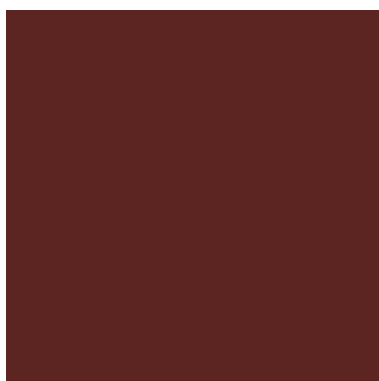


## Materials Science 2017



14<sup>th</sup> International Conference and Exhibition on

## **MATERIALS SCIENCE AND ENGINEERING**

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# Scientific Tracks & Abstracts

## Day 1

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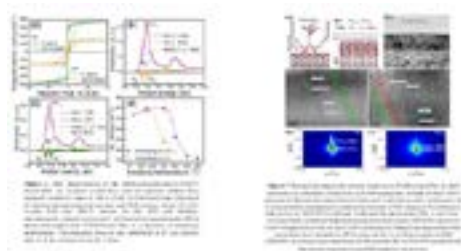
November 13-15, 2017 | Las Vegas, USA

## High-magnetization oxide spinel ferrite films

**Jun Ding**

National University of Singapore, Singapore

Tetragonal half-metallic magnets find broad applications in spintronics owing to the optimized magnetization and magnetic anisotropy. Herein, a low-temperature thermal decomposition method is utilized to grow new stabilized tetragonal ferrite films. Tetragonal  $\text{Fe}_3\text{O}_4$ -based film possesses high saturation magnetizations of  $\sim 1$  Tesla and tetragonal Co-doped  $\text{Fe}_3\text{O}_4$ -based film exhibits high energy product of  $\sim 10.9$  MGOe with perpendicular magnetocrystalline anisotropy. A combined experimental and first-principles study reveals that carbon interstitials ( $\text{C}_i^{\text{B}}$ ) and oxygen vacancies (VO) form  $\text{C}_i^{\text{B}}\text{-V}_\text{O}$  pairs which stabilize the tetragonal phase and meanwhile enhancing the magnetization. The high magnetization is attributed to the spin flipping on FeA as a result of the  $\text{C}_i^{\text{B}}\text{-V}_\text{O}$ -induced atomic migration and lattice distortion. The novel stabilized tetragonal ferrite films with high and tunable magnetization and magnetic anisotropy largely extends the applications of half-metallic spinel ferrites and novel energy harvest devices.



## Biography

Dr Jun Ding is Professor at Department of Materials Science & Engineering, National University of Singapore. He has been working on functional materials (particularly magnetic materials) over 25 years. His current research is focusing on additive manufacturing (3D printing) with the emphasis of advanced functional and multi-functional devices.

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## Impact of the residual flux reduction on the internal corrosion behavior for the automotive brazed heater cores

Philippe Da Silva and Vincent Joubier  
Valeo THS, France

The Nocolok® flux is used in the worldwide technology of heat exchangers to remove the aluminum oxide during the controlled atmosphere brazing. This flux (mixture of Potassium (K), Aluminum (Al), Fluorine (F)) is known to react with corrosion inhibitors of coolants. Furthermore, the several temperature cycles, the coolant ageing and the inhibitors consumption have an impact on the internal corrosion behavior of heat exchangers. That is the reason why car manufacturers ask to reduce the residual flux amount inside parts. The challenge of VALEO is to minimize the flux quantity while maintaining a good brazing quality and also staying at high level of robustness and reliability. A method to quantify the residual flux inside exchangers has been developed. The impact of the residual flux reduction on the internal corrosion behavior has been studied thanks to an internal corrosion reliability test developed by VALEO. This test called DECLIC (Degraded Coolant for Internal Corrosion test) will give us the benefit or not to reduce the flux quantity inside parts during the brazing process.

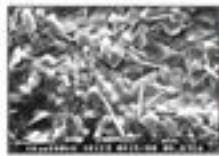


Figure 1: Flux residues with SEM at 500X



Figure 2: Corrosion on tube

### Biography

Philippe Da Silva is 36 years old and has been working for VALEO since 2006. He is a VALEO material expert since 2011. He is specialized in aluminum exchangers and also in corrosion tests. He has written 4 publications on the corrosion topics applied on automotive brazed Heat Exchangers.

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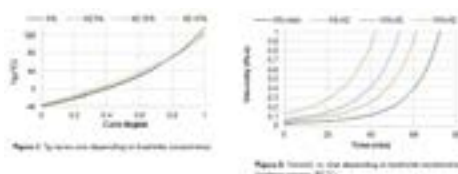
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## Influence of boehmite nanoparticle on the curing kinetics and rheology of an epoxy matrix for liquid composite molding process

Dilmurat Abliz, Tatjana Artys and Gerhard Ziegmann  
Clausthal University of Technology, Germany

Modifying the resin matrix with nano-scale additives is especially attractive in the liquid composite molding (LCM) processes in order to increase the matrix performance, by effectively reducing the shrinkage and improving the mechanical properties without compromising the flow and impregnation behavior of the matrix. Main target of this paper is to characterize and model curing kinetics and rheological behavior of the boehmite (AlOOH) nanoparticle-modified epoxy matrix, regarding to the application in LCM processes for fabrication of fiber-reinforced plastics (FRP), which are not yet covered in the literature. Based on the curing behavior and rheological characteristics, the curing kinetics and rheology of the boehmite nanoparticle-filled epoxy matrix is modelled by Kamal-Sourour and Castro-Macosko models, separately. Based on the cure kinetics, the boehmite nanoparticles showed an accelerating effect on the reaction up to a cure degree of about 0.82. However, then the T<sub>g</sub> of the reference system becomes higher than that particle-filled suspensions, indicating an inhibiting effect of the nanoparticle on the cure and negative effect on T<sub>g</sub>. The final T<sub>g</sub> value showed a reverse trend with the particle content: the higher the particle concentration, the lower the final T<sub>g</sub>, indicating a decreased network stability of the particle filled suspension compared to that by the reference system. According to the rheological investigations, the effective processing time is inevitably decreased by about 28 % at 10 wt% and 40 % at 15 wt% boehmite concentration. The effects of the nanoparticles on the curing kinetics and rheology of the matrix exert extra requirements and restrictions on the processing strategies and parameters considering the decreased impregnation length for the fabrication of FRP structures.



### Biography

Dilmurat Abliz is a PhD student in the Clausthal University of Technology and working as a scientific assistant since 2012 in the Institute of Polymer Materials and Plastics Engineering, TU Clausthal. His main research focus lies in the material, process and property characterization and modelling/simulation regarding nanoparticle-modified epoxy matrix for application in high-performance fiber-composites. This work originates from the Research Group Program FOR 2021 "Acting Principles of Nano-Scaled Matrix Additives for Composite Structures" funded by the German Research Foundation (DFG: ZI 648/42-1; ZI 648/43-1).

