

## DS 6: Thin Film Applications

Time: Monday 15:00–18:15

Location: H 0111

DS 6.1 Mon 15:00 H 0111

**Chalkopyrite thin film solar cells conditioned with RbF** — ●TIM KODALLE<sup>1</sup>, MARC DANIEL HEINEMANN<sup>1</sup>, HASAN ARIF YETKIN<sup>1,2</sup>, IVER LAUERMAN<sup>1</sup>, RUTGER SCHLATMANN<sup>1,3</sup>, and CHRISTIAN ALEXANDER KAUFMANN<sup>1</sup> — <sup>1</sup>PVcomB/Helmholtz-Zentrum Berlin, Germany — <sup>2</sup>Technical University Berlin, Germany — <sup>3</sup>Hochschule für Technik und Wirtschaft Berlin, Germany

We investigate the impact of an RbF post deposition treatment (PDT) on the material and device properties of Cu(In,Ga)Se<sub>2</sub> thin-film solar cells in dependence of both the PDT's parameters (e.g. the duration of the PDT) and the copper to group III elemental ratio ( $[\text{Cu}]/([\text{Ga}]+[\text{In}]) = \text{CGI}$ ).

A clear trade-off between increasing open-circuit-voltage ( $V_{\text{OC}}$ ) and decreasing fill factor ( $FF$ ) with longer RbF-deposition could be observed. We propose a model explaining the gain in  $V_{\text{OC}}$  by an increased carrier concentration and the formation of an (Rb,Na)-In<sub>x</sub>Se<sub>y</sub> surface layer during the PDT. Additionally we build a model to explain the decreasing  $FF$  based on the generation of additional acceptor-like defects at the buffer/window-interface by temperature-induced alkali-migration during sputtering of the window layer.

Furthermore we investigate the performance of the optimized PDT on absorbers with varied CGI. Here we find, that the PDT is most efficiently when being applied to thin films close to stoichiometry. Thereby we were able to overcome the  $FF$ -loss and increase the maximum efficiency up to 17.5%, which is about 1.1% (abs.) higher than the reference value.

DS 6.2 Mon 15:15 H 0111

**Metal thin films as plasmonic support for surface enhanced vibrational spectroscopy and optofluidics** — ●DIMITRA GKOGKOU, CHRISTOPH KRATZ, NORBERT ESSER, EUGEN SPEISER, and KARSTEN HINRICHS — Leibniz-Institut für Analytische Wissenschaften -ISAS- e.V., Department Berlin, Schwarzschildstr. 8, 12489 Berlin, Germany

We present metal nanosland films that exhibit plasmonic resonances in the visible and infrared region of the spectrum. These different resonances correspond to adjacent areas of an Au gradient layer and provide surface enhanced Raman scattering (SERS) and surface enhance infrared absorption (SEIRA) signals, dependable on the thickness of the layer. In that way, all vibrational information of an adsorbed molecule can be acquired by a line scan on a single substrate. Also presented is the integration of this combinatorial substrate with a microfluidic setup that allows for the in-situ investigation of  $\mu\text{L}$  volumes. Ultra low detection limits of analytes were achieved, i.e. submonolayer sensitivity demonstrated in situ for monolayer self-assembly.

The presented optofluidic platform is a sensing device that has possible applications in sensitive and label-free biosensing, lab-on-a-chip devices, or molecular imaging tools for biochemical analyses.

DS 6.3 Mon 15:30 H 0111

**Fully sprayed, ITO-free, flexible organic solar cells** — ●MARIUS LOCH<sup>1</sup>, FLORIN LOGHIN<sup>1</sup>, KAMYAR BAGHVAND<sup>1</sup>, PAOLO LUGLI<sup>2</sup>, and MARKUS BECHERER<sup>1</sup> — <sup>1</sup>Lehrstuhl für Nanoelektronik, Technische Universität München, Theresienstrasse 90, 80333 Munich, Germany. — <sup>2</sup>Faculty of Science and Technology, Free University of Bozen-Bolzano, Universitätsplatz 5, 39100 Bolzano, Italy

