Congrès 2018, Toulon

11, 12 & 13 septembre
Session : Advanced functional nanomaterials
Keywords: Atomic layer deposition; Titania; Titanium Tetraisopropoxide; annealing

An investigation of the response of atomic layer deposited Titania to annealing: impact of deposition and annealing temperatures on the refractive index

Maïmouna W. Diouf[1, 2], Maxime E. Dufond[1], Jacques Kools[2], Lionel Santinacci[1]

1. Aix-Marseille Université, CNRS, Centre Interdisciplinaire de Nanoscience de Marseille, France
2. Encapsulix SAS, Simiane-Collongue, France

Titania thin films were grown from Titanium Tetraisopropoxide (TTIP) and water at substrate temperatures of 80°C and 120°C. Films were subsequently annealed in air from 200 to 450°C. The refractive index and thickness evolution with annealing temperature and duration were investigated by spectroscopic ellipsometry. A refractive index increase associated with a thickness decrease has been observed up to a saturation value. The saturation value of the refractive index and the minimum annealing duration needed to reach it depend both on deposition temperature and annealing temperature.

Samples deposited from TDMAT/water at 120°C and TTIP/ water at 200°C were also explored for comparison. No evolution of thickness was observed for those films.

It has been concluded that annealing leads to the release of the ligands that are incorporated in the film during deposition from TTIP at low deposition temperatures. That causes both the shrinkage and the increase of the refractive index.

Films have further been characterized by X-ray diffraction and environmental ellipsometry porosimetry.

11, 12 & 13 septembre
Session: Nanomaterials
Keywords: Photooxidation, thin film, ALD, TiO_2

On the Stability of the n-Si/TiO_2 Photoelectrodes: Effect of the Atomic Layer Deposition Conditions

M. E. Dufond[1], G. Loget[2] et L. Santinacci[1]

1. Aix Marseille Univ, CNRS, CINaM, Marseille, France
2. Institut des Sciences Chimiques de Rennes, UMR 6226 CNRS, Université de Rennes 1, France

Due to their intermittent nature, the development of renewable energies is limited. An efficient way to store and to transport this energy is required. In this context photoelectrochemical water splitting into H_2 and O_2 appears as a leading approach. To achieve this goal a hybrid photoanode n-Si/TiO_2 is prepared using Atomic Layer Deposition (ALD). In this study, the impact of the ALD process (temperature of the reaction chamber, precursor nature…) on the long-term chemical and photoelectrochemical stability is investigated. To assess this long-term stability, a sequence composed of a waiting steps in the electrolyte at rest potential and cyclic voltammetries measurements is developped. Surprisingly, stability variations are observed on TiO_2 thin films grown in the so-called ALD window. This stability is directly correlated to the measured refractive index that depends on the process temperature as well as on the precursor used during the deposition. The decrease of the electrode efficiency is attributed to a degradation phenomenon that proceeds through the oxidation/reduction of the interfacial SiO_2 layer during the waiting time. It leads to the destruction of the protective TiO_2 layer. The optimized deposition conditions are therefore identified.

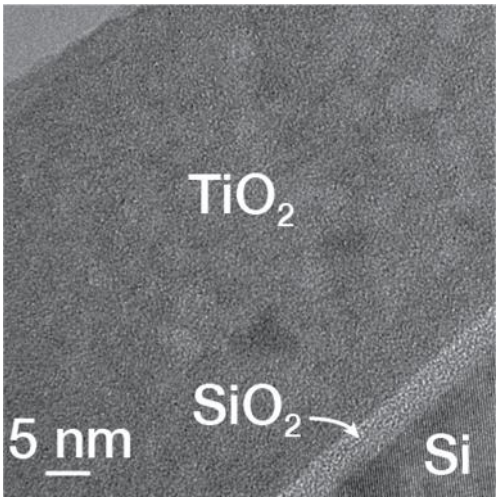

Figure 1: TEM cross section of a TiO_2 layer grown on Si by ALD at 120°C using titanium tetraisopropxide

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Session : Nanomatériaux avancés pour la photonique
Keywords: silicon nanocrystals ; boron doping ; evaporation ; photoluminescence

Photoluminescence of $SiO_{1.5}$ alloys doped with boron

F.Trad, M. Stoffel, X. Devaux, A. Bouché, M. Vergnat, H. Rinnert

Université de Lorraine, CNRS, IJL, F-54000 Nancy, France

Silicon nanocrystals (Si NCs) are the subject of an intense research activity, due to their optical and electronic properties. Actually, as in the case of bulk semiconductors, the fine tuning of their optical and electronic properties is related to the effective capability to control doping, i.e. incorporation of atoms such as phosphorous or boron within these nanostructures.