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## Accelerated corrosion test for exhaust gas recirculation exchangers

Vincent Renault<sup>1</sup>, Anne-Gaëlle Villemiane<sup>1</sup> and Shayma El-Hafa<sup>2</sup><sup>1</sup>Valeo THS, France<sup>2</sup>MCA Ingénierie, France

The VALEO strategy focuses on two areas. First is to develop innovative technologies related to the reduction of CO<sub>2</sub> emissions and intuitive driving. The second is the geographical expansion in high growth regions. In the field of new heat exchanger integration within the EGR LP loops such as the Charge Air Cooler (CAC), it appeared that the condensation of aggressive chemical solution can occur. This condensation can lead to part material corrosion and that may create some issues in the field (leak, loss of thermal performance...). Different studies have already been carried out in order to develop specific tests for corrosion resistance evaluation. Most of these tests concern only small samples tested by immersion. The final product in its vehicle architecture could not be tested. The project was to develop and adapt a new Charge Air Cooler heat exchangers test bench for corrosion resistance evaluation of. A patent has been submitted on this specific test bench (n° FR3012217 A1). Thanks to the capabilities of the test benches, we reduced test duration considerably compared with other test methodologies such as immersion tests. Specific gas flow rate, condensate chemical flow rate injection and temperature were adapted to reach dew points leading to condensation of chemical mixtures inside the CAC. The repeatability of the corrosion test results was investigated. Condensate mixtures can be very aggressive for CAC corrosion resistance. Test bench conception in stainless steel and PTFE allow us to use very low or very high pH. That is necessary to adapt the condensate mixture with the real condensates extracted during engine tests by OEM. We compared the corrosion test results obtained on the CAC following the corrosion tests with parts from the vehicle. Then, test duration and the vehicle mileage were correlated in order to draw a reliability curve.



### Biography

Vincent Renault is 29 years old and has been working for VALEO since 2007. He is specialized in materials and corrosion test bench development. He is metallurgical department manager for VALEO Thermal Systems materials laboratory.

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## Cleaner production practices for resource optimization

**Sampath Kumar M C**

B.M.S College of engineering Bangalore, India

This Paper describes the studies conducted on application of best practices in cleaner production at industry level and its visible beneficial impact on the surrounding environment and ground water. The industrial zone had many medium and large scale industries and posing many challenges in resource utilization. The studies involved many industry specific issues such as non-compliance to adoption of green chemistry concepts to process and impediments in application of cleaner technologies to various activities in the industries. The characterization included evaluation of energy consumption, hazardous waste management and water quality indices for ground water. The studies were supplemented with estimation of carbon credits and justified by environmental economics. Studies were made effective by creating a decision making model and support system using remote sensing and GIS tools for locating the industries and optimizing resource conservation. Such green initiatives have brought a distinct change in work practices in industrial areas and community at large.

### Biography

Sampath kumar M.C. is faculty at the civil engineering Department at B.M.S College of engineering Bangalore, India. He is involved in Teaching, research and environmental application activities. His area of interest is in the field of remote sensing and GIS for natural resources conservation.

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## Accelerated corrosion test for exhaust gas recirculation exchangers

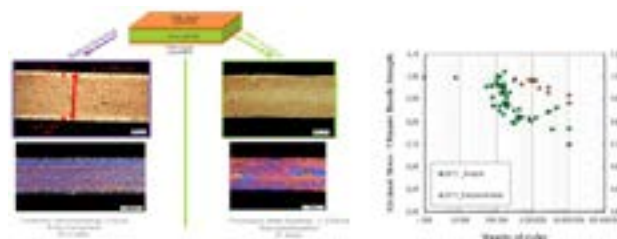
Anne-Gaëlle Villemiane<sup>1</sup>, Josselin Paturaud<sup>2</sup>, Armelle Danielou<sup>3</sup>, Jean-Yves Buffière<sup>2</sup> and Damien Fabregue<sup>2</sup>

<sup>1</sup>Valeo THS France

<sup>2</sup>INSA Lyon, France

<sup>3</sup>Constellium Ing. C-Tec, France

Economic and environmental drivers are leading to exchanger weight reduction for automotive applications. The consequence is a material downgauging and some critical conditions reached. One of the exchanger's main failure modes is induced by transient differential dilatations between the exchanger components. In this work, a detailed characterization of the cyclic damage mechanisms in car heat exchangers has been undertaken in order to improve their reliability. The studied material is a very thin (<0.3 mm) aluminum sheet composed of 3 layers (4XXX /3XXX/ 4XXX) (figure 1) compared to the same aluminium sheet made of 1 layer (3XXX), brazed in similar conditions to those of real components. Fatigue tests at constant stress amplitude have been performed at room temperature to show the influence of the clad in the fatigue resistance. Tensile properties between the clad alloy and the unclad alloy are strictly identical. However, the Wöhler curve shows a high fatigue resistance for the unclad material compared to the clad one. (Figure 2). Fractography analysis on the 3 layer alloy reveals that the crack initiation is intergranular on the clad side and occurs on the specimen face because the clad is harder than the core which weakened the grain boundaries leading to multifissuration initiation and propagation. Cracks stopped for about 50% of the fatigue life then there is a transgranular propagation of the crack until failure. Concerning the unclad material, the elements Cu, Fe, Si, Mn and Ti are better distributed in the alloy thickness leading to a less modified surface state and decreasing the site initiation number and therefore the multifissuration. Thanks to microstructure, tomography and surface rupture analysis a fatigue damage mechanisms can be proposed, showing the residual clad layer key influence on the crack initiation.



## Biography

Anne-Gaëlle Villemiane is an expert in fatigue and fractography. She has been working for Valeo for 10 years and she is head of the Material Laboratory. She has worked on 3 PhDs specialising in fatigue and has written 8 publications on the topic applied on automotive problematic. She has obtained a PhD in 2006 on the determination of the niobium effect on the oxidation mechanisms of ternary titanium aluminides. This study was conducted from first seconds (20 s) to long term oxidation times (2000 h).

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## Hydrothermally grown nanoflowered WO<sub>3</sub> thin films on etched ITO for electrochromic studies

**Anamika V Kadam**

D Y Patil College of Engineering and Technology, India

**Abstract:** Herein, we present, for a first time, an electrochromic film of WO<sub>3</sub> fabricated on a ITO by etching process, adopting a low-cost, facile and template-free fabrication process. By using hydrothermal method, we obtained WO<sub>3</sub> films with a simplified architecture (ITO/HCl/WO<sub>3</sub>) in which HCl supports WO<sub>3</sub> to form adhesive layer. Compared to ITO/WO<sub>3</sub> configuration, the ITO/HCl/WO<sub>3</sub> configuration exhibited a strong enhancement in terms of roughness, porosity, open-tunnel structure, current density and coloration efficiency (about 179cm<sup>2</sup>C<sup>-1</sup>). Moreover, electro-optical characterization illustrates high transmittance modulation (about 49% at 630 nm) with excellent stability, making it attractive for a practical application.