Organic solar cells are a promising candidate for a future of ubiquitous, low-cost solar power harvesting. While this promise is founded on easily scalable, large-area solution processing techniques, most of the scientific research community uses small-scale deposition methods convenient for the lab like spin coating in inert atmosphere and vacuum processing, which are not scalable. In this work, we use an automated spray roboter in ambient conditions to deposit all layers of the solar cell (reflective electrode, transparent electrode, active material blend and blocking layers). The layers are independently optimized and eventually put together in one fully sprayed device. By replacing brittle and expensive indium tin oxide (ITO) with silver nanowires (AgNW) and conductive polymers (PEDOT:PSS) for the transparent electrode, the use of flexible foil substrates is enabled and mechanical stability is studied by bending tests.

DS 6.4 Mon 15:45 H 0111

**Effect of cation stoichiometry on electric properties of thin-film varactors with Ba<sub>x</sub>Sr<sub>1-x</sub>TiO<sub>3</sub> tunable dielectric and highly conducting SrMoO<sub>3</sub> electrodes** — ●LUKAS ZEINAR<sup>1</sup>, PATRICK SALG<sup>1</sup>, ALDIN RADETINAC<sup>1</sup>, DOMINIK WALK<sup>2</sup>, PHILIPP KOMISSINSKIY<sup>1</sup>, HOLGER MAUNE<sup>2</sup>, ROLF JACOBY<sup>2</sup>, and LAMBERT ALFF<sup>1</sup> — <sup>1</sup>Materials Science, TU Darmstadt, Germany — <sup>2</sup>Microwave Engineering and Photonics, TU Darmstadt, Germany

We present Au/Pt/Ba<sub>x</sub>Sr<sub>1-x</sub>TiO<sub>3</sub>/SrMoO<sub>3</sub> varactor heterostructures utilizing single crystalline Ba<sub>x</sub>Sr<sub>1-x</sub>TiO<sub>3</sub> films grown epitaxially by pulsed laser deposition on a highly conducting thin\*film oxide SrMoO<sub>3</sub> bottom electrodes with a room-temperature resistivity of 30  $\mu\Omega\text{cm}$ . The stoichiometry of the dielectric Ba<sub>x</sub>Sr<sub>1-x</sub>TiO<sub>3</sub> was tuned to achieve the desirable high tunability and low losses of the varactors at room temperature. Influence of the cation stoichiometry of the Ba<sub>x</sub>Sr<sub>1-x</sub>TiO<sub>3</sub> films on their Curie temperature and room-temperature dielectric permittivity was investigated. The changes of the Ba<sub>x</sub>Sr<sub>1-x</sub>TiO<sub>3</sub> out-of-plane lattice parameter by 2% and the corresponding changes of the Ba-Sr and (Ba,Sr)-Ti cation ratios by 6 and 11%, respectively, were observed by varying the laser energy fluence in the range between 0.3 and 1.4 J/cm<sup>2</sup>. Tunability and leakage current of the varactors were investigated by a vector network analyzer at frequencies between 300 MHz and 10 GHz. Fine tuning of the Ba<sub>x</sub>Sr<sub>1-x</sub>TiO<sub>3</sub> cation stoichiometry allows high relative tunability of the varactors up to 80% and reduction of the varactor leakage current by up to three orders of magnitude down to 10 nA.

DS 6.5 Mon 16:00 H 0111

**The Influence of Crystallographic Order on Ferrimagnetic Response of Spinel ZnFe<sub>2</sub>O<sub>4</sub> Thin Films** — ●VITALY ZVIAGIN, YOGESH KUMAR, CHRIS STURM, ISRAEL LORITE, PABLO ESQUINAZI, MARIUS GRUNDMANN, and RÜDIGER SCHMIDT-GRUND — Universität Leipzig, Felix-Bloch-Institut für Festkörperphysik, Linnéstr. 5, Leipzig