We present in this study the preparation method, the structure and the optical properties of $SiO_{1.5}$ thin films doped with boron.

The alloys were prepared by co-evaporation of SiO and SiO_2 from two electron-beam guns in an ultrahigh vacuum chamber. Boron was introduced during the evaporation from a Knudsen cell for the low boron contents and from an electron beam gun for the high boron contents. The films were annealed at different temperatures until 1100°C in order to obtain the dismutation of SiO which results in Si nanocrystals embedded in a SiO_2 matrix.

The structure and the optical properties were studied by infrared absorption spectrometry and by photoluminescence experiments. Infrared absorption spectrometry allows us to observe an absorption band at 1380 cm^{-1} attributed to the O-B bonds. For low annealing temperatures, the photoluminescence spectra show bands attributed to defects. For high annealing temperatures greater than 700°C, a band attributed to the Si nanocrystals appears near 800 cm^{-1}. This band disappears for high boron contents.

Session Nanophonics, Advanced nanomaterials for photonics

Keywords: 'transition metal dichalcogenides' 'solar cell' 'high efficiency photovoltaic' 'van der Waals heterojunction'

Proposal of a dual-gated $WTe_2/MoSe_2$ van der Waals tandem solar cell

N. Cavassilas[1], D. Logoteta[1], Y. Lee[2], F. Michelini[1], M. Lannoo[1], M. Bescond[3], M. Luisier[2]

1. Aix-Marseille Université, CNRS, Université de Toulon, IM2NP UMR 7334
2. Integrated Systems Laboratory, ETH Zürich
3. LIMMS, CNRS-Institute of Industrial Science, UMI 2820, Université de Tokyo

We propose and numerically investigate, through a multi-scale approach, a tandem solar cell based on a van der Waals heterostructure composed of two monolayers of transition metal dichalcogenides. The electronic connection between the two subcells is obtained *via* tunneling through the van der Waals heterojunction which is electrostatically controlled by means of a dual-gate. Furthermore, by adjusting the dual-gate voltages, the photocurrents in the two subcells can be matched and the tandem cell performances optimized. Assuming an optimal absorptance, as expected in light-trapping systems, we predict that a power conversion efficiency of 30.7%, largely exceeding that of the single subcells, can be achieved.

11, 12 & 13 septembre
Nano-optics
Keywords: ZnO nanoparticles, photoluminescence, doping, PL QY

Doped ZnO Nanoparticles for WLED Application

Y. Zhang[1], A. Apostoluk[1], B. Masenelli[1], S. Daniele[2], N. Le Bail[2], C. Theron[2], T. Cornier[2]

1. Université de Lyon, Institut des Nanotechnologies de Lyon (INL, UMR CNRS 5270), Institut National des Sciences Appliquées de Lyon (INSA Lyon), France
2. Université de Lyon, Institut de Recherches sur la Catalyse et l'Environnement de Lyon (IRCELYON, UMR CNRS 5256), Université Claude Bernard Lyon 1, France

ZnO can have excellent optical properties as a wide bandgap semiconductor with numerous intrinsic defects. The visible photoluminescence (PL) of ZnO originating from defects makes it a promising candidate for optoelectronic applications, such as white light emitting diodes (WLEDs). Since the industrialized WLEDs materials are dominated by rare-earth based phosphors, which are expensive and environmentally-unfriendly, ZnO provides a cheap and "green" way out for lighting devices. In our previous study, a hybrid sphere structure of ZnO nanoparticles and polyacrylic acid (PAA) matrix fabricated through a hydrolysis method has proven an efficient material emitting intensively in the visible range. [1] Herein, various dopants are introduced into ZnO hybrid structure in the same manner in order to optimize the photoluminescence of ZnO nanoparticles. Effects of dopant nature, size and valence are investigated at different doping concentrations at room temperature. The emission color of doped ZnO nanoparticles can be tuned in a wide visible range between yellow and green and the photoluminescent quantum yield (PL QY) can be improved by specific doping.

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Keywords: porous hybrid materials, solid electrolytes, Li-ion batteries

Design of lithium-ion conducting organic/inorganic hybrid porous materials as solid electrolytes for Lithium batteries

Ephrem Tefere WELDEKIDAN, Virginie HORNEBECQ, Chrystelle LEBOUIN

Aix-Marseille University (AMU), MADIREL (UMR 7246), Electrochemistry of Materials Group (ELMA), Marseille, France

Organic-inorganic composite polymer electrolytes have offered the possibility to have attractive properties of inorganic oxides (mechanical and thermal stability) and organic polymers (ductility, flexibility and processability) in a single solid material. However, the performance of such kind of electrolytes is still far from that required for practical applications.