### Biography

Dr. Anamika Vitthal Kadam has completed her PhD at the age of 31 years from Bharti Vidyapeeth University, Pune, MH, and India. She is working as Assistant Prof in D.Y. Patil Engg and Tech, Kolhapur, MH, India and having guideship of D.Y. Patil University. Se has published more than 25 papers in national and international journals and achieved a project under young scientist scheme with one minor research project.

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## Spinorbitronics at interfaces for THz emission

H. Jaffrès<sup>1</sup>, T.-H. Dang<sup>1</sup>, H. Nond<sup>2</sup>, Q. Barbedienne<sup>1</sup>, S. Collin<sup>1</sup>, N. Reyren<sup>1</sup>, Nicolas<sup>1</sup>, J.-M. George<sup>1</sup>, L. Vila<sup>3</sup>, J. Tignon<sup>2</sup>, L. Divay<sup>4</sup>, P. Bortolotti<sup>4</sup>, S. Dhillon<sup>2</sup><sup>1</sup>Unité Mixte de Physique CNRS-Thales, France<sup>2</sup>Université Paris Diderot-Sorbonne Paris Cité, France<sup>3</sup>Spintec, Institut Nanosciences et Cryogenie, France<sup>4</sup>Thales Research & Technology, France

Spin-Hall Effects at short lengthscale in bulk heavy metals like Pt or W and spin-orbit related phenomena like Inverse-Edelstein Effect at interfaces are presently at the basis of new spintronics functionalities. Combined with RF-spin-pumping Ferromagnetic Resonance (FMR) pumping, spin-orbit give rise to AC and DC spin-to-charge current conversion. Those combined techniques enable to probe the interface quality and physical properties. In the same way, in an extended description out-of FMR resonance, it was recently reported that THz emission of relatively high power may be realized in the same kind of heterostructures composed of ferromagnetic (FM) and non-FM metal films via dynamical spin-to charge conversion and time-dependent spectroscopy (TDS). In that mind, we will present our last results of THz emission provided by optimized growth bilayers composed of a high-spin orbit material in contact with a ferromagnetic layer Co/Pt, NiFe/Au:W). Those bilayers state-to-the art model systems in experiments combining RF-spin pumping and spin-to-charge conversion by ISHE. Here, experiments consist in exciting magnetization and spin-currents within the FM layer via femtosecond laser excitation and measuring, in the picosecond timescale, the relaxation of the correlated spin and charge currents responsible for THz dipolar emission. The THz emission provided by these spintronics bilayers reaches the power of ZnTe semiconductor technology. We will display the first THz emission results obtained on -Sn/InSb topological insulators. Moreover, in order to study the SHE spin-current profiles and address their properties in those [Co,Ni]N/Pt and [Co,Ni]N/Au:W multilayers, we have analyzed their Anomalous Hall effect (AHE) signals showing up a characteristic AHE spin-inversion from Pt to Au:W samples. We analyze our results in the series of samples: the exact conductivity profile across the multilayers via the 'extended' Camley-Barnas approach and the spin current profile generated by spin-Hall effect. We will discuss the role of the generalized spin-mixing conductance on the spin-transport properties and spin-orbit torques.

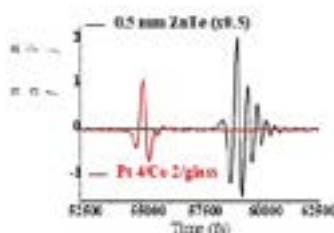


Figure 1: Time-Dependent Spectroscopy (TDS) THz signal of Pt/Co 2/glass. The signal is centered around 8000 fs and shows a sharp peak. The x-axis ranges from 8100 to 8200 fs, and the y-axis ranges from -1 to 1. The legend indicates '0.5 mm ZnTe (x8.5)' and 'Pt 4Co 2/glass'.

## Biography

Dr. Henri Jaffrès completed his Ph.D. at the Physics Department of the Institut National des Sciences Appliquées (INSA) - University Toulouse III, France, in 1999. Then he joined the Unité Mixte de Physique CNRS-Thales, Palaiseau, France as a postdoc (2000–2001) before joining the CNRS at the same institute. His work focuses on spintronics, spin injection, spin transport, and spin transfer in semiconductor spintronics devices with electrical and optical detection in III-V heterostructures, as well as spin-Hall effect and spin-pumping in group IV semiconductors.

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## Crystal growth of Si based on the Na-Si binary phase diagram

Haruhiko Morito

Tohoku University, Japan

Phase diagram provide essential information for the conditions of materials synthesis and crystal growth. Although many binary phase diagrams were reported in the last century, that for Sodium (Na) and Silicon (Si) has not yet been established. In 2009, our group has presented a Na-Si binary phase diagram with the results of thermal analyses and morphology observation. In the present study, we demonstrated the crystal growth of Si from the Na-Si solution based on the Na-Si phase diagram. As shown in the Na-Si binary phase diagram (Fig. 1), Si is dissolved in a Na melt at 1173 K. Since the boiling point of Na is 1154 K at 1 atm and the vapor pressure of Na is relatively high above 973 K, Na can be removed from the products by evaporation. The Na-Si mixture (molar ratio Na/Si = 3:2) was heated at 1173 K. Na evaporation changed the composition of the sample toward the liquidus line at around 55 mol% Si at 1173 K, allowing crystallization of supersaturated Si to begin. After Na evaporation, single crystal of Si was obtained as shown in Fig. 1. Likewise, various Si crystals such as Si film, porous bulk Si and Si micro-tube were prepared by using a Na-Si solution. Furthermore, the efficient removal of impurities in Si for the solar cell was demonstrated by dissolution and recrystallization in a Na melt at low temperature. Recently, we succeeded in the crystal growth of Si clathrates by using a Na-Sn flux. These compounds have been widely studied due to their unique open-framework structures of Si polyhedrons.

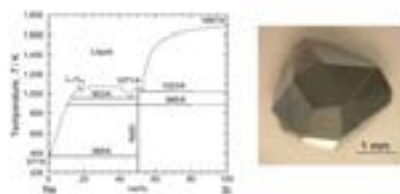


Figure 1: Na-Si binary phase diagram (left) and the single crystal of Si prepared from Na-Si solution (right).