We present the dielectric function of normal spinel ZnFe<sub>2</sub>O<sub>4</sub> (ZFO) grown at different pressures and temperatures on SrTiO<sub>3</sub> (100) substrate by pulsed laser deposition. Electronic transitions visible in the diagonal element of the dielectric tensor are assigned to transitions involving Fe<sup>2+</sup>, Fe<sup>3+</sup> and Zn<sup>2+</sup> cation 3d and 4s orbitals. Transitions from O<sub>2p</sub> to tetrahedrally coordinated Fe<sup>3+</sup> cation, located at  $\sim 3.5\text{eV}$ , and between octahedrally coordinated Fe<sup>2+</sup> cations, located at  $\sim 0.9\text{eV}$ , give evidence to disorder in the normal spinel structure. Growth temperature dependent investigation has shown a direct correlation between saturation magnetization at 5 K and the amplitude of the former mentioned transition, likely due to the dominant nature of the oxygen mediated coupling between Fe<sup>3+</sup> located on two different lattice sites.[1] Annealing films at temperatures greater than 250 °C in argon and oxygen atmospheres facilitates a decrease in the ferrimagnetic response and is explained by reordering of the disordered spinel structure toward ordered normal state. A direct correlation between the disorder cation transition contributions to the dielectric function and room temperature ferrimagnetic response is shown.

[1] V. Zviagin et al., Appl. Phys. Lett. **108**, 13 (2016)

DS 6.6 Mon 16:15 H 0111

**Unsupervised Hebbian learning experimentally realized with analogue memristive crossbar arrays** — ●FINN ZAHARI, MIRKO HANSEN, HERMANN KOHLSTEDT, and MARTIN ZIEGLER — Chair of Nanoelectronics, Faculty for Electrical Engineering and Information Technology, Kiel University, Germany

Memristive devices are promising candidates to emulate synaptic behaviour in neuromorphic circuits in an efficient manner. Even though in the last couple of years a variety of materials and device structures were employed to fabricate memristive devices, there is still a gap between promising computing schemes and their hardware realization with memristive devices. We show that so called double barrier memristive devices can be integrated into crossbar architectures without the need for additional selector devices. These ionic memristive devices show a non-filamentary interface-based resistive switching behaviour with a high I-V nonlinearity and asymmetry as well as self-rectifying and self-limitation characteristics. They are used to realize selector-device-free 16x16 crossbar-arrays with 256 memristive devices. A local Hebbian learning scheme was utilized to perform unsupervised learning of visual patterns to demonstrate the applicability of the selector-free

crossbars within a mixed signal circuit consisting of double barrier memristive devices as hardware synapses und software neurons.

Financial support by the German Research Foundation through FOR 2093 is gratefully acknowledged.

### 15 min. break.

DS 6.7 Mon 16:45 H 0111

**Bottom-up Synthesis and Characterization of Mesoporous Al-Modified Hematite Thin Film Photo-Anodes** — ●AHMED CHNANI and STEFFEN STREHLE — Ulm University, Institute of Electron Devices and Circuits, Albert-Einstein-Allee 45, 89081 Ulm

Hematite ( $\alpha$ -Fe<sub>2</sub>O<sub>3</sub>) is an earth abundant, low-cost and non-toxic n-type semiconductor being in the research focus for the assembly of efficient photo-anodes in the field of solar fuel production by water splitting. Despite a suitable band structure and sufficient water splitting stability, there are various critical issues that need to be resolved including for instance the short charge carrier lifetime that is significantly misaligned with the optical absorption length, an overall low electrical conductivity as well as a low surface charge transfer kinetics.

In this paper, aluminium is added to hematite as a sustainable strategy to reduce the defect state density while simultaneously increasing the charge carrier concentration. For the studies, thermally evaporated Fe(Al) thin films with roughly 200 nm in thickness were utilized. By rational control of a plain thermal oxidation process under ambient conditions, non-porous to mesoporous Al-modified hematite thin films were prepared. The experiments show that mesoporous thin films show not only efficient light trapping but also an overall increased electrical conductivity and an increased photoactivity in comparison to non-porous thin films, plain hematite electrodes and even in comparison to high-density hematite nanowire arrays. The complete surface band structure was reconstructed to evaluate the surface defect states by utilizing a Kelvin probe as well as ambient photoelectron spectroscopy.

