniques were used to understand morphology.

2:40pm **TF-WeA3 Properties of Grain Boundaries in Cu(In,Ga)Se₂**, D. Hebert, A. Hall, A. Aquino, C.H. Lei, I.M. Robertson, A. Rockett, University of Illinois, Urbana-Champaign

CuInSe₂ (CIS) and related materials yield the highest performance thin film solar cells and show excellent promise for very high efficiency multijunction devices if adequate single junction devices can be produced. One of the primary questions concerning the nature of these devices is the optoelectronic behavior of grain boundaries in the material. We have

grown epitaxial bicrystals of these materials on polished GaAs bicrystalline substrates and have studied the grain boundaries by a variety of methods including atomic force microscopy, Kelvin probe force microscopy, position-dependent photoluminescence, cathodoluminescence, transmission electron microscopy, Hall effect and other methods. The bicrystals show distinct differences in the two grains, one of which has a nearly (100) surface orientation while the other has a nearly (110) orientation. The latter is highly faceted. The grain boundary is fully dense. The (110) grains show a lower energy luminescence characteristic of subgap emission from deep defect states, while the (100) grain show higher energy luminescence. No distinct behavior directly connected with the grain boundary is evident in any of the measurements. Furthermore, there is no measurable chemical change in the CIS chemistry at the grain boundary that might account for surface state passivation. Although this negative result is surprising, it is consistent with the observation that grain boundaries are inactive in the devices. This confirms the evidence that grain boundaries are surprisingly innocuous in this material.

3:00pm **TF-WeA4 Growth and Characterization of In_xGa_{1-x}N (0 ≤ x ≤ 1) Thin Films Grown by MOCVD for Photovoltaic Applications**, J. Mangum, O. Kryliouk, University of Florida; A. Davydov, National Institute of Standards and Technology; T.J. Anderson, University of Florida

Recently the electronic band gap of indium nitride (InN) has been revealed to be 0.7 eV in marked contrast to the previously accepted value of ~2.1 eV. By varying the band gap of InN with the incorporation of gallium to form In_xGa_{1-x}N, the optimal band gap energy for either a single cell or tandem cell combination is possible. Furthermore, the high absorption coefficient and radiation hardness make InN and In_xGa_{1-x}N attractive materials for photovoltaics. In_xGa_{1-x}N films on Si (111) and Al₂O₃ (0001) substrates were grown by metal organic chemical vapor deposition (MOCVD) at low temperatures (T < 600 °C) over the entire compositional range (0 ≤ x ≤ 1). The lattice parameter was determined from XRD measurements of the as-grown films. The films were also characterized by PL, SEM, and Hall measurements. An In_xGa_{1-x}N based solar cell device structure is proposed that is assessed by device modeling as well! as quantum efficiency measurements.

3:20pm **TF-WeA5 Thin Film Deposition Technologies Enabling a New Generation of 3-D Integrated All-Solid-State Batteries**, P. Notten, Philips Research and Eindhoven University of Technology, The Netherlands; R.A.H. Niessen, J.H.G. Op het Veld, Philips Research Laboratories, The Netherlands
INVITED

It is anticipated by the electronic industry that smart Autonomous Devices, enabling future Ambient Intelligence inside offices and houses, will play a dominant role in our future life. Characteristic of these Autonomous Devices is that these should operate independently, meaning that the energy supply must be guaranteed wirelessly. This implies that both energy scavenging and electrochemical energy storage are of crucial importance for these devices. It has been reported that all-solid-state Li-based rechargeable batteries can be frequently charged and discharged. These thin-film batteries were, however, planar structured and include a dynamic metallic lithium anode. The thin film geometries were grown, by making use of physical deposition techniques. However, the geometric energy density of these devices is unfortunately relatively low due to its planar structure. Interestingly, it has recently been discovered that the amount of Li which could be reversibly intercalated and de-intercalated in thin film Silicon electrodes is about 10 times higher than in conventional graphite electrodes, making these anodes much more energy dense and, compared to metallic Li, mechanically more robust. Silicon is a well-known substrate material nowadays widely applied in the electronic IC-industry, allowing a high degree of component integration. One of the latest developments is the integration of capacitors into Si wafers; 3-D structured high surface area substrates are obtained by either physical or wet-chemical etching, enabling the beneficial deposition of high surface area electrode structures. Based on the various above-mentioned developments a new battery concept is proposed to come to fully 3-D integrated, all-solid-state, rechargeable batteries, revealing a high energy density. This concept will be based on the Li-intercalation chemistry of Silicon and LiMeOx. In the present presentation the details of this challenging 3-D integrated battery concept will be disclosed and the electrochemistry of Li-intercalation in Silicon will be reported

