

## Functional Thin Films and Surfaces Room Golden State Ballroom - Session CP

### Functional Thin Films and Surfaces (Symposium C) Poster Session

**CP-1 Cross-Linking Processes in Antimicrobial UV-Sol-Gel and Thermal-Sol-Gel Systems Initiated by Atmospheric Pressure Plasma Characterized by FTIR**, *Simon Chwatal (Simon.Chwatal@joanneum.at)*, *J. Lackner, W. Waldhauser*, Joanneum Research Forschungsgesellschaft GmbH, Austria; *M. Stummer*, INOCON Technologie GmbH, Austria; *H. Steiner*, Aerospace & Advanced Composites GmbH, Austria; *A. Coclite*, Graz University of Technology, Austria

The versatile adjustability of the sol-gel chemistry is a great technological advantage over other coating systems, especially due to the usability of organic and inorganic precursors as well as the variation of the reaction control and drying, curing, compaction. Alongside the many promising possibilities for producing functional coatings using the sol-gel process, challenges remain by (1) the temporal stability of sol-gel systems, (2) sensitivity of sol-gel systems to slight fluctuations in the ambient conditions during production but also processing, (3) crack formation caused by shrinkage during drying and curing, and (4) widely required curing temperatures of up to 180 °C for several minutes to hours. The last two challenges can be solved by very quick plasma curing instead of using UV or heat-based, long-lasting processes separately. Plasma combines both high and short UV and temperature impacts on the sol-gel system. INOCON Technologie GmbH has developed and patented a hot gas atmospheric pressure plasma source for exactly this purpose. In the current work, special attention is given to the atomic bonding and cross-linking processes initiated by the hot plasma and the occurring interactions. In order to better show the influence of both main plasma characteristics, a thermal and a rather new UV curing sol-gel system developed by Aerospace & Advanced Composites GmbH are used once. FTIR analyses are a base for evaluating and providing information about the intensity and position of the peaks. They also show the progress of the curing process. The hardness of the layer is an indicator of the degree of cross-linking. The harder the system, the better the atomic structures are linked together.

In addition to these studies, the antimicrobial effect of the sol-gel systems is also tested. The biocidal effect should be further enhanced by applying zinc or copper particles on the cured sol-gel layer within a subsequent process step. Alongside the experiment and optical spectroscopy, gas flow simulations, with the software ANSYS, are used to include information on the processes within the plasma, initiated by gases, flow rates, plasma jet power, and admixed precursors. Therefore, INOCON Technologie GmbH carried out a CFD-simulation model. The temperature plays an important role here, must be estimated beforehand, since critical temperatures lead to discoloration or even decomposition in the layer, and thus renders the result unusable. For this purpose, a transient thermal simulation is conducted to take the influence of the curing speed into account.

**CP-2 Crystallization and Vitrification Kinetics by Design: The Role of Chemical Bonding**, *Matthias Wuttig (wuttig@physik.rwth-aachen.de)*, RWTH Aachen University, Germany

Controlling a state of material between its crystalline and glassy phase has fostered many real-world applications. Nevertheless, design rules for crystallization and vitrification kinetics still lack predictive power. Here, we identify stoichiometry trends for these processes in phase change materials, i.e. along the GeTe-GeSe, GeTe-SnTe, and GeTe-Sb<sub>2</sub>Te<sub>3</sub> pseudo-binary lines employing a pump-probe laser setup and calorimetry. We discover a clear stoichiometry dependence of crystallization speed along a line connecting regions characterized by two fundamental bonding types, metallic and covalent bonding. Increasing covalency slows down crystallization by six orders of magnitude and promotes vitrification. The stoichiometry dependence is correlated with material properties, such as the optical properties of the crystalline phase and a bond indicator, the number of electrons shared between adjacent atoms. A quantum-chemical map explains these trends and provides a blueprint to design crystallization kinetics.