DS 6.8 Mon 17:00 H 0111

**Large-scale self-assembling of nanostructures by controlled dewetting of ultra-thin silicon films on insulators** — ●MARCO SALVALAGLIO<sup>1</sup>, RAINER BACKOFEN<sup>1</sup>, MEHER NAFFOUTI<sup>2,3</sup>, THOMAS BOTTEIN<sup>2</sup>, MARIO LODARI<sup>4</sup>, THOMAS DAVID<sup>2</sup>, ABDELMALEK BENKOUIDER<sup>2</sup>, IBTISSEM FRAJ<sup>3</sup>, LUC FAVRE<sup>2</sup>, ANTOINE RONDA<sup>2</sup>, ISABELLE BERBEZIER<sup>2</sup>, DAVID GROSSO<sup>2</sup>, MARCO ABBARCHI<sup>2</sup>, MONICA BOLLANI<sup>4</sup>, and AXEL VOIGT<sup>1</sup> — <sup>1</sup>TU-Dresden, 01062 Dresden, DE — <sup>2</sup>CNRS - IM2NP, 13397 Marseille, FR — <sup>3</sup>Université de Monastir, 5019 Monastir, TN — <sup>4</sup>IFN-CNR, L-NESS, 22100 Como, IT

Thin solid films are rarely stable when annealed even below their melting temperature. Under the action of surface diffusion, atoms move away from the edges of thin films leading to their retraction and breaking. This process occurs in ultra-thin silicon films on insulator (UT-SOI), limiting their applications in several microsystems. Moreover, the self-assembled structures forming at the end of the process show too large randomness in positioning and size dispersion to be exploited for targeted applications. Here, thanks to a synergistic theoretical and experimental investigation, we illustrate a method to control the dewetting of UT-SOI, delivering nanostructures with determined positions, sizes and shapes [1]. 3D phase-field (PF) simulations, accounting for surface diffusion-limited kinetics, are adopted to enlighten the mechanism underlying the process and assess the outcomes of experiments. Indeed, we demonstrate that a fine control over the final structures is achieved when combining patches with an ad hoc initial patterning of the thin film. [1] M. Naffouti et al., Science Adv. 3, eaao1472 (2017).

DS 6.9 Mon 17:15 H 0111

**Growth of large sized 2D molybdenum sulfide flakes at the air-liquid interface** — XIAOLING ZENG, TALHA NISAR, MARLIS ORTEL, ●TORSTEN BALSTER, and VEIT WAGNER — Jacobs University Bremen, Campus Ring 1, 28759 Bremen, Germany

Layered transition metal chalcogenides, especially MoS<sub>2</sub>, are promising materials for catalysis as well as semiconducting layers in thin film transistors. Since the 1st transistors were produced with mechanically exfoliated MoS<sub>2</sub> flakes, new deposition processes for large area and atomically thin layers are needed to enable new generation electronic devices.

In this investigation, we have developed a cheap, wet chemical deposition process, which takes advantage of growth on a liquid surface. For this purpose, a saturated solution of ammonium tetrathiomolybdate

(ATTM) in deionized water was prepared by heating and ultrasonication. After two hours of cooling period molybdenum sulfide flakes were formed in solution at the air-liquid interface with a lateral size of more than 150 μm. These flakes were transferred onto a SiO<sub>2</sub>/Si substrate in a Langmuir-Blodgett like deposition process. The thickness of the flakes ranged from a single monolayer to 5 monolayers as confirmed by AFM and Raman spectroscopy. XPS and TEM reveal, that with post growth thermal treatment flakes of high quality are obtained.