## Biography

Haruhiko Morito received his PhD in engineering from Tohoku University in 2007. He is currently working as an associate professor at the Institute for Materials Research of Tohoku University. The main objective of his research is to develop an emerging material which has a new function and new physical properties. In particular, he has developed new functional ceramics containing alkali metals. He has also developed a new crystal growth process based on the binary phase diagram of sodium and silicon. He has synthesized the various silicon-based materials by the sodium flux method.

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### Plenary Talk

Day 2

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## Alexander G Ramm

Kansas State University, USA

### Wave scattering by many small impedance particles and creating materials with a desired refraction coefficient

The theory of acoustic and electromagnetic (EM) wave scattering by one and many small impedance particles of arbitrary shapes is developed. The basic assumptions are:  $a \ll d \ll \lambda$ , where 'a' is the characteristic size of particles, 'd' is the smallest distance between the neighboring particles, ' $\lambda$ ' is the wavelength. This theory allows one to give a recipe for creating materials with a desired refraction coefficient. One can create material with negative refraction: the group velocity in this material is directed opposite to the phase velocity.

- One can create a material with a desired permeability.
- Equation is derived for the EM field in the medium in which many small impedance particles are embedded.
- Similar results are obtained in [6] for heat transfer in the media in which many small particles are distributed.
- The theory presented in this talk is developed in [1]-[6].

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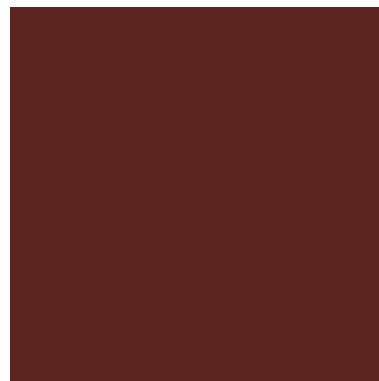
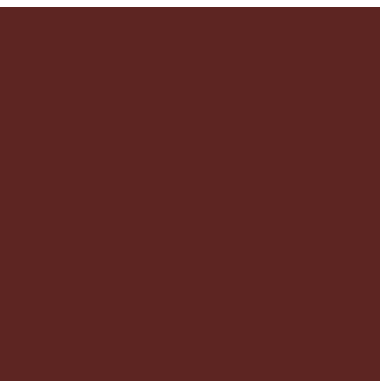
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#### Biography

A.G.Ramm was born in USSR and emigrated to USA in 1979. he is a US citizen, professor of mathematics at KSU, an author of more than 660 papers in mathematical and physical Journals, of 15 monographs, and an editor of 3 books. His scientific interests include differential and integral equations, operator theory, mathematical physics, especially scattering theory and inverse problems, numerical analysis, especially methods for solving ill-posed problems, various problems of applied mathematics and theoretical engineering. Professor A.G.Ramm was awarded many honors, including Fulbright Research Professorships in Israel and Ukraine, Mercator Professorship, NATO and DAAD professorships and grants, Khwarizmi international award, distinguished professorships in some countries and distinguished lectureships of London Mathematical Society and Hong Kong Mechanical society, and many other honors and awards. He gave invited plenary talks at many conferences throughout the world.

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## Young Research Forum

Day 2

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## Flexible organic field effect transistors with enhanced electrical properties

**Davoud Dastan**

Cornell University, USA

Bottom-gate top-contact organic field effect transistors (OFET's) have been fabricated on flexible substrates. Organic/inorganic materials are used as gate dielectric to enhance the output and transfer characteristics of the fabricated devices. Rutile titania nanoparticles (NP's) were prepared using solvothermal technique and incorporated into poly vinyl alcohol (PVA) to improve the capacitance and therefore dielectric constant of the host matrix. The composite films were exposed to ozone treatment and the gold contacts were thermally made on top of the films through a shadow mask. The gate dielectric was treated with a self-assembled monolayer (SAM) of octadecyltrichlorosilane (OTS) and then an active layer of copper phthalocyanine (CuPc) was deposited on top of the films. The output and transfer characteristics of the fabricated FET's were measured using semiconductor parameter analyzer. OFET's treated with a SAM of OTS exhibited higher mobility, on-off current ratio, and lower threshold voltage than the devices without a SAM of OTS treatment.

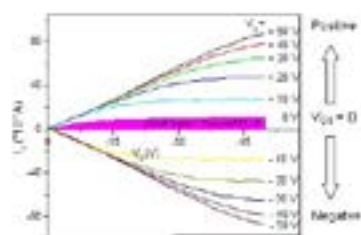


Figure 8: Output transfer characteristics of OFET treated with a SAM of OTS for various applied gate voltages

### Biography

Davoud Dastan has his expertise in the area of materials science. His expertise in materials science includes synthesis, characterization of nanomaterials for energy applications. He has the experience of synthesizing semiconductor oxides nanoparticles and thin films, fabricating solar cells, metal-insulator-semiconductors (MIS) structures, and organic field effect transistors using hybrid materials such as organic/inorganic materials. He has got several competitive grants during his research and has an ever growing potential for exploring his interest in materials science and nanotechnology.

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## Microstructural characterization of Mg-SiC nanocomposites produced by powder metallurgy techniques

Daniela Penther, Sepideh Kamrani, Alireza Ghasemi, Ralf Riedel and Claudia Fleck  
Technische Universität Berlin, Germany

In the present study, the microstructure of newly developed magnesium matrix composites reinforced with SiC nanoparticles was investigated. To produce Mg-SiC nanocomposites, magnesium powder and various volume fractions of SiC particles with an average diameter of 50 nm were co-milled by a high energy planetary ball mill. The milled powder was compacted by a hydraulic hand-operated press followed by cold isostatic pressing and sintering. Finally, the nanocomposites were hot extruded to eliminate porosity and achieve full density. Scanning electron microscopy, energy dispersive x-ray analysis and x-ray diffraction were used to characterize the microstructure and texture of the magnesium matrix and the distribution of the SiC-reinforcements after extrusion. Further, transmission electron microscopy analyses were performed to study the grain size of the magnesium matrix and the interface between the SiC nanoparticles and the magnesium matrix. All developed nanocomposites revealed a uniform distribution of the SiC nanoparticles in the magnesium matrix. No evidence of porosity or interfacial products between the SiC nanoparticles and the magnesium matrix were found, indicating a well-bonded interface. The used powder metallurgy techniques allow to produce dense nanostructured Mg-SiC nanocomposites.

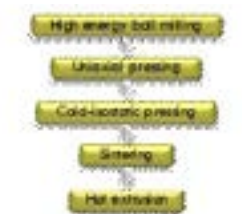


Fig. 1 Powder metallurgy techniques used to produce compact Mg-SiC nanocomposites.