C. Persch, M. Müller, A. Yadav, N. Honne, J. Pries, S. Wei, P. Fantini, E. Varesi, F. Pelizzer, M. Wuttig, *The Role of Chemical Bonding to Design Crystallization and Vitrification Kinetics*

**CP-3 Theoretical and Experimental Study to Simplify AgZn Alloy IR Refractive Index Calculation**, *Daniel Lin (ding@labforinvention.com)*, *T. Ding, G. Ding*, Labforinvention, USA

#### Abstract

The optical refractive index and electrical resistivities of Silver Zinc alloy were studied experimentally by a co-sputtering method. The theories on alloys refractive index currently are too complex, dependent on too many factors, so it can still only be a semi-practical prediction. In this study, a new method was developed to simplify the calculation of silver alloy IR refractive index by comparing silver refractive index at the same deposition condition, specifically: (1) theoretically, the refractive index ratio  $n_{\text{alloy}}/n_{\text{Ag}}$  between silver and its alloy at IR region is assumed to cancel out most factors so that it only depends on free electron density  $n_e$  and the film resistivity  $\rho$ ; further, only dependent on alloy concentration and resistivity  $\rho$ ; (2) Experimentally, this assumption was approximately met by: the deposition conditions between sputtering Ag and its alloy were identical except the alloy with an additional tiny Zinc co-sputtering power; (3) The experimental results agreed well with this simplified calculation. Further discussions are compared with the literature on how the zinc electrons contribute to the optical and electrical properties in low Zn concentration AgZn alloy (<10%) found in this study.

**CP-6 Sputter Deposited Advanced Anode Functional Layers for Solid Oxide Fuel Cells**, *K. Steier, Justyna Kulczyk-Malecka (j.kulczyk-malecka@mmu.ac.uk)*, *P. Kelly*, Manchester Metropolitan University, UK

Solid oxide fuel cells (SOFCs) convert the chemical energy stored in fuels, such as hydrogen and gaseous hydrocarbons, directly into electrical power and thermal energy through electrochemical reactions. State-of-the-art SOFC anodes consist of a cermet of nickel and yttria-stabilised zirconia (YSZ) to increase the reactive sites at the anode/electrolyte interface.

Nanostructured Ni-YSZ functional layers has been produced using reactive pulsed DC magnetron co-sputtering of metallic targets of zirconium-yttrium and nickel. Whilst recent studies show the deposited Ni-YSZ films from a single Ni-YSZ compound target, we present the co-deposition from decoupled Ni and Zr-Y targets, which allows the deposition of Ni-YSZ with a graded composition of nickel within the structure.

The sputtering process was performed in an oblique angle deposition mode, to deliberately generate columnar nanostructures, in mixed argon/oxygen atmospheres. Deposition parameters, such as deposition angle and deposition pressure have been studied to determine their influence on the structural and morphological properties in the context of their application as SOFC anode functional layers. The obtained films were characterised by SEM, EDS and XRD. We found that sputter deposited YSZ films led to a higher porosity within the YSZ scaffolds with increasing deposition angle and pressure. During the co-sputtering of Ni and Zr-Y, Ni was oxidised to NiO and then subsequently transformed to catalytically active nickel during the reduction in hydrogen, facilitating the required porosity for the gas transport.

Furthermore, two designs of Ni-YSZ anodes were deposited onto a spark plasma sintered YSZ electrolyte-supported button cell coupled with a commercial LSM cathode. The first design used a constant Ni composition and the second comprised of a graded Ni content within the structure. Finally, both configurations have been tested in fuel cell mode under hydrogen and air flows for anode and cathode, respectively, to characterise the performance of the functional layers.

**CP-8 Unraveling the Bisignate and Broadband Chiroptical Response from All-Dielectric Distorted L-Shape Metamaterials**, *Ufuk Kilic (UFUKKILIC@UNL.EDU)*, *M. Hilfiker, S. Wimer, A. Ruder, E. Schubert, C. Aryropoulos, M. Schubert*, University of Nebraska-Lincoln, USA

With a broad variety of nanofabrication technologies available, structures with different morphologies and subwavelength scale dimensions were proposed as strong candidates to manipulate light from visible to infrared spectral regions. [1,2]. Of particular interest, all-dielectric three-dimensional nanostructures have been frequently reported as prominent contestants which can tackle both the lossy nature of metals and the insufficient broadband chiral response of their planar thin film configurations [1,3].