Wednesday Afternoon, November 15, 2006

4:00pm **TF-WeA7 Fabrication and Fuel Cell Performance of Ultra-Thin Yttrium-Doped Barium Zirconate Films**, *J.H. Shim, T.M. Gür, F.B. Prinz*, Stanford University

Acceptor-doped perovskites such as yttrium or gadolinium-doped barium cerate (BaCeO_3), strontium cerate (SrCeO_3) and barium zirconate (BaZrO_3) have been intensively studied as potential proton conducting electrolytes for fuel cells due to their high ionic conductivity for protons. However, instability in acidic gas environment such as carbon dioxide has limited practical usage of most of the doped cerates. Only yttrium doped barium zirconate (Y:BaZrO_3) has shown high proton conductivity combined with sufficient chemical stability. However, Y:BaZrO_3 is difficult to be densified using conventional sintering processes. This adversely affects their conductivity and mechanical strength. Furthermore, most Y:BaZrO_3 membranes that have been reported in the literature have been fabricated at thicknesses exceeding few tens of microns, which limits their use in low temperature applications because of its high area specific resistance (ASR). In this work, we report fabrication of nano-scale Y:BaZrO_3 films using an optimally-conditioned pulsed laser deposition technique. The thin films are prepared on single crystal magnesium oxide substrates or silicon nitride-buffered single crystal silicon wafers. Structural qualities of the film including crystallinity, density, and film composition are investigated using the X-ray photoelectron spectroscopy (XPS), X-ray diffraction (XRD) and reflection (XRR) measurements. With the ultra-thin Y:BaZrO_3 membrane, we have fabricated fuel cells and measured the performance in terms of voltage-current relations. @FootnoteText@ @footnote 1@ Iguchi, S. et al., 2004 Fuel Cell seminar, Nov. 1-5, San Antonio, TX, USA (2004)@footnote 2@ Kreuer, K. D. Annual Review of Materials Research 33, 333-359 (2003)@footnote 3@ P. Babilo & S. M. Haile, J. Amer. Cer. Soc. 88, 2362-2368 (2005).

4:20pm **TF-WeA8 Growth and Electrochemical Properties of Li-Ni-Co-Al Oxide Films**, *C.V. Ramana*, University of Michigan; *K. Zaghib*, Institut de Recherches d'Hydro-Quebec; *C.M. Julien*, Université Pierre et Marie Curie

There is a constantly increasing demand for miniaturized high energy density batteries to power microsystems such as microsensors, smart cards, implantable medical devices, intelligent labels, and so on. From this view point, there has been particular interest in solid-state lithium batteries fabricated by thin-film technology. The present work deals with the growth and electrochemical properties of the $\text{Li}(\text{Ni},\text{Co},\text{Al})\text{O}_2$ films grown using pulsed laser deposition (PLD). The investigations revealed that the the growth and microstructure of the films is highly dependent on the substrate material, the growth temperature, and the gas pressure during ablation. The charge-discharge process conducted in Li-microcells demonstrates that effective high specific capacities can be obtained with films 1.35 μm thick. Stable capacities of 83 and 92 $\mu\text{Ah}/\text{cm}^2$ are available in the potential range 4.2-2.5 V for $\text{LiNi}_{0.8}\text{Co}_{0.2}\text{O}_2$ and $\text{LiNi}_{0.8}\text{Co}_{0.15}\text{Al}_{0.05}\text{O}_2$ films, respectively. A comparison of the electrochemical performance of microcells using films deposited on Si and Ni is also made. The results obtained will be presented and discussed.

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