### Biography

Daniela Penther has her expertise in powder metallurgy techniques including high energy ball milling, diverse pressing techniques and sintering of metals. She started studying and analyzing composites by SEM (EDS, EBSD), XRD and TEM during her diploma thesis in the collaborative research centre "TRIP-Matrix-Composite" supported by German Research foundation (DFG) at TU Bergakademie Freiberg, Germany. During her PhD she is currently producing Mg-SiC nanocomposites by powder metallurgy techniques and analyzing their microstructure as well as their fatigue behavior in a project supported by DFG at Technische Universität Berlin, Germany.

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## Modification of Surfaces with Carboxymethylthio Ligands Towards Chelate-Assisted Extraction of Copper

**John Onyango Adongo**

Humboldt-Universität zu Berlin, Germany

Copper (Cu) is an essential metal in biological systems; however, at concentrations beyond threshold limits, not only can it kill aquatic organisms but also it can become highly toxic to humans. Copper can bind onto certain organic ligands via coordination mechanisms. Electrochemical grafting of aryl diazonium derivatives have successfully been used to modify substrates by introducing layers of various organic functional groups onto metallic and semiconducting substrate surfaces.<sup>1</sup> Strategies involving functionalization of substrates with large-molecular-weight oligomers and peptides via diazonium grafting routes for extraction of heavy metal ion (HMI) pollutants have been reported. Some of these methods involve introduction of chelating groups in more than a single step. However, a simpler one-step quick grafting of low-molecular-weight HMI - chelating agents may not only present some cost reduction advantages towards devising kits for HMI extraction but also permit the fabrication of relatively thinner layers with optimal surface grafting with excellent chelation efficiency. Silicon is one of the most abundant materials on the earth's crust and its suitable surface chemistry has motivated organic functionalization efforts towards developing a wide range of applications. The purpose of this study is to explore a one-step functionalization strategy for introducing carboxymethylthio (CMT) chelating groups via direct electrografting of the diazonium cation 4-[(carboxymethyl)thio]benzenediazonium cation, (4-CMTBD), onto Si surface, leading to fabrication of the Si-(4-CMTB) surface. The investigation of Cu chelation is also studied.

**Finding:** The fabricated surface, Si-(4-CMTB), is capable of chelating Cu ions from aqueous solutions at trace amounts as shown by Raman spectroscopy.<sup>2</sup>

**Conclusion & Significance:** The surfaces may be of potential engineering interests for HMI sensing and/or extraction. This study offers positive contributions in the fields of environmental protection, forensic diagnostics, biosensing, and mineral prospecting among other related disciplines.

### Biography

John Onyango Adongo is a doctoral candidate registered at Humboldt-Universität zu Berlin, Germany. He conducts collaborative research within the surface sciences group of Dr. Jörg Rappich based at the Institut für Si-Photovoltaik, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH. He currently holds a tutorial fellow position at the chemistry department, Egerton University, Kenya. As a material scientist, his doctoral research focusses on the design, fabrication and testing of potentially renewable HMI – chelating surfaces incorporating silicon as the substrate material. The approach for functionalizing substrate surfaces majorly involves the facile electrografting method achieved via electroreduction of aryl diazonium salts.

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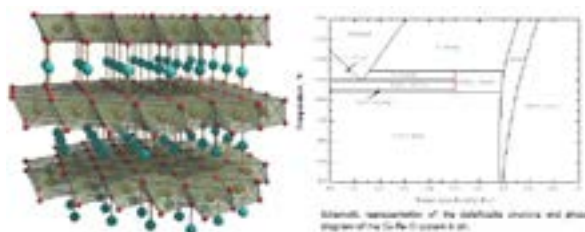
# MATERIALS SCIENCE AND ENGINEERING

November 13-15, 2017 | Las Vegas, USA

## Thermal-structural and elemental analysis of Cu-Fe-O system coupled with available thermodynamic modeling

Juliano Schorne Pinto, Laurent Cassayre and Antoine Barnabé  
CIRIMAT Université de Toulouse UPS, France

The Cu-Fe-O system has a great technological interest in the copper industry, as well as the development of catalytic compounds and transparent devices. The  $\text{CuFeO}_2$  phase (delafossite) and  $\text{Cu}_x\text{Fe}_{3-x}\text{O}_4$  phase (spinel) exhibit remarkable electrical, magnetic, optical and optoelectrical properties. Therefore, an in-depth understanding of the stability of the delafossite structure becomes of particular interest for fundamental research and for instance, its applications to the development of efficient p-type TCOs. The purpose of this study is reviewed the structural and thermodynamic information and phase equilibria of the Cu-Fe-O system in addition to checking the consistency of the available thermodynamics models with the experimental data. First, several of these models based on the CALPHAD method were reviewed and differences were highlighted. Moreover, several experimental procedures were employed to establish the relationships among temperature, lattice parameter, and stoichiometry of mixed oxides. In situ HT-XRD (High-temperature X-Ray Diffraction) and TGA/DTA measurements, Rietveld refinement were used to provide thermo-structural information in the range of 50° to 1100°C from stoichiometric mixture of CuO and  $\text{Fe}_2\text{O}_3$  single oxides. Plasma Sintering (SPS) followed by adjusted post-annealing treatments were used to stabilize delafossite phase in different Copper/Iron gradient and analyzed by Electron Probe Micro-Analyzer (EPMA). The HT-XRD demonstrated that the spinel phase started to be formed from 750° and increases the amount of Cu after 900°C ( $\text{CuFe}_{3-x}\text{O}_4$ ). In addition, the variation of lattice parameters of spinel phase was determined by Rietveld refinement and compared with those of different molar ratios. Contrary to all the models, EPMA coupled with local structural analysis showed that delafossite phase could be stabilized with a substantial degree of cationic non-stoichiometry. These results were related to available thermodynamics models providing an improved understanding of this system, new information has generated to implement the existing data. The need to develop and improve a new model is considered.



### Biography

Juliano Schorne Pinto is a Ph.D. student at Université de Toulouse and research associate at the CIRIMAT and Laboratoire de Génie Chimique. He has obtained his Master's degree in Materials Science and Engineering at Université of Montpellier (France) and bachelor's degree in Materials Engineering from the Federal University of Rio Grande do Sul (Brazil). He has experience in the synthesis and characterization of nanostructured materials with photocatalytic activities, carbon nanotubes and thermodynamic modeling of systems using the CALPHAD method.