DS 6.10 Mon 17:30 H 0111

**Magnetron sputtered refractory metal thin films on NiTi and their influence on the phase transition behaviour of NiTi** — ●FABIAN SEIFRIED<sup>1</sup>, HELMUT RIEDEL<sup>2</sup>, HARALD LEISTE<sup>1</sup>, RUTH SCHWAIGER<sup>1</sup>, SVEN ULRICH<sup>1</sup>, HANS JUERGEN SEIFERT<sup>1</sup>, and MICHAEL STUEBER<sup>1</sup> — <sup>1</sup>KIT IAM-AWP, Eggenstein-Leopoldshafen, Germany — <sup>2</sup>TU Wien WWWT, Wien, Austria

In this study, pseudo-elastic Ni 50.8 at.%-Ti alloy sheets of 1000 microns thickness were coated with 10 microns thick refractory metal thin films, by non-reactive d.c. magnetron sputtering. These thin films were characterized with regard to their microstructure and selected mechanical properties. Microstructural characterization of the thin films included X-Ray Diffraction and Scanning Electron Microscopy analyses. Mo thin films grow in a densely packed, (110) textured b.c.c. structure with columnar grains on the NiTi substrate. Ta and Nb thin films grow as well in a dense columnar structure; however they show X-Ray diffraction peaks of various lattice planes of the b.c.c. structures (i.e. no texture). Considering the specific thin film/substrate thickness ratio (1:100) of the samples, the mechanical properties of both the thin films and thin film/substrate composites were investigated on different length scales, using nano- and microindentation techniques. To evaluate the potential impact of the surface coating and the deposition process on the phase transformation behaviour of the NiTi shape memory alloy, differential scanning calorimetry analyses were done. Conclusions and recommendations will be given for potential thin film materials as radiopaque coatings on NiTi substrates for medical applications.

DS 6.11 Mon 17:45 H 0111

**Focused electron beam induced multi-tip deposition for energy harvesting from the green-house radiator.** — ●KOOBS HANS WILFRIED PETER — Ernst Ludwig Strasse 16, Ober-Ramstadt, Germany

A cross-lines grid with 0,5 μm cell-width is proposed to harvest IR radiation from the green house gases in the earth atmosphere. According to NASA-measurements 340 W/m<sup>2</sup> reach the earth in the IR-regime. A nanogranular Pt/C material can be used in a detector-matrix to harvest this energy, by collecting IR quanta with nanocrystalline Pt/C compound material in form of electron-hole Bosons. Very large numbers of Bosons can be stored in such energy layers. Applying a field gradient allows to move the Bosons to the end of the material layer, where the Bosons release an electron each, and the resulting hole can form a new Boson again. Electrons are emitted in a coherent fashion. The small-area experiment shall prove the principle of the energy harvesting capability. Large areas of collector fields shall follow, built with the principle of glass coating machines with massive parallel ion beam sources to deposit the Pt/C absorber structure layers.

DS 6.12 Mon 18:00 H 0111

**Modelling of the vertical deflection of ferroelectric bending tongues** — ●JULIETTE CARDOLETTI<sup>1</sup>, ALDIN RADETINAC<sup>1</sup>, JULIAN WALKER<sup>2</sup>, PHILIPP KOMISSINSKIY<sup>1</sup>, SUSAN TROLIER-MCKINSTRY<sup>2</sup>, and LAMBERT ALFF<sup>1</sup> — <sup>1</sup>Technische Universität Darmstadt, Institute of Materials Science, Alarich-Weiss-Straße 2, 64287 Darmstadt, Germany — <sup>2</sup>Materials Research Institute, Pennsylvania State University, University Park, PA, 16802, USA

With the acute need for miniaturisation of devices and components, the use of bending tongues (cantilevers or wider beams) based on piezoelectric ceramics is increasing. Due to its large piezoelectric coefficient, PbZr<sub>0.52</sub>Ti<sub>0.48</sub>O<sub>3</sub> (PZT) is the most commonly used material, but it is also ferroelectric (i.e. the polarisation direction can be switched between discrete crystallographically allowable orientations by an external electric field). This particularity should be taken into account when modelling the vertical deflection of bending tongues.

To date, bending tongue based devices have been modelled from a static and dynamic point of view without simulating the ferroelectric switching occurring in grains [1]. However, various papers attempted to describe ferroelectric switching based on different approaches, for ex-

ample based on a switching criterion accounting for mechanical work and electrical work contributions to the switching process [2].

The here described modelling program, based on Hwang's switching

criterion [2], aims to bridge the gap between the previous approaches by describing the vertical deflection of a bending tongue while taking into account ferroelectric switching at the grain scale.