## Fundamentals and Technology of Multifunctional Materials and Devices
## Room Golden West - Session C3+C1-WeM

### Thin Films for Energy-related Applications I/Optical Metrology in Design, Optimization, and Production of Multifunctional Materials

**Moderators: Per Eklund**, Linköpings Universitet, **Tushar Shimpi**, Colorado State University, USA

8:20am **C3+C1-WeM-2 Avoiding Blistering of Magnetron Sputtered Thin Film CdTe Photovoltaic Devices***, J Walls, F Bittau, R Greenhalgh, A Abbas,* ***Peter Hatton****, R Smith,* Loughborough University, UK

Magnetron sputtering is an industrially scalable technique for thin film deposition. It provides excellent coating uniformity and the deposition can be conducted at relatively low substrate temperatures. It is widely used in the manufacture of solar modules. However, its use for the deposition of thin film CdTe photovoltaics results in unusual problems. Blisters appear on the surface of the device and voids occur in the CdTe absorber. These problems appear after the cadmium chloride activation treatment at $400^{0}$C. The voids often occur at the p-n junction interface causing catastrophic delamination. This problem has been known for more than 25 years, but the mechanisms leading to blistering have not been understood. Using High Resolution Transmission Electron Microscopy we have discovered that during the activation process, argon trapped during the sputtering process diffuses in the lattice to form gas bubbles. The gas bubbles grow by agglomeration particularly at grain boundaries and at interfaces. The growth of the bubbles eventually leads to void formation and blistering. Switching the working gas to xenon overcomes these problems.

8:40am **C3+C1-WeM-3 Electrochromic Device Based on $WO_3$/NiO Complementary Electrodes Prepared by Using Vacuum Cathodic Arc Plasma***,* ***Po-Wen Chen****,* Institute of Nuclear Energy Research, Taiwan

Smart windows based on electrochromic (EC) materials, which are controlled to change their optical properties of reflectance, transmittance, and absorption can be effectively reduced the heating or cooling loads of building interiors. Electrochromism can produce interesting phenomenon based on redox reaction that gives a reversible, persistent changing in color, thus with an optical modulation by a small applied DC voltage pulse difference. In this study, we prepared a complementary electrochromic device (ECD) with ITO/$WO_3$/$LiClO_4$-PC/NiO/ITO structure was assembled. This work focues on the influence of thickness of NiO layers on the ECD electrochemical and optical properties. For the fabrication of ECD, $WO_3$ and NiO electrode films were used as the cathodic and anodic coloring materials, which are fabricated by vacuum cathodic arc plasma (CAP). We achieve a high performance electrochromic elecrode, producing porous deposited by the CAP technique is promising smart window for potential electrochromic application. Our results are observed the highest oxidation/reduction ion diffusion coefficient ($9.38x10^{-9}$ / $8.12x10^{-8}$ $cm^2/s$, respectively) with NiO(60 nm)/ITO films, meaning that enhanced electrochromic properties compared to the other samples. The performance of the 5×5 $cm^2$ ECD demonstrated optical contrast of 52 % and switching times 4.6 sec and 8.1 sec for coloring and bleaching state at the wavelength of 633 nm. During the durability test, the transmittance cahnge (ΔT) of ECD remained 45% after 2500 cycles, which was about 85% of original state.

9:00am **C3+C1-WeM-4 Influence of Film Thickness on Growth, Structure and Properties of Magnetron Sputtered ITO Films***,* ***Andrius Subacius,*** Manchester University, UK*; É Bousser,* École Polytechnique de Montréal, Canada*; B Baloukas,* Polytechnique Montreal, Canada*; S Hinder, M Baker,* Surrey University, UK*; D Ngo,* Manchester University, UK*; C Rebholz,* Cyprus University, Cyprus*; A Matthews,* Manchester University, UK

Indium tin oxide (ITO) is one of the most widely used transparent conducting oxides due to its electrical conductivity and optical transparency, and it can be used for many applications, such as LEDs, flat-panel displays, smart windows and architectural windows. As typical for transparent conducting films, there is a trade-off between conductivity and transparency.

In this work, the effect of film thickness on the evolution of growth, microstructure and electrical and optical properties was studied. ITO coatings with different thickness values (200, 800 and 3000 nm) were deposited onto unheated soda lime glass substrates by r.f. sputtering from a ceramic ($In_2O_3$:$SnO_2$, 90:10 wt.%) target. X-ray diffraction (XRD), transmission Kikuchi diffraction (TKD) and transmission electron microscopy (TEM) analysis revealed an increase in crystallinity with growing ITO film thickness. While the 200 nm thin film appeared amorphous in XRD measurements, the 800 and 3000 nm coatings were found to be crystalline. The 3000 nm thick film displayed preferred orientations in the (440) and (400) directions. In the case of the 200 nm film, TKD results showed local crystallinity with 50-200 nm grains imbedded in an amorphous or possibly nanocrystalline matrix. The luminous transmittance in the visible range was found to decrease with increasing film thickness from 81.7 % for the 200 nm film down to 70 % for the 800 nm one and 44.6 % for the 3000 nm film. On the other hand, electrical resistivity values only slightly decreased with increasing film thickness from $6.15\times10^{-4}$ Ω·cm to $5.36\times10^{-4}$ Ω·cm and $5.23\times10^{-4}$ Ω·cm for 200 nm, 800 nm and 3000 nm films, respectively.

9:20am **C3+C1-WeM-5 Metal/Semiconductor Superlattice Metamaterials: A New Paradigm in Solid-State Energy Conversion***,* ***Bivas Saha,*** Jawaharlal Nehru Centre for Advanced Scientific Research, India **INVITED**

Since the 1960s, researchers exploring the potential of artificially-structured materials for applications in quantum electronic devices have sought combinations of metals and semiconductors that could be combined on the nano-scale with atomically-sharp interfaces. Early work with multilayers of polycrystalline elemental metals and amorphous semiconductors showed promise in tunneling devices. More recently, similar metal/semiconductor multilayers have been utilized to demonstrate novel optical metamaterials. These metal/semiconductor multilayers, however, are not amenable to atomic-scale control of interfaces. We developed the first epitaxial metal/semiconductor multilayer and superlattice heterostructures that are free of extended defects. These rocksalt nitride superlattices have atomically sharp interfaces and properties that are tunable by alloying, doping and quantum size effects. Furthermore, these nitride superlattices exhibit exceptional mechanical hardness, chemical stability and thermal stability up to ~1000̊C.

In this presentation, I will describe the growth, structural characterization and transport properties of nitride metal/semiconductor superlattices including (Ti,W)N/(Al,Sc)N and (Hf, Zr)N/ScN. ScN and $Al_xSc_{1-x}N$ ($x$ < 0.82) are rocksalt semiconductors in thin film and bulk form that can be doped preferentially with *n*-type or *p*-type carriers. $Al_xSc_{1-x}N$ can also be stabilized in rocksalt phase for high AlN mole fractions by lattice-matched epitaxy. TiN, ZrN, HfN and similar transition metal nitride films can be good metals with carrier concentrations approaching $10^{22}$ $cm^{-3}$. Potential applications of these single crystalline superlattice and thin films in thermoelectric devices and plasmonic metamaterials will be discussed. Furthermore, recent experimental efforts to employ these superlattices as model materials for investigating the fundamentals of heat transport in nanostructured materials will be addressed.

Reference:

1. B. Saha, A. Shakouri and T. D. Sands, "Rocksalt Nitride Metal/Semiconductor Superlattices: A New Class of Artificially-Structured Materials". *Appl. Phys. Rev. 5, 021101 (2018).*

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