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# MATERIALS SCIENCE AND ENGINEERING

November 13-15, 2017 | Las Vegas, USA

## The improved photoelectrochemical properties using $\alpha$ -hematite -molybdenum disulfide nanostructured material

Hussein Alrobei and Manoj K Ram  
University of South Florida, USA

The alpha ( $\alpha$ )- hematite ( $\text{Fe}_2\text{O}_3$ ) nanomaterials are attractive due its optical, electrical, and photoelectrochemical (PEC) properties. Several transition metal ions (Ti, Al, Pt, Zn etc.) have been doped to enhance low conductivity, surface kinetic, carrier diffusion, and decreasing of the photocorrosion. However, little attention is paid to dope dichalcogenide 2D- molybdenum disulfide ( $\text{MoS}_2$ ) with  $\alpha\text{-Fe}_2\text{O}_3$ . The  $\text{MoS}_2$  has shown interesting photo-activity due to its bonding, chemical composition and doping properties. So, we have synthesized nanocomposite  $\alpha\text{-Fe}_2\text{O}_3\text{-MoS}_2$  using sol-gel technique. The  $\alpha\text{-Fe}_2\text{O}_3\text{-MoS}_2$  nanomaterial was characterized using combination of physical techniques such as SEM, X-ray diffraction, UV-vis, FTIR and Raman techniques, respectively. The photocurrent, electrode/electrolyte interface of  $\alpha\text{-Fe}_2\text{O}_3\text{-MoS}_2$  nanocomposite films were investigated using electrochemical techniques. The rhombohedral structure with lower band gap is obtained using X-ray diffraction and UV-vis measurements for  $\alpha\text{-Fe}_2\text{O}_3\text{-MoS}_2$  films. Besides,  $\alpha\text{-Fe}_2\text{O}_3\text{-MoS}_2$  film revealed improved hydrogen production compared to  $\alpha\text{-Fe}_2\text{O}_3$  as well as aluminum doped  $\alpha\text{-Fe}_2\text{O}_3$  nanostructured films. Later, mechanism of photoelectrochemical water splitting in nanocomposite  $\alpha\text{-Fe}_2\text{O}_3\text{-MoS}_2$  films is understood through band diagram.

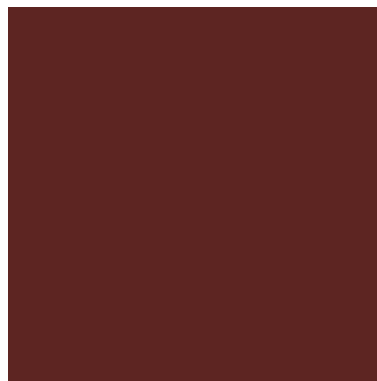
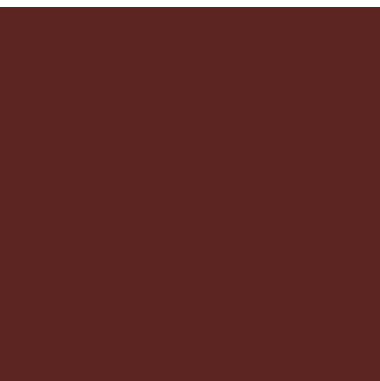
### Biography

Hussein Alrobei is a Ph.D student under the supervision of Manoj K Ram. He has background in the field of photoelectrochemical, advanced materials, polymers and energy. He has been involved on photoelectrochemical properties on various metal oxides, polymers and conducting polymers, and recently his patent on nano-hybrid structured regioregular polyhexylthiophene blend films for production of photoelectrochemical energy has been approved.

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### Scientific Tracks & Abstracts

Day 3

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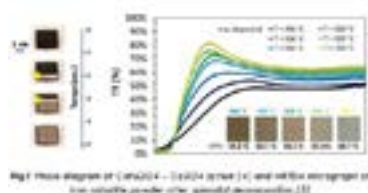
# MATERIALS SCIENCE AND ENGINEERING

November 13-15, 2017 | Las Vegas, USA

## p-type TCO thin films of Delafossite $\text{CuCrO}_2$ :Mg by rf sputtering with conventional thermal and ultra-rapid laser annealing

A Barnabe, Y. Thimont, L Presmanes, I Sinnarasa and P. Tailhades  
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Currently there is a lack of a p-type materials with comparable combinations of high conductivity and transparency to established n-TCO. This technological gap imposes many constraints on the conception and performance on optoelectronic devices which require a transparent hole injection, collection or transport layer. For p-TCO, it is first necessary to deposit the resultant material as a thin film on a transparent substrate. This has been already published using a large range of deposition conditions and technics. However, the main p-TCO performance still needs improvements to, in fine, reach that of their n-TCO counterparts. Second, proper control of the substrate temperature is required and may become an important issue for realistic applications since conventional or flexible substrates are required. The growth of  $\text{CuCrO}_2$ :Mg delafossite thin film on quartz substrate by rf sputtering is first reported in this work. The deposition leads to a nanocrystalline phase. Delafossite characteristic diffraction peaks were obtained as a function of the thermal treatment. The electrical conductivity was optimized until  $1.6 \text{ S cm}^{-1}$  with an optical transmittance of 63% in the visible range. The transport properties were analyzed by Seebeck and Hall measurements, integrated spectrophotometry and optical simulation. The second part of this work is focused on the post laser annealing which was carried out by varying the scan speed, power and number of pass of the laser beam on films deposited on various polymer, conventional glass and quartz substrates. The laser annealing affects the microstructure, sheet resistance, and optical transmittance of the  $\text{CuCrO}_2$ :Mg thin films. From the present work it can then be concluded that the preparation of efficient p-type TCO thin films based on Delafossite structure could be obtained at temperatures compatible with the use of cheap substrates such as flexible polymer or conventional glass slides.



### Biography

A. Barnabé is a professor at the CIRIMAT laboratory (Mixed Oxide Valency research group), Paul Sabatier University, France. He received his PhD degree in chemistry of materials from University de Caen-Basse Normandie (France) in 1999. He held a post-doctoral position in Northwestern University, Evanston (USA), in 2000. His current research interests are mainly focused in functional metal oxide powders, ceramics and thin films prepared by PVD technique. He first worked on TEM characterization of giant magnetoresistance manganites then moves to complex oxides with new optoelectronic properties. For the last decade, he has developed transparent conductive oxides (n- and p-type) and gas-sensing layers for the CO<sub>2</sub> detection sputtered oxide thin films. He's in charge on the SEM/TEM/EPMA/SIMS characterization center R. CASTAING in Toulouse. To date, all these works have led to 63 publications, 2 patents, and more than 80 communications (hindex = 22, sum of the times cited > 1400).

