

Thursday Afternoon Poster Sessions

Energy Frontiers Topical Conference

Room: Southwest Exhibit Hall - Session EN-ThP

Energy Frontiers Topical Conference Poster Session

EN-ThP1 N-doped TiO₂ Photocatalytic Thin Films : Synthesis with Controlled Nitrogen Partial Pressure and Study on Their Catalytic Activity, J.-H. Boo, S.-J. Cho, C.-K. Jung, Y.-H. Song, Sungkyunkwan University, Republic of Korea, S.-S. Kim, Paichai University, Republic of Korea

We have deposited N-doped TiO_xN_y thin films on Si(100) substrates at 500°C using PEMOCVD method. Titanium iso-propoxide was used as precursor with different nitrogen flow rate to control oxygen and nitrogen contents in the films. Changes of chemical states of constituent elements in the deposited films were examined by XPS analysis. The data showed that with increasing nitrogen flow rate, the total amounts of nitrogen and titanium were increased while that of oxygen was decreased, resulting in a binding energy shift toward high energy side. The characteristics of film growth orientation and structure as well as morphology change behavior were also analyzed by XRD, TED, TEM, AFM, and SEM. Deposition at higher nitrogen flow rate results in finer clusters with a nano-scale grain size and a slower growth rate.

In order to elevate photocatalytic activity of the as-grown N-doped TiO_xN_y films, argon and oxygen plasmas ignited by atmospheric discharge at 300 W were also used within 5 min. at room temperature. Photocatalytic activity was evaluated by the measurements of the contact angle, UV-Visible spectroscopy. In this work, the effect of the plasma on the improvement of hydrophilic property of N-doped TiO_xN_y photocatalysts has mainly been investigated. Superhydrophilic property and smooth surface morphology appeared in the UV light irradiation with O₂ plasma treatment.

Keywords : N-doped TiO_xN_y Thin Film, Photocatalyst, PEMOCVD, Atmospheric Plasma, Surface Modification

EN-ThP2 Optical and Electrical Properties of Transparent Conducting B-doped ZnO Thin Films Prepared by Various Deposition Methods, J.-I. Nomoto, S. Hotta, T. Miyata, T. Minami, Kanazawa Institute of Technology, Japan

Recently, transparent conducting impurity-doped ZnO films with a high transmittance in the near-infrared region have attracted much attention for transparent electrode applications in thin-film solar cells. It is necessary to achieve a reduction of the plasma resonance frequency resulting from a decrease of carrier concentration. However, in order to maintain a low resistivity in impurity-doped ZnO films, any decrease in carrier concentration should be compensated by an appropriate increase of mobility. In this paper, we describe the preparation of transparent conducting B-doped ZnO (BZO) thin films with a lower carrier concentration as well as a higher Hall mobility by various deposition methods. BZO thin films were prepared on low temperature glass substrates by dc or rf magnetron sputtering deposition, pulsed laser deposition (PLD) and vacuum arc plasma evaporation methods. The optical and electrical properties were evaluated in BZO thin films prepared with various thicknesses up to about 3 μm and doped B contents (B/(B+Zn) atomic ratio) up to 5 at.%. In addition, long-term resistivity stability was evaluated with exposure to a highly moist environment (air at 85% relative humidity and 85°C) as well as an oxidizing atmosphere at a high temperature (air at a temperature up to 250°C). In the moisture-resistance tests, the BZO thin films exhibited an increase in resistivity during long-term testing; increasing the thin film thickness tended to lessen this increase in resistance, irrespective of the deposition method. In the heat-resistance tests, the resistivity of thin films thicker than approximately 200 nm was found to be stable for 1000 h at a testing temperature up to 200°C. A Hall mobility of 42 cm²/Vs and a carrier concentration of 3.4×10²⁰ cm⁻³ were obtained in a BZO thin film prepared by PLD. Resistivities of 4-6×10⁻⁴ Ωcm were obtained in 500 nm-thick-BZO thin films prepared with a B content of 1 at.%, irrespective of deposition methods. The low-resistivity BZO thin films exhibited an average transmittance in the visible range above 80 %; transmittances were above 80% at a wavelength of 1100 nm and 75% at 1300 nm.