In our work, we have developed hybrid porous polymer-silica electrolytes based on PEO and mesoporous silica matrix through two fabrication methods. In the first case, mesoporous PEO-silica hybrid particles have been fabricated through diblock copolymer templated sol-gel synthesis method at room temperature. The selective removing of the hydrophobic blocks of the template resulted in non-organized pores inside hybrid materials. Textural properties, nanostructured and chemical structure of the hybrid porous materials will be presented. Furthermore, the electrochemical properties of the Li-salt loaded materials will be discussed to demonstrate the feasibility of our materials as solid electrolytes. Second, surfactant templated mesoporous silica films have been fabricated on conductive substrates via electro-assisted self-assembly method. Well-ordered and vertically oriented mesochannels of 3nm size are obtained when the templates are let soluble in HCl/ethanol solution at room temperature. The permeability, morphology and nanostructure of the films will be presented.

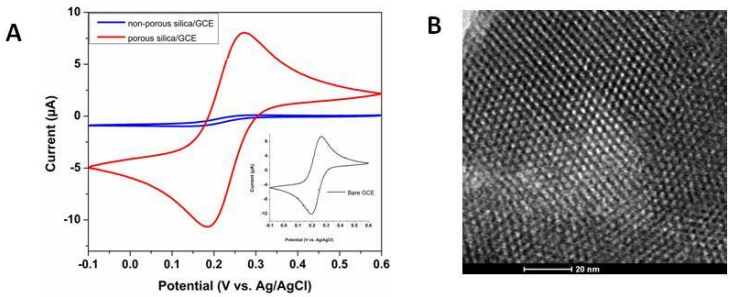

Figure 1: A) cyclic voltammogram recorded on silica film modified GCE before (blue) and after removing the template and B) TEM image of silica film after removing CTAB template.

Light-weight and Flexible Carbon Nanotubes (CNT) Tissues as Anode Materials for Flexible Li-ion Microbatteries

Vinsensia Ade SUGIAWATI[1], Florence VACANDIO[1], Yair EIN-ELI[2], Thierry DJENIZIAN[3]

1. *Aix Marseille Université, CNRS, MADIREL UMR 7246, F-13397, Marseille Cedex 20, France.*
2. *Department of Materials Science and Engineering, TECHNION, Haifa 3200003, Israel.*
3. *Ecole Nationale Supérieure des Mines de Saint-Etienne, 13541, Gardanne, France.*

Currently, flexible power sources are gaining immense interests due to their potential applications in the next-generation flexible and wearable electronics, such as implantable medical devices, smart cards, electronic skin, sensors, RFID tags, and more [1]. As an allotrope of graphite, carbon nanotubes (CNT) tissues are also capable of accommodating Li-ions as well as exhibits significantly higher reversible charge-discharge capacity than the commercial graphite (372 mAh/g). Due to its remarkable properties such as Li-ion storage capability, excellent mechanical property and high electronic conductivity, CNT tissues have been considered as competitive anode materials for flexible microbatteries [2]. In this work, the electropolymerization of the p-sulfonated poly (allyl phenyl ether) (SPAPE) polymer electrolyte into CNT tissues has been performed via cyclic voltammetry (CV) technique. Prior to cell assembly, the anode pre-lithiation process was employed to reduce a high irreversible capacity of the CNT tissues. Interestingly, the results show the irreversible capacity can be reduced about 87% after direct pre-lithiation and the SPAPE-coated CNT gives much higher reversible capacity (508 mAh/g, 187 µAh/cm^2) compared to pristine CNT (355 mAh/g, 130 µAh/cm^2) at 10C rate, even after 500 cycles.

Keywords: CNT tissues, Anode, Flexible microbatteries, Electropolymerization, Pre-lithiation

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Session: Nanophotonics
Keywords: 'Mid-IR Nanoantennas', 'SEIRA', 'Gas sensing', 'Hybrid materials' ,'Zeolites'

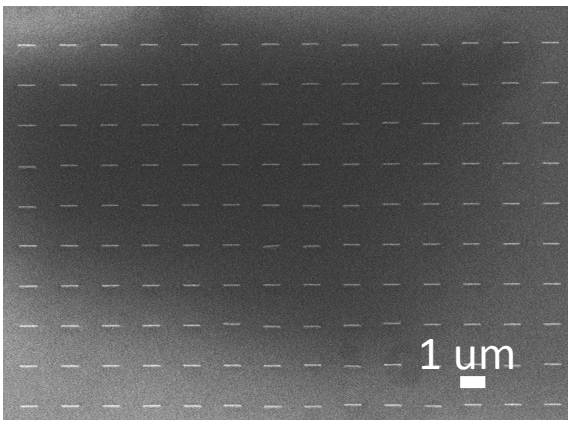
SEIRA detection of benzene at ppb levels mediated by resonant nanoantennas

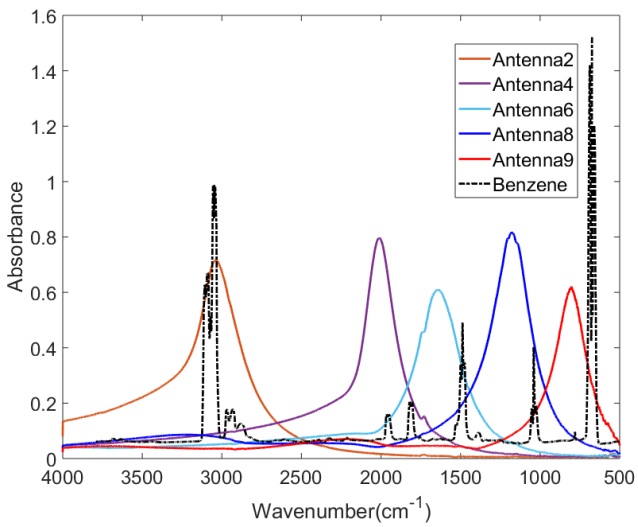
J. Nunez[1], J. Grand[3], S. Mintova[3], A. Boersma[1], B. Sciacca*[1,2]

1. TNO, HTC 25 Eindhoven, Netherlands
2. CINaM, Campus de Luminy, 13288 Marseille, France
3. ENSICAEN, Université de Caen, 14050 Caen, France

*sciacca@cinam.univ-mrs.fr

The detection of volatile organic compounds (VOC) at trace levels (ppb), such as **benzene**, is expected to have a role of increasing impact in the field of environmental monitoring for health related issues. Commercial portable low-cost sensors typically monitor changes (such as conductance) in a responsive material. These approaches can be very sensitive for a specific VOC target (ppb range), but they often lack of versatility and/or selectivity.
Spectroscopic techniques in the mid infrared (3-20 um) are able to detect the *unique* fingerprints of molecular transitions, but they are strongly limited by the extremely weak light-matter interaction (a^3/λ), thereby requiring long optical paths to boost the signal to noise ratio for applications where *ppb* levels of detection are required.
The use of **resonant nanoantennas** to boost the sensitivity (Surface Enhanced Infrared Absorption – **SEIRA**) has been so far limited to the detection of organic monolayers adsorbed on the antennas surface, where the field enhancement is the highest.
We will present a new approach, that enables to **extend** SEIRA to the detection of **gases**.
This is based on the combination of a *concentrating inorganic material*, such as zeolites to trap gas molecule and locally increase the concentration (***chemical enhancement***), with *phased array of resonant nanoantennas* to locally boost light-matter interaction (***photonic enhancement***).
Experimental data show that with this *hybrid system* an absorbance **enhancement >10^7** is obtained. This allows to detect benzene at concentrations as low as **10 ppb** in 1-2 minutes, and to discriminate it from other VOCs such as toluene.





Theoretical Design of New Small Molecules Thiophene and Oxathiazole based D-π-A organic dyes for efficient dye-sensitized solar cells (DSSCs)

T. Abram, R. Kacimi, L. Bejjit, M. Bouachrine*

MEM, High School of Technology (ESTM), University Moulay Ismail, Meknes, Morocco.
*Corresponding Author. E-mail: tayeb87abram@gmail.com or bouachrine@gmail.com;

Abstract

Four series of dyes were studied theoretically and characterized by functional density theory (DFT) and time-density functional theory (TD / DFT) using the B3LYP method and the 6-31G base set (d, p) to systematically explore the structure-property relationship of dyes with the D-π-A architecture and the performance of dye sensitized solar cells. These new compounds based on Thiophene and Oxathiazole bound to cyanoacrylic acid 2 as the acceptor and the electron donor unit has varied. The key parameters associated with the short circuit current density Jsc and the open circuit photovoltage Voc have been characterized and analyzed in detail. All assay results show that DM2 dye should be the best candidate to manufacture dye-based solar cells because of the better electronic property low energy gap and optimal optical absorption bung (wide absorption band of 300 to 900 nm for the adsorbed dye) in neutral and doping states and other exceptional parameters.

Keywords*:* Thiophene, Oxathiazole,DFT, TD/DFT, Dyes solar cells