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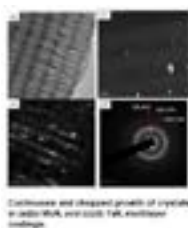
# MATERIALS SCIENCE AND ENGINEERING

November 13-15, 2017 | Las Vegas, USA

## Single element transition metal nitride protective sputtering coatings with versatile structural features

F.B. Wu, Y.H. Yang, J.Y. Xiang, K.Y. Liu and Z.X. Lin  
National United University, Taiwan

Transition metal nitride, TMN, coatings had been proved to be excellent protective surface layers in recent decades owing to their promising corrosion resistance, high hardness and modulus, good adhesion onto various substrates, and pronounced tribological behavior. Tremendous efforts were made on characteristic enhancement of the nitride coatings with multicomponent and multilayer features for the past decade. In this work single element nitride films, including TaN, MoN, and HfN, were and were manipulated to form amorphous, crystalline, preferred structures by RF magnetron sputtering and dedicated parameter control. Through input power and source gas ratio modulation, TaN with amorphous/crystalline altering layer stacking, i.e. an a-TaN/cTaN multilayer coating, could be produced with tougher behavior. Less tribological failures for the multilayer TaN coatings, like scratch cracking and peeling, during scratch and dry sliding wear were observed as compared to single layer coatings. Likewise, superior mechanical properties and corrosion resistance were obtained for single element HfN multilayer film with HfN nanolayers deposited under various RF input powers. More promising effect on adhesion enhancement was found for the nanocrystalline/preferred-orientation-crystalline MoN multilayer coatings. The continuity of column structure found in single layer nitride coatings could be effectively suppressed by nanolayered stacking of single element nitride layers with different structure features. The modulated multilayer features were also beneficial to the mechanical characteristics. The effects of the modulation on mechanical characteristics of the multilayer nitride coatings, such as hardness, modulus, adhesion strength, and tribological behavior, were demonstrated and discussed.



### Biography

Fan-Bean Wu, Ph.D, graduated from Department of Materials Science and Engineering of National Tsing Hua University, Taiwan, in 2002. He has been recognized as a dedicated researcher in hard protective coating and specialty glass fields. As a faculty in Department of Materials Science and Engineering in National United University, Taiwan, and a society member in both Committees of Taiwan Association of Coatings and Thin Films, TACT, and Taiwan Ceramics Society, TCS, he has served as department chairperson, director of Editing committee, and vice-director of Member committee and received Awards of Outstanding Teaching, Outstanding Service, several research conferences and innovation expos. He welcomes all kinds of research collaboration and is willing to put efforts on developments in any interesting topics concerning coatings/surface technology/glass/material process technologies.

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# MATERIALS SCIENCE AND ENGINEERING

November 13-15, 2017 | Las Vegas, USA

## New DGEBA-based epoxy resins toughened with liquid silicones

Daniela Rusu, Sophie Bistac and Christelle Delaite  
LPIM - Université de Haute-Alsace, France

**Statement of the Problem:** Epoxy coatings topic is experiencing a continuous renewal and still presents a great potential to produce new advanced functional materials exhibiting self-healing, shape memory or other functional properties such as transparent-to-opaque transitions. Epoxy coatings can be widely formulated by tailoring the epoxy resin/hardener partners upon the performance requirements for the end product. However, these materials exhibit naturally low impact resistance because of their high crosslinking density. The usual approach to toughen epoxy thermosets is to add either elastomers or thermoplastic modifiers, but this is also lowering their overall mechanical performances. Methodology & Theoretical Orientation: New epoxy-silicone coating formulations are proposed based on diglycidyl ether of bisphenol-A epoxy resin (DGEBA) and 5-amino-1,3,3-trimethylcyclohexanemethanamine (IPDA) as hardener. Several block and grafted copolymers with a silicone part were added to the epoxy matrix or to epoxy-silicone blends, at different silicone contents. Their effect on the morphology and dispersion effectiveness was studied by scanning electron microscopy (SEM). The influence of liquid silicone inclusions on epoxy curing kinetics and on final thermomechanical properties of epoxy-modified networks was investigated using differential scanning calorimetry (DSC) and dynamic mechanical thermal analysis (DMTA). Thermal stabilities of the new formulations were analyzed by thermogravimetric analysis (TGA). Findings: The morphological evolution of epoxy-toughened networks was used to understand and explain the differences in curing kinetics and impact properties of the epoxy-modified networks with different contents of liquid silicone. Conclusion & Significance: A new strategy for preparing epoxy coatings was presented. Varying the chemical structure of silicone copolymers allows tailoring the morphology and morphological evolution of the silicone inclusions during curing and so, the impact resistance of the epoxy-silicone modified coatings.

### Biography

Daniela Rusu (M.Sci., Ph.D., HDR in Materials Science) is a Polymer Scientist at the Université de Haute-Alsace, Laboratoire de Photochimie et d'Ingénierie Macromoléculaires (LPIM), Mulhouse, France. Her research and teaching activities focuses on multiphase polymer systems (polymer blends, nanostructured materials, gels, composites...), in understanding the processing-structure-properties relationships and tailoring these complex polymer materials for targeted applications (biomedical applications, food packaging, transport, coatings...). Her current research focuses on advanced polymeric materials for coating, and biodegradable polymers for medical and industrial applications. She co-authored 10 book chapters and over 100 articles on multiphase polymer systems, in different peer-reviewed journals and proceedings. She is an active referee for peer-reviewed journals and a scientific expert for EU Framework Program Horizon 2020 for Research and Innovation.

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# MATERIALS SCIENCE AND ENGINEERING

November 13-15, 2017 | Las Vegas, USA

## Hydrogen storage characteristics of nanostructured $\text{La}_{0.75}\text{Ce}_{0.25}\text{Ni}_5$ alloy grinded by sonication process

Shrok Allami and Mutawer Redah

Ministry of Science and Technology, Iraq

$\text{La}_{0.75}\text{Ce}_{0.25}\text{Ni}_5$  alloy was purchased from Whole Win (Beijing) Materials Sci and Tech. com., Ltd. The nanocrystalline alloy was obtained by grinding the alloy powder in sonicator under different periods. Particle size distribution, surface morphology and structure were studied by laser diffraction, SEM and XRD respectively. The surface area measured by BTU method. The hydrogen storage properties were examined by PCT measurement. The enthalpy ( $\Delta H$ ) and entropy ( $\Delta S$ ) of the alloy indicate that the thermodynamic performance of the nanocrystalline alloy is improved by increasing surface area and diffusion ability of hydrogen in the nanocrystalline microstructure. Short diffusion path of hydrogen in the nanocrystalline microstructure, resulting in better overall hydrogen storage properties, improved the hydrogenation-dehydrogenation reactions of the nanocrystalline alloy. The obtained hydrogen storage capacity was 4.23% (mass fraction), and the amount of hydrogen desorption was 3.74%.

### Biography

Shrok Allami is a scientific researcher in ministry of science and technology/ renewable energy directory/ department of hydrogen and biofuel. She has completed her PhD at 2007 from University Technology, Iraq. She has published more than 25 papers in reputed journals, participates at more than 16 national and international conferences as researcher and at their committees, and has been serving as an editorial board member in Iraqi scientific journals.