EN-ThP3 Enhanced Performance of Dye-Sensitized Solar Cell by Inorganic/Organic Core-Shell Formation using Dip-Coating Method, M.J. Shin, J.M. Kim, H.J. Kim, B. Hong, Sungkyunkwan University, Republic of Korea

Dye-sensitized solar cell (DSSC) is considered as alternative to traditional solar cells due to its environment-friendly energy conversion capability and

low fabrication cost. However, DSSC still suffers from efficiency loss due to a high recombination rate between the injected electrons and the oxidized dye or ions in electrolyte.

In this work, we present a very efficient but simple method is presented to improve the efficiency of DSSC using inorganic/organic core-shell electrode. This core-shell electrode consists of an inner nanoporous TiO₂ matrix covered with an aminopropyltriethoxysilane (APS) monolayer. It is relatively easy to control the shell density by controlling the concentration of APS using the dip-coating method. We confirmed that the efficiency of DSSC with TiO₂/APS core-shell instead of conventional TiO₂ was significantly dependent on the shell density. Relative change in surface chemistry with APS concentration was investigated by various analysis methods. The power conversion efficiency under AM 1.5 G spectral illumination of 100 mWcm⁻² was improved by 20 % (from 4.37 % to 5.28 %) when APS concentration was optimized. This TiO₂ nanoparticles covered with APS are supposed to increase dye adsorption on TiO₂ surface and to prevent interfacial recombination of charge carriers. For the various analysis, it was used UV-absorbance spectroscopy, FT-IR (Fourier transfer IR), EIS (Electrochemical Impedance spectroscopy), TOF-SIMS (Time-of-Flight Secondary Ion Mass Spectrometry) and HR-TEM (High Resolution-Transmission Electron Microscope).

EN-ThP4 Characteristics of Undoped ZnO as Window Layer for CIGS Thin Film Solar Cell using Nano-Inks, E.C. Choi, J. Chang, D.Y. Jung, B. Hong, Sungkyunkwan University, Republic of Korea

ZnO is a very useful material as II-VI compound semiconductor with a wide band gap of 3.3 eV and a property of native n-type semiconductors. It has been studied actively due to its excellent optical, electrical and structural properties suitable for many applications such as transparent conductive oxide (TCO), solar cell window layer and surface acoustic wave (SAW) devices. In particular, n-type and undoped ZnO films are used as the window layer of GIGS solar cell (n-ZnO/-ZnO/CdS/CIGS/Mo/glass).

The surface morphology of CIGS film deposited on Mo/glass substrate by liquefied deposition method using nano-inks is severely uneven and the film has many crevices. Also, the CBD-CdS layer with the thicknesses of about 50 nm does not perfectly cover the surface of the CIGS layer. Consequently, these crevices, which remain before the TCO deposition, lead to the formation of shunt path between TCO and CIGS layers.

Therefore, in this study, we investigate the role of undoped ZnO film with high resistivity to prevent the shunt path between TCO and CIGS layers, and ZnO films are deposited varying the thickness and the plasma power to investigate characteristics of undoped ZnO film for CIGS solar cell. It is confirmed that the efficiency of CIGS solar cell depends on the properties of the undoped ZnO films. The films are deposited using magnetron sputtering system in argon ambient and are analyzed using Hall measurement, UV-visible spectrometer and XRD.

EN-ThP5 Effect of Hydrogen and Deuterium Gas on the Thermionic Electron Emission from Nitrogen Doped Diamond Films, M. Zumer, V. Nemanic, B. Zajec, Jozef Stefan Institute, Slovenia, R.J. Nemanich, F.A.M. Koock, Arizona State University

Nitrogen doped, hydrogen terminated diamond films have shown a work function of less than 1.5 eV and thermionic electron emission has been detected at temperatures as low as 300 °C. This report explores the influence of hydrogen and deuterium gas on the electron emission using a triode setup with an applied electric field that ranges from low values to 4 MV/m. The extracting grid and phosphor screen were set to the same potential. The hydrogen terminated, nitrogen doped diamond films were deposited on 25 mm diameter molybdenum substrates by microwave plasma assisted chemical vapour deposition. The process involves a nucleation layer, nitrogen doped layer and surface termination which were all optimized to enhance the emission. The thermionic electron emission from 300 to 500 °C was quite intense. A typical average emission current density at 500 °C was of the order of 2E-6A/cm² at a base pressure of the order of 10⁻⁷ mbar. The emission was relatively stable exhibiting only a weak tendency to decrease with time. The emission was relatively uniform across the surface as opposed to the intense emission sites often observed in field emission. When hydrogen was leaked into the chamber, the emission current density increased by greater than an order of magnitude as the pressure was increased from UHV to 10⁻⁵ mbar. Results indicated that atomic hydrogen generated by a nearby Bayard-Alpert ionization gauge induced the effect. An identical leak rate of deuterium causes a similar but less intense increase of the emission current. At both cases, the initial UHV of the thermionic emission was restored by establishing again the UHV. The question of whether the hydrogen (deuterium) improves the surface through bonding and forming a NEA or whether it assists in the charge

transfer process is assessed. These results should guide the development of an efficient thermionic cell for direct conversion of heat to electricity.

EN-ThP6 Hot Electron Transfer from Semiconductor Nanocrystals. *W. Tisdale*, University of Minnesota, **K. Williams**, University of Texas at Austin, *B. Timp, D. Norris, E.S. Aydil*, University of Minnesota, *X.-Y. Zhu*, University of Texas at Austin

In typical semiconductor solar cells, photons with energies above the semiconductor bandgap generate hot charge carriers that quickly cool before all of their energy can be captured, a process that limits device efficiency. Although fabricating the semiconductor in nanocrystalline morphology can slow this cooling, the transfer of hot carriers to electron/hole acceptors has not yet been thoroughly demonstrated. We use time-resolved optical second harmonic generation to observe hot electron transfer from colloidal lead selenide nanocrystals (PbSe NCs) to a titanium dioxide electron acceptor (TiO₂). With appropriate chemical treatment of the nanocrystal surface, this transfer occurs much faster than expected. Moreover, the electric field resulting from sub-50 femtosecond charge separation across the PbSe-TiO₂ interface impulsively excites coherent vibrations of the TiO₂ surface atoms, whose motions can be followed in real time.

EN-ThP7 Synthesis and Characterization of Free-Standing Si Nanocrystals using PECVD. **R. Chaukulkar**, *B.N. Jariwala, S. Weeks*, Colorado School of Mines, *N.J. Kramer*, Eindhoven University of Technology, Netherlands, *S. Agarwal*, Colorado School of Mines

Si nanocrystals (NCs) (size <5nm) are generating an increased interest as a material to be used in third generation photovoltaics (PVs) owing to their size-dependent band gap, visible photoluminescence and multiple exciton generation (MEG). Synthesis of both liquid and gas phase NCs have been reported in the literature. We synthesize the Si NCs using a capacitively-coupled SiH₄/Ar plasma generated using radio-frequency power. The Si NCs are characterized using *in situ* attenuated total reflection Fourier-transform infrared spectroscopy (ATR-FTIR) and *ex situ* techniques such as transmission electron microscopy (TEM), energy-dispersive X-ray spectroscopy, infrared spectroscopy, photoluminescence spectroscopy, Raman spectroscopy and X-ray diffraction. The size of the NCs can be controlled by varying the residence time in the plasma volume. The residence time is adjusted to attain a particle size of 5nm collected on a grid. The crystallinity of the NCs depends on the amount of rf power put in the plasma. By varying the input rf power we were successful in demonstrating the transition from amorphous to crystalline nanoparticles using X-ray diffraction and TEM.

EN-ThP8 Physical Properties of Zinc Oxide Thin Films for Hybrid Solar Cell Application. *S.-H. Nam, M.-H. Kim*, Sungkyunkwan University, Republic of Korea, *S. Kim*, Paichai University, Republic of Korea, *B. Hong, J.-H. Boo*, Sungkyunkwan University, Republic of Korea

Zinc oxide (ZnO) films have been investigated in recent years as transparent conducting oxide layers, because of their good electrical and optical properties in combination with large band gap, abundance in nature, and absence of toxicity. Zinc oxide thin films were prepared at deposition thickness in the range of 50 nm to 150 nm by RF magnetron sputtering on glass substrates with pure zinc oxide target. The crystallinity nanostructure and surface morphology of zinc oxide thin films were investigated by X-ray diffraction (XRD), scanning electron microscopy (SEM). As the thickness of the films increased, the grain size and surface roughness increased. Also, we studied the optical-electrical properties of the zinc oxide thin films such as carrier concentration, mobility, and resistivity by hall measurement. As changed by thickness of zinc oxide thin films, concentration become increasing. But mobility and resistivity become decreasing.

EN-ThP9 Al and N co-doped ZnO:(Al,N) Thin Films for Solar Driven Hydrogen Production. *S. Shet*, National Renewable Energy Laboratory

ZnO thin films with significantly reduced bandgaps were synthesized by doping N and co-doping Al and N at 100°C. All the films were synthesized by radio-frequency magnetron sputtering on F-doped tin-oxide-coated glass. We found that co-doped ZnO:(Al,N) thin films exhibited significantly enhanced crystallinity as compared to ZnO doped solely with N. ZnO:N, at the same growth conditions. Furthermore, annealed ZnO:(Al,N) thin films exhibited enhanced N incorporation over ZnO:N films. As a result, ZnO:(Al,N) films exhibited improved photocurrents than ZnO:N films grown with pure N doping, suggesting that charge-compensated donor-acceptor co-doping could be a potential method for bandgap reduction of wide-bandgap oxide materials to improve their photoelectrochemical performance.

EN-ThP10 Optical and Thermal Studies on CdSe Quantum Dots and Rods. *H. Awad, S. Abdallah*, Ain Shams University, Egypt, *K. Easawib, S. Negm*, Benha University, Egypt, **H. Talaat**, Ain Shams University, Egypt

CdSe nanoparticles have attracted a great deal of scientific interest recently, because of the sensitivity of their optical and non-radiative properties to their size and shape, and their applicability in high efficiency photovoltaic solar cells [1]. As the size of a material falls to the nanometer length scale, the material properties become sensitive not only to the particles size, but also to their shapes. The optical (band gap width) and thermal properties of different sized CdSe quantum dots (QDs) and nano rods (NRs) of different aspect ratios have been characterized and compared using photoacoustic (PA) techniques. CdSe colloidal nanocrystals were prepared by the method of Talapine et al. [2], on the other hand, CdSe nanorods were prepared according to Manna et al [3]. A conventional PA setup with (PAR model 6003) PA cell was used to measure the optical absorption spectrum, and the thermal parameters. The PA absorption spectra for CdSe QDs and NRs in Figures (1.a) and (2.a), respectively, show a significant red shift in all cases as the nanoparticles increase in size. We used the second-derivative technique, to determine the peaks positions for QDs and NRs (Figure (1.b) and (2.b), respectively). The lowest energy transition is between 1S(e) and 1S_{3/2}(h) states in case of QDs and between 1S(e) and 1S_{1/2} states in case of NRs. The UV-Vis absorption spectra were also obtained for the samples and give a comparable values for the first excitonic transition peaks. The band gap of the nanoparticles $E_g(\text{NC})$ is determined by the energy of the lowest 1S(e)-1S_{3/2}(h) transition corrected for the coulomb e-h interaction, NOTE: WE ARE UNABLE TO INCLUDE FORMULAS where m_{hh} is the heavy hole mass, e is the electron charge, and ϵ is the dielectric constant for bulk CdSe. The QDs radii were found to be within 2.52 nm and 2.86 nm in agreement with the dimensions obtained by XRD. In the case of NRs, the radial dimensions determined in the same way, were found to be between 2.28 nm and 2.89 nm in good agreement with STM measurements, which gave the rod lengths as 19-50 nm. The second peak in the PA spectra could be described by the transition coupling the 1P_e electron state with the 1P_{1/2} hole state. Furthermore, the thermal parameters of the CdSe nanoparticles (diffusivity α , effusivity e and conductivity k) as determined by PA technique for both the QD's and NR's show an increase by almost an order of magnitude from the bulk values, however, there is no observable variations between the QD's and the NR's thermal parameters.

NOTE: WE ARE UNABLE TO INCLUDE FIGURES

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EN-ThP11 Study of Optical and Thermal Properties Of CdTe Quantum Dots Using Photoacoustic Spectroscopy. *A. Badawi, N. Al-Hosiny*, Taif University, Saudi Arabia, *S. Abdallah*, Taif University, Saudi Arabia and Ain Shams University, Egypt, *S. Negm, H. Talaat*, Ain Shams University, Egypt

Semiconductor nanoparticles are currently of great interest for their industrial applications in a variety of optoelectronic devices specially solar cells. Recently, CdTe semiconductor quantum dots (QDs) have become one of the promising materials for high efficiency photovoltaic solar cell. Therefore, massive attention has been devoted to investigate their optical and thermal properties in order to improve the performance of the solar cell. In this work, CdTe QDs were fabricated by the chemical solution deposition (CD) technique [1]. Four samples of increasing time of growth leading to different sizes labeled (a-d) were obtained The sizes of these samples were estimated using transmission electron microscope (TEM); as an sample (d) is shown in Fig. (1)

NOTE: WE ARE UNABLE TO INCLUDE FIGURES

Photoacoustic spectroscopy (PA) was employed to study both the optical and thermal properties of the samples at room temperature and modulation frequency $f = 15\text{Hz}$. Fig (2) show the PA spectra for the four different particle sizes samples (a-d) in the wavelength range 400–700 nm. The absorption edges shift towards lower energy region with increasing size , from (a) at 540 nm to (d) at 595 nm. The PA spectra give typical results with those obtained by regular UV-Vis absorption, though the samples were in colloidal form for UV-Vis and in powder form for the PA. The sizes of the CdTe nanocrystals were calculated using the effective mass approximation (EMA) model [2].

NOTE: WE ARE UNABLE TO INCLUDE FORMULAS

where m^* is the reduced electron-hole mass, E_g is the bulk crystal band gap, R is the average radius of the nanocrystal, $E_{g(\text{nano})}$ is the lowest energy for electronic transition and h is the Planck's constant. The calculated average

diameters of CdTe nanocrystal show an increase from 2.13 nm for (a) to 2.43 nm for (d), in agreement with the values determined by TEM.

NOTE: WE ARE UNABLE TO INCLUDE FIGURES

The PA technique was also employed to investigate the thermal properties of the CdTe QDs which are of great importance to solar energy conversion. The powder of each sample size was compressed into a disk. The PA signal amplitude was recorded at various chopping frequencies for each sample (depth profile analysis) using the Argon laser at wavelength 514 nm. The plot of \ln PA amplitude versus the \ln f. (Fig. 3) shows a distinct change in slope, at the characteristic frequency (f_c) where the sample changes from being thermally thick to thermally thin. The thermal diffusivity (D), was then calculated using the relation [4].

NOTE: WE ARE UNABLE TO INCLUDE FORMULAS

where L is the thickness of the sample. The calculated diffusivity varies from 0.65 cm²/s for (a) to 0.38 cm²/s for (d). These values of the thermal diffusivity are at least one order of magnitude larger than the bulk value (0.05 cm²/s) [4]. Our results are in agreement with the results of other authors [4,5], where the decrease in thermal diffusivity with increasing the particle size is attributed to the decrease in the population of phonons.

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EN-ThP12 CdTe Quantum Dots Sensitized TiO₂ Electrodes for Photovoltaic Cells, A. Badawi, N. Al-Hosiny, S. Abdallah, Taif University, Saudi Arabia, S. Negm, H. Talaat, Ain Shams University, Egypt

Semiconductors quantum dots (QDs) has been paid much attention in QDs sensitized solar cell because of their high potential in light harvesting under visible region along with particle size tuning properties. CdTe semiconductor quantum dots (QDs) have become one of the promising materials for high efficiency photovoltaic solar cell [1]. It has a high extinction coefficient ($4.4 \times 10^4 \text{ M}^{-1} \text{ cm}^{-1}$) at 370 nm and valence band, conduction band, and band gap energies of -3.9, -5.5, and +1.6 eV, respectively, would behave as sensitizers capable of effectively injecting electrons into TiO₂ NPs (band gap: 3.4 eV)[2]. CdTe QDs were fabricated by the chemical solution deposition (CD) technique [3]. In this article we describe the preparation and photovoltaic characterization of CdTe quantum dot-sensitized solar cells (QDSSCs). We coated Fluorine doped Tin Oxide (FTO) substrates with 20 nm-diameter TiO₂ nanoparticles (NPs) by the doctor blade method. Then, the as prepared CdTe quantum dots of different sizes were deposited on the TiO₂-coated substrates by the chemical bath deposition (CBD) technique for various periods of dipping times under ambient conditions. Other FTO substrates were coated with platinum to form the counter electrode, while the electrolyte containing Γ/Γ_3 redox species was sandwiched between the two electrodes. The I-V characteristic curve of the QDSSCs was measured under AM1.5-simulated sunlight at 100 mW/cm². As a result, the open-circuit photovoltage V_{oc} and the short circuit photocurrent density J_{sc} were about 0.48 volts and 300 $\mu\text{A}/\text{cm}^2$ respectively. The fill factor FF and efficiency for energy conversion η of the photovoltaic cell were calculated to be about 0.48 and 0.113 %, respectively. Our results are comparable with that obtained by Guo-YuLan et-al [2].

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