Here, we propose a simplistic chiral nano-platform: all-dielectric distorted L-shape metamaterials so-called *nanoboomerangs*. Thanks to glancing angle deposition, a recently emerging bottom-up fabrication technique with precise sample stage manipulation ability, we successfully assembled achiral silicon columnar structures and fabricated three-dimensional, highly

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porous, superlattice-type, distorted L-shape metamaterial. Using Mueller matrix generalized spectroscopic ellipsometry technique, we performed the chiroptical characterization of the *nanoboomerangs* which exhibit extremely broadband, large, tunable, and bisignate chiroptical response. We believe that this new metamaterial platform can be a strong candidate for a myriad of next generation photonic integrated technological applications including but not limited to chiral sensors, drug-delivery systems, and chiral-topological insulators.

## References:

1. Kilic, U., *et al.*, *Advanced Functional Materials*, 31(20), 2010329, (2021).
2. Kilic, U. *et al.* *Sci. Rep.* 7:1–11(2019).
3. Yang, X. *et al.* *Sci. Rep.* 7:1:1-9 (2017).

**CP-10 Microstructured Electrodeposition of Copper Templated by Photo-Induced Monolayer Patterning, David Sconyers (david.j.sconyers2.civ@army.mil), C. Longo, J. Maurer, US Army DEVCOM AC, Benet Laboratories, USA**

Materials presenting surfaces with antiviral or antibacterial properties represent a growing area of interest due to the threat of future global pandemics. Surface morphologies that are hostile to the adhesion and replication of microorganisms are a commonly employed defense system found in nature. Defined textures and patterns of this kind can be emulated artificially via directed electrodeposition of transition metals from aqueous solutions onto electrically conductive substrates relevant to human use. Here, we carry out the electrochemical generation of such surfaces, driven by the selective coating of self-assembled monolayers (SAMs) of alkylphosphonates and alkoxy silanes onto mild steel. Photo-induced monolayer patterning (PIMP) subsequently generates defect sites in these engineered coatings, characterized through Fourier-transform infrared spectroscopy (FTIR), matrix-assisted laser desorption/ionization time-of-flight mass spectrometry (MALDI-TOF) and contact angle (CA) measurements. The exposed steel at these defect sites provide points of nucleation for the electrochemical reduction of copper, and have been shown to generate deposits that exhibit variable microstructure.

**CP-12 Ag Segregation in Co-sputtered ZrCuAlNi:Ag Thin Films, M. Steinhoff, D. Holzapfel, S. Karimi Aghda, D. Neuß, P. Pöllmann, M. Hans, RWTH Aachen University, Germany; D. Primetzhofer, Uppsala University, Sweden; J. Schneider, Clio Azina (clioazina@gmail.com), RWTH Aachen University, Germany**

The development of nanocomposites opens the door for new functional materials which combine the properties of two or more constituents. Herein, we report on the formation of Ag-reinforced thin film metallic glass nanocomposites by a hybrid direct-current magnetron sputtering and high-power pulsed magnetron sputtering process. The effects of Ag-content, substrate temperature and substrate bias potential on the phase formation and morphology of the nanocomposites were investigated.

While applying a substrate bias potential did not strongly affect the morphological evolution of the nanocomposites, the Ag content dictated the size and distribution of Ag surface segregations, while the bulk of the film remained featureless. However, at higher substrate temperatures, increased Ag contents led to the formation of lamellar-shaped Ag segregations in the bulk and that of a polycrystalline Ag layer at the surface, both of which were due to thermally enhanced surface diffusion.

The electrical resistivity of the produced nanocomposites was strongly affected by the segregations as a significant decrease was observed for the dual-phase systems, supporting the combination of properties of the metallic glass matrix and metallic reinforcement.

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