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# MATERIALS SCIENCE AND ENGINEERING

November 13-15, 2017 | Las Vegas, USA

## Rational design of novel Cu-containing catalysts for effective CO<sub>2</sub> conversion

**Qiang Sun**

Peking University, China

The environmental pollution caused by massive carbon dioxide emissions has become one of the main obstacles to the national health and economic development. It is now an urgent problem to develop novel CO<sub>2</sub> conversion catalysts. According to current research, Cu electrode is reported to be the best CO<sub>2</sub> reduction catalyst among the commonly used metal electrodes. However, bulk Cu electrode is also faced with a few problems like high overpotential, poor selectivity on products and low reaction efficiency due to scaling relationships. In order to develop new Cu-based CO<sub>2</sub> reduction catalysts, we will focus on geometric optimization of low dimensional nanomaterials and study their catalytic performances. The introduction of Cu atom, Cu<sub>2</sub> dimer, Cu nanowires and nano-flakes to one or two dimensional organic or inorganic systems may bring unique catalytic characteristic and break the limits of bulk Cu electrode. These well-distributed Cu nanostructures are easier to controll and may show novel physical and chemical effects including size effect, geometric effect, substrate effect, magnetic effect, curvature effect and spatial confinement effect, which may improve CO<sub>2</sub> catalytic reduction.

### Biography

Dr. Qiang Sun is a professor at Peking University, China. His current research interest is in computational materials design for energy and environment applications. These include hydrogen storage, lithium batteries, solar energy, CO<sub>2</sub> capture and conversion.

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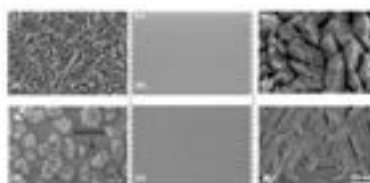
# MATERIALS SCIENCE AND ENGINEERING

November 13-15, 2017 | Las Vegas, USA

## Effect of TMAI pretreatment of sapphire substrate on the properties of MOCVD grown AlN epilayers

Talal M Al tahtamouni<sup>1</sup>, Haiding Sun<sup>2</sup>, Feng Wu<sup>2</sup>, Nasir Alfaraj<sup>2</sup>, Kuang-Hui Li<sup>2</sup>, Xiaohang Li<sup>2</sup>, Young Jae Park<sup>3</sup>, Theeradetch Detchprohm<sup>3</sup>, Russell D. Dupuis<sup>3</sup><sup>1</sup>Qatar University, Qatar<sup>2</sup>King Abdullah University of Science and Technology, Saudi Arabia<sup>3</sup>Georgia Institute of Technology, USA

The growth of high quality AlN epitaxial films relies on precise control of the initial growth stages. In this work, we investigated the influence of trimethylaluminum (TMAI) pretreatment of sapphire substrates on the properties, impurity incorporation and growth mode change of AlN films grown by metalorganic chemical vapor deposition (MOCVD). Without the pretreatment, no trace of carbon was found at AlN/sapphire interface and the residual oxygen resulted in N-polarity. With 5s pretreatments, carbon started to be incorporated, forming scattered carbon-rich zones due to the decomposition of TMAI. It was discovered that carbon attracted surrounding oxygen impurity atoms and consequently, suppressed the formation of N-polarity. With 40 s pretreatment, a significant presence of carbon clusters at the AlN/sapphire interface occurred, which attracted considerable co-existed oxygen. While preventing the N-polarity, the carbon clusters served as random masks to further induce a 3D growth mode, creating Al-polar AlN nanocolumns with different facets. The properties of AlN and epitaxial growth mode change are discussed



SEM plan-view images of morphological changes of Samples 1, 2 and 3, including (a) - (c) before and (d) - (f) after MOCVD growth, respectively

### Biography

Prof. Al tahtamouni is an associate professor at Department of Material Science and Technology in Qatar University. His research mainly concentrates on design, material growth and property study of III-nitride-based deep UV optoelectronic devices. He conducted the research on design, growth and testing of deep-UV light-emitting diodes (LEDs) and MOCVD growth of polar and nonpolar Group-III nitrides epilayers and quantum well structures. He also received many awards and honors, such as DFG Fellowship Research grant at Ulm University and Fulbright Research Award at Texas Tech University. Al tahtamouni's research work on deep ultra violet materials and device structures resulted in a series of technical publications in the world leading journals and conferences. Many of his papers have been published in Applied Physics Letters, widely considered one of the top international journals in this research area.

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# MATERIALS SCIENCE AND ENGINEERING

November 13-15, 2017 | Las Vegas, USA

## Injectable antimicrobial collagen/nanohydroxyapatite hydrogel scaffolds for bone regenerative applications

Ahmed Abd El-Fattah and Sherif Kandil  
Alexandria University, Egypt

Bone is a complex, highly organized living organ forming the structural framework of the body. It is a naturally existing composite that is composed of an inorganic mineral phase of hydroxyapatite (60% by weight) and an organic phase of mainly type I collagen. Bone defects are a serious illness that may result after a pathological process has destroyed vital components of the bone. Recently, Injectable hydrogels have been used in bone regenerative applications, because of their high tissue-like water content and moldable features. Such injectable hydrogels are of particular significance because drugs, cells, proteins, and bioactive agents can be essentially incorporated into polymer solutions before administration. In this work antimicrobial injectable hydrogel scaffolds based on a biopolymer matrix composed of collagen, reinforced with the nanohydroxyapatite (nHA), were prepared. The chemical structure, morphology, and swelling ratio as well as mechanical and viscoelastic properties of the prepared hydrogel scaffolds were investigated. For drug-release tests, gentamicin, an antibiotic drug, was entrapped within the scaffold, and the drug-release profile was examined. The results revealed that the incorporation of the nHA particles into the collagen hydrogel enhanced the mechanical and biodegradable properties and also cause a reduction in both the hydrogel porosity and swelling ratio. Furthermore, the rheological studies showed that the collagen/nHA hydrogel scaffolds is non-Newtonian viscoelastic material with more elastic dominance and exhibited higher stiffness. These properties make the injectable hydrogel of potential interest as biomimetic scaffold for bone regeneration operations in diverse applications. Consequently, this collagen/nHA hydrogel scaffold will provide an opportunity to translate lab research to the market and to apply the principles of tissue engineering in the clinical settings.



Photographs of collagen/nHA hydrogels in 3D and injectable forms (a) bulk 3D hydrogel scaffold form compressed by fingers, (b) injectable hydrogel scaffold delivered in a syringe, and (c) SEM image.

### Biography

Ahmed Abd El-Fattah research work is focused on preparing nanoparticles and nanofibers block copolymers with different architectures and compositions. Polymeric materials (hydrogel scaffold) with a range of different final properties were obtained by selecting suitable synthetic strategies. Moreover, those nano copolymers used as drug delivery systems and scaffolds for tissue engineering applications. They were loaded with various bioactive agents (antimicrobial, anticancer, and photosensitizer) and their release profiles were studied.

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### Notes: