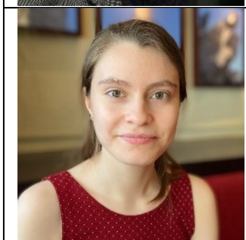
VÁCUO 2023
Workshop

June 30, 2023
Anfiteatro VA1, Pavilhão de Engenharia Civil, Instituto Superior Técnico (IST), Avenida Rovisco Pais, Lisboa

The **VÁCUO 2023 Workshop** aims to bring together Portugal-based scientists in an intimate meeting that promotes discussion on deposition methods, materials synthesis and characterization techniques using vacuum technologies. The 2023 edition will be held on Friday June 30 between 2-6 pm at IST, Lisbon. The topics of the Workshop will focus on solar cells, plasma effects on surfaces, ion implantation, hydrogen leak detectors, tribological and decorative coatings for the industry, biomedical coatings, metal-semiconductor-metal structures membranes, amongst other topics.

Programme:

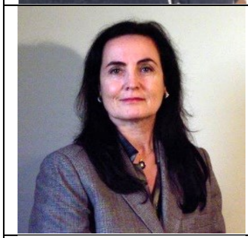
14:00–14:05 **Foreword:** Carlos Tavares, *SOPORVAC*

	14:05-14:20 **Decorative coatings on plastic parts.** *Martin Andritschky* Physics Department, University of Minho
	14:20–14:35 **Leaking in cork stoppers** *Carolina Adame* CEFITEC, Department of Physics, Nova School of Science and Technology
	14:35-14:50 **Systems for the deposition of magnetic heterostructures (sensors and memories)** *Paulo Freitas* INESC MN, University of Lisbon

14:50-15:05

Study of the Biofunctionalization of Alumina for Implants

Mikhael Rodarte
CEMMPRE, Department of Mechanical Engineering, University of Coimbra
Department of Mechanical Engineering, Federal University of São João del Rei



15:05-15:20

Ultrathin oxides and atomically sharp interfaces: in-situ surface/interface studies

Ana Cristina Silva
CEFITEC, Department of Physics, Nova School of Science and Technology

15:20-15:35

Optimisation of Ga_2O_3 membrane based MSM structures for optical and electronic sensors

Miguel Pedro
INESC MN, University of Lisbon

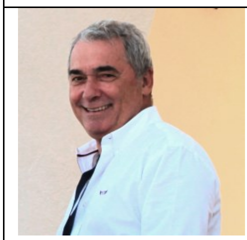
15:35-15:55

The effect of target-substrate distance and deposition pressure on the properties of W-S-C coatings deposited by magnetron sputtering

Albano Cavaleiro
CEMMPRE, Department of Mechanical Engineering, University of Coimbra

COFFEE BREAK

15:55-16:15



16:15-16:30

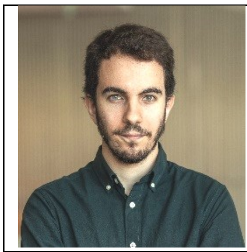
Study of aluminosilicate films co-doped with (Tb^{3+}, Er^{3+}) / Yb^{3+} by ion implantation

Eduardo Alves
Instituto de Plasmas e Fusão Nuclear, Instituto Superior Técnico, Universidade de Lisboa

16:30-16:45

Atomic wall recombination in oxygen-containing plasmas

Pedro Viegas
Instituto de Plasmas e Fusão Nuclear, Instituto Superior Técnico, Universidade de Lisboa

	16:45-17:00 **The Impact of High-Performance Transparent Substrates on Bifacial Solar Cells Performance** *André Violas* INL – International Iberian Nanotechnology Laboratory, Braga
	17:00-17:15 **Fabrication and Optimization of Intrinsic/Doped a-Si:H Layers for High-Efficiency HIT Solar Cells** *Ghulam Abbas* CENIMAT|i3N, Department of Materials Science, NOVA School of Science and Technology
	17:15-17:30 **Bacterial adhesion on sputter-deposited a-C:H:N coatings for Orthodontics** *António Frois* CEMMPRE, Department of Mechanical Engineering, University of Coimbra
	17:30-17:45 **Traceability of Hydrogen Leak Detectors** *Orlando Ferreira* CEFITEC, Departamento de Física da Faculdade de Ciências e Tecnologia da Universidade Nova de Lisboa
	17:45-18:00 **Experimental and numerical study of the reaction pathways in low-pressure CO_2-CH_4 glow discharges** *Tiago Silva* Instituto de Plasmas e Fusão Nuclear, Instituto Superior Técnico, Universidade de Lisboa

www.soporvac.pt

VÁCUO 2023

BOOK OF ABSTRACTS

Decorative coatings on plastic parts

Martin Andritschky[1], Jorge Ferreira[2]

[1] *Centro de Física, Universidade do Minho, Portugal*
[2] *KLC* Marinha Grande, Portugal
**corresponding author: martin.andritschky@fisica.uminho.pt*

The colour of a decorative coating is the first and most important feature. Optical interference coatings allow the production of all rainbow colours. In contrast to most paints or lacquers those colours are also very lively. On the other hand, interference colours are part of an optical stack consisting in a substrate, a reflective metal layer, a transparent layer and, in most cases necessary, a transparent protective layer. Frequently the substrate is injection moulded and to hide surface defects require a base coat. Within the frame of this work we are using a transparent PC as substrate, a transparent UV cured laquer as base coat, Ti metal layer which serves both as an adhesion and as an optically reflective layer, TiO_2 as transparent interference layer and SiO_2 as transparent protective layer. The optical properties n_{Ti} and k_{Ti}, n_{TiO2}, t_{TiO2} and n_{SiO2}, t_{SiO2} (k_{TiO2} and k_{SiO2} are frequently very small), where by n being the refractive index, k the extinction coefficient and t the thickness of the respective material. Within the frame of this work, we deposited Ti and TiO_2 by reactive magnetron sputtering and SiO_2 by PECVD with HMDSO as a precursor. It is almost impossible to predict the colour of a three-layer coating experimentally, therefore, we determined the optical properties of each layer individually, determined the deposition rate experimentally and simulated the reflectivity of the coating. Fig. 1 shows the optical properties of the three materials Ti, TiO_2 and SiO_2.

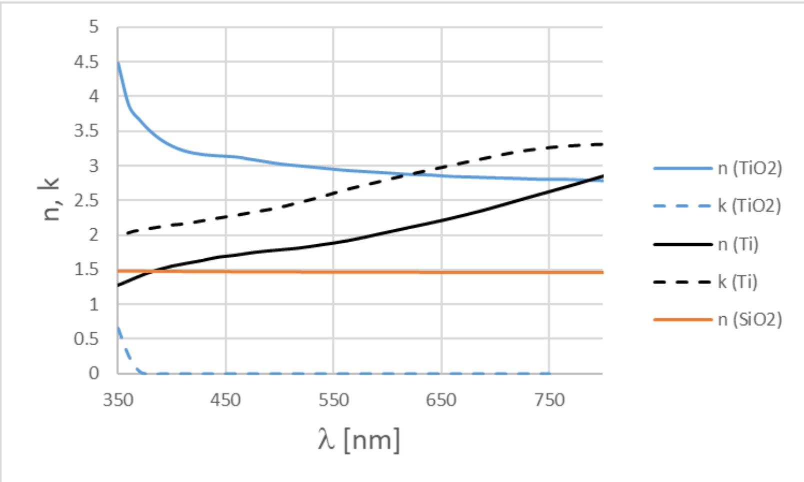


Figure1 - Optical properties n, k =f(l) of the 3 layers employed in the simulation.

Based on these characteristics the specular reflectance of three coating was simulated, as shown in Fig. 2. The first stack consisting in a Ti layer and a 145 nm thick TiO_2 layer and the second in the same layers with an additional 150 nm SiO_2 protective.

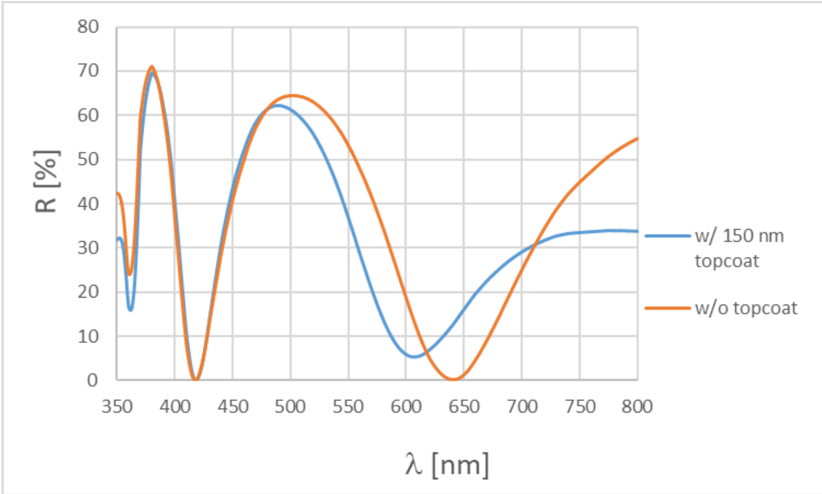


Figure 2 - Reflectance spectra of Ti + 145nm TiO_2 w/ and w/o a protective 150 nm SiO_2 topcoat.

The main reflectance intensity is found in the configuration indicated for wavelengths in the greenish part of the light spectrum.

Fig 3a shows a photo of the stack deposited on top of a molded transparent PC part. At the edges of the samples the coating deposition was not uniform, resulting a thinner TiO_2 layer, giving origin to bluish shades.

a) b)

Figure 3 - a) Photo of a transparent PC sample with Ti + 145nm TiO_2 w/ 150 nm SiO_2 topcoat.
b) Photo of a transparent PC sample with Ti + 105 nm TiO_2.

Conclusions

Very intense and lively coloured coatings can be produced by optical interference coatings. The intensity is related to the refractive index of the transparent (TiO_2 oxide) layer. SiO_2 protective layers can be deposited on top of the transparent TiO_2 layer without causing, when choosing the right thickness, significant changes to the colour of the optical stack. The coating colour is very sensitive to variations of the optical thickness. The coatings require a tight control of the deposition conditions to guarantee reproducibility. Coating of 3 D parts is therefore problematic.

Leaking in cork stoppers

Carolina Adame*, Orlando Teodoro

CEFITEC, Department of Physics, Nova School of Science and Technology, 2829-516 Caparica, Portugal
**Corresponding author e-mail: c.adame@campus.fct.unl.pt*

The passage of gas through a cork stopper in a wine bottle is an important factor to be considered in wine conservation. Excessive intake of oxygen into the bottle can spoil wines by oxidation. Preliminary studies on the permeability of cork suggest that the gas transference in wine bottles might not be entirely due to gas passing through the bulk of the cork stopper, but also due to lateral leaks in the bottleneck/cork stopper interface.
Typically, cork stoppers used in wine bottles receive surface treatments with paraffin and silicones, mainly to reduce friction during the insertion of the cork into the bottle. However, the effect of these treatments on possible lateral leaks is not well understood.
In this work, vacuum metrology techniques were applied to study the transmission of gases in cork stoppers in bottlenecks. Empty bottles were sealed with natural and micro-granulated cork, with and without surface treatments. The bottlenecks were cut off the bottles and mounted on a homemade apparatus built to apply a He to the "outside" of the bottleneck, and the gas crossing the bottleneck was detected and quantified by He mass spectrometry.
Sealing compounds were applied to the interface in cork stoppers with higher leak rates, reducing the leak rate by an order of magnitude, and confirming that these leak rates are due to interface leaks.
The comparison of leak rate data of natural cork stoppers of the same quality with and without surface treatments revealed that the surface treatments are determining in the sealing of bottles, with the untreated cork stoppers presenting leak rates well above those admissible for wine storage, while the majority of surface treated cork stopper having leak rates below the detection limit of the equipment employed.

Study of the Biofunctionalization of Alumina for Implants

M. Rodarte[1*], D. Santo[2], D. Cavaleiro[2], R. Balestra[1], S. Carvalho[2,3]

[1]Department of Mechanical Engineering, Federal University of São João del Rei
[2]CEMMPRE, Mechanical Engineering Department, University of Coimbra, 3030-788 Coimbra, Portugal
[3]Laboratory of Tests, Wear and Materials, IPN, LED & MAT—Instituto Pedro Nunes, Rua Pedro Nunes, 3030-199 Coimbra, Portugal
*Corresponding author e-mail: mikhaelbrener@hotmail.com

Implants play a crucial role in improving quality of life, allowing individuals to restore lost function or enhance capabilities. Alumina is a bioceramic widely used in medicine due to its bioinert characteristics, biocompatibility and good mechanical compression properties. Scaffolds can have interconnected and well-distributed porous structures that favor bone/implant adhesion due to tissue growth within the pores. The biomimetic method can be used to cover alumina scaffolds with a bioactive layer of hydroxyapatite (HAp), a calcium phosphate that contributes to bone regeneration. In this study, the objective was to create porous samples that presented osseointegration capacity and non-inflammatory characteristics. Such samples showed biological properties due to HPa crystals that grew due to the biomimetic bioative layer.

Futhermore by deposition of silver (Ag) and silver oxide (AgO) by magnetron sputtering is possible to achieve a surface with antimicrobial activity. Indeed, it is well known that Ag and AgO have important bactericidal properties that reduce inflammatory reactions. Porous alumina pellets were produced using ammonium bicarbonate as a pore former, and the samples were mixed, compacted, and sintered, resulting in a porosity of 55%. The biomimetic layer was performed by immersing the samples in a simplified solution (SS) of calcium chloride dihydrate and disodium phosphate dihydrate. Then, the samples went through the Ag and AgO NPs deposition process, resulting in layers with thicknesses of 50 nm and 100 nm, respectively. We performed bioactivity assays by immersing the samples in Simulated Body Fluid (SBF) to assess HAp growth on the coating. Throughout the process, SEM and EDS analyzes were carried out, in addition to wettability and microbiological tests. We conclude that the sample production method was effective, observing a greater growth of HAp after the bioactivity test. In addition, microbiological tests demonstrated inhibition of microbial growth in the coated samples compared to the samples without the metallic coating. Therefore, we can conclude that this work is extremely important in the search for more effective production methods for materials used in implant dentistry, considering the essential biological characteristics necessary for this purpose.

References

[1] ANDRETO, C. A. Estudo Da Produção De *Scaffold* De Alumina Revestido Por Fosfato De Cálcio Através Do Método Biomimético. Dissertação de Mestrado. Universidade Federal de São João del Rei – UFSJ. 2021.

Ultrathin oxides and atomically sharp interfaces: in-situ surface/interface studies.

Ana G Silva[1, *] **Kjeld Pedersen**[2], **Zheshen Li**[3] **and Per Morgen**[4]

[1]*Cefitec, NOVA School of Science & Technology, New University of Lisbon, Campus da Caparica, 2829-516, Portugal.*
[2]*Aalborg University, Fredrik Bajers Vej 7K, 9220 Aalborg, Denmark.*
[3]*Physics and Astronomy Department, Aarhus University, Nordre Ringgade 1, 8000 Aarhus C, Denmark.*
[4]*Department of Green Technology, University of Southern Denmark, Campusvej 55, 5230 Odense, Denmark.*
*Corresponding author: acs@fct.unl.pt

In-situ high-resolution high surface/interface sensitivity synchrotron photoelectron spectroscopy studies of the mechanisms underlying the growth of the ultrathin films, $Sn/SiO_2/Si$ and SiC/Si, nanoparticles/SiO_2, and ultrathin oxides, SiO_2, Al_2O_3 will be presented and discussed. Oxidation mechanisms of Si and Al films is investigated under UHV conditions and with highly controlled and reproducible Si deposition and oxygen exposure conditions. For metals evaporation e-beam sources were used. As for SiC remote microwave plasma was implemented. Very low deposition rates of Si, Al and Sn allowed to follow the mechanism and the formation of the intermediate interfaces. Experiments were conducted at room and high temperatures, depending on the mechanism to be studied and the system to be analyzed. All steps of the processes, films growth, oxide-films, and oxidation, were carried out in an ultra-high-vacuum chamber and all followed in-situ by synchrotron photoemission spectroscopy carried out using the SGM-beamline with a SCIENTA analyzer at ASTRID1 and in the MAT-beamline with a SPECS analyzer at ASTRID2 synchrotron radiation sources (Denmark). Spectra of core-levels Si 2p, Al 2p, Sn 3d, C 1s, O1s at different photon energies, 130 eV, 350 eV and 610 eV, were acquired in all steps.

Acknowledgement
Ana G Silva acknowledges the support from EU (CALIPSO 312284). Portuguese science foundation through the project UID/FIS/00068/2019. The authors thank the technical staff at ASTRID for their support and effort during the experiments and for the good work environment at ASTRID.

References

[1] Ana G. Silva, Kjeld Pedersen, Zheshen Li, Jeanette Hvam, Rajnish Dhiman and Per Morgen, Growth of aluminum oxide on silicon carbide with an atomically sharp interface, J. Vac. Technol. A, 35, 01B142 (2017); http://dx.doi.org/10.1116/1.4972774

[1] Ana G. Silva, Kjeld Pedersen, Zheshen Li, Per Morgen, Applied Surface Science 353 (2015) 1208–1213, http://dx.doi.org/10.1016/j.apsusc.2015.07.024

[3] Ana G. Silva, Kjeld Pedersen, Zheshen Li, Per Morgen, Thin Solid Films 520 (2011) 697–699, doi:10.1016/j.tsf.2011.04.189

Optimisation of Ga_2O_3 membrane based MSM structures for optical and electronic sensors

M. C. Pedro[1,2*], D. M. Esteves[1,2], D. R. Pereira[1,2], L. C. Alves[2,3,4], K. Lorenz[1,2,4], M. Peres[1,2,4]

[1]INESC MN, Rua Alves Redol 9, Lisbon, Portugal
[2]IPFN, Instituto Superior Técnico, University of Lisbon, Av. Rovisco Pais 1, Lisbon, Portugal.
[3]C2TN, Instituto Superior Técnico, University of Lisbon, Estrada Nacional 10, Bobadela, Portugal.
[4]DECN, Instituto Superior Técnico, University of Lisbon, Estrada Nacional 10, Bobadela, Portugal.
**corresponding author e-mail: miguel.cardoso.pedro@tecnico.ulisboa.pt*

The β phase of gallium oxide (β-Ga_2O_3), is an emergent wide bandgap semiconductor, with promising technological applications, such as solar-blind ultraviolet photodetectors and sensors. Due to the monoclinic structure of β-Ga_2O_3, its crystal has easy cleavage along the (100) plane, allowing for exfoliation to be done. In particular, it is possible to induce controllable strain profiles in (100)-oriented crystals using ion implantation. This leads to the self-rolling of a thin layer, creating a microtube (left figure) that can be transferred to a desired substrate by a conventional pick and place technique. The microtube can then be unrolled through thermal annealing, which relaxes the strains and removes defects created by the implantation. The result is a nanomembrane of bulk-like crystalline quality on a selected substrate. In this work, metal-semiconductor-metal (MSM) structures based on these membranes were prepared on Si/SiO_2 and Al_2O_3 substrates. For the evaluation and optimisation of the metal-semiconductor junction, structures with different sputtered metals were tested and characterised. By testing structures employing Ti/Au contacts after different thermal treatments, it was often found that the initially Schottky rectifying contacts change into ohmic upon 500 ºC rapid thermal annealing, returning then to rectifying for higher temperatures (right figure). To better understand this transition, the electrical characterisation of these structures was complemented with Rutherford backscattering spectrometry and X-ray diffraction. These structures were also tested as photodetectors and as field effect transistors. Preliminary results show a response of the structures to UV light and, in particular for those supported on Si/SiO_2, a response of the current flow to the applied gate voltage.

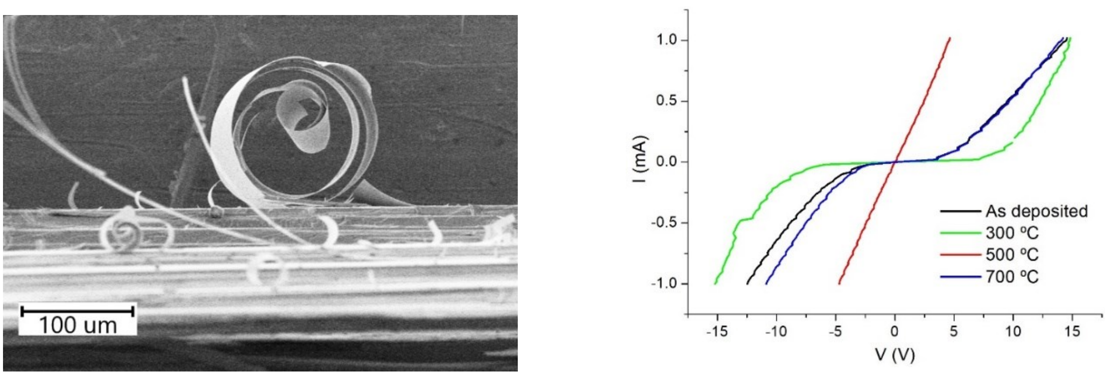


Figure 1- Left: Scanning electron microscopy image of the surface of a β-Ga_2O_3 crystal where several microtubes can be found. Right: I-V curves measured for an MSM structure after annealing at different temperatures.

The effect of target-substrate distance and deposition pressure on the properties of W-S-C coatings deposited by magnetron sputtering

Todor Vuchkov [1,2], Manuel Evaristo[1], Talha Bin Yaqub [1,2], Albano Cavaleiro [1,2]

[1]Surface engineering group (SEG) of the Centre for Mechanical Engineering, Materials, Products and Processes.
University of Coimbra, Portugal
[2]IPN - LED & MAT - Instituto Pedro Nunes, Laboratory for Wear, Testing and Materials, Rua Pedro Nunes, Coimbra, Portugal
**corresponding author e-mail: albano.cavaleiro@dem.uc.pt*

Nanocomposite coatings consisting of an amorphous carbon matrix (a-C) with nanocrystallites of transition metal dichalcogenides (TMD) embedded in it can provide protection against friction and wear in different operating environments, from vacuum to humid ambient air conditions [1]. These types of coatings are often deposited in smaller laboratory scale deposition units and there is a lack of information regarding their deposition in larger (semi-) industrial deposition units. Therefore, in this study we will present the synthesis of carbon-alloyed TMD-based coatings deposited by closed-field unbalanced magnetron sputtering in semi-industrial conditions. The focus of the study was the effect of the target-substrate distance and the deposition pressure on the properties of the coatings. The coating studied was tungsten-sulfur-carbon (W-S-C). The relationships established between the deposition procedure and the compositional and microstructural properties will be presented. Furthermore, the tribo-mechanical properties of the coatings will also be presented and correlated with the deposition procedure and their structural and compositional properties. The characterization techniques employed include scanning electron microscopy with wavelength dispersive spectroscopy (SEM/WDS), X-ray diffraction, scratch testing, nanoindentation. Additionally, the tribological performance was assessed in various conditions like ambient conditions with standard temperature and humidity, at elevated temperature (200°C) and in dry N_2 environment. This work will present the strong effect of the deposition procedure (e.g. the target-to-substrate distance) on the tribological properties of these types of coatings.

References

[1] Polcar T, Cavaleiro A. Review on self-lubricant transition metal dichalcogenide nanocomposite coatings alloyed with carbon. Surf Coatings Technol 2011;206:686–95. doi:10.1016/J.SURFCOAT.2011.03.004.

Study of aluminosilicate films co-doped with (Tb^{3+}, Er^{3+}) / Yb^{3+} by ion implantation

D. Faye[a], M. Dias[a], R. E. Rojas-Hernandez[b], Luís F. Santos[b], Rui M. Almeida[b], E. Alves[a]

[a] *IPFN, Instituto Superior Técnico, Universidade de Lisboa, 2695-066 Bobadela, Portugal*
[b] *Centro de Química Estrutural, Instituto Superior Técnico, Universidade de Lisboa*
Av. Rovisco Pais, 1049-001 Lisboa, Portugal

**corresponding author e-mail: ealves@ctn.tecnico.ulisboa.pt*

Harvesting solar energy demands efficient solar cells working over the larger region of the solar spectrum possible. The extension of the wavelength region is viable through the use of frequency converting phosphors. Rare earth (RE) elements fulfil this criteria and in particular the Erbium/Ytterbium pair allows a good coverage from the near-infrared (NIR) to visible up conversion (UC) luminescence at room temperature. In this study we report the structural and optical properties of aluminosilicate films grown by sol-gel (SG) spin-coating deposition technique and co-doped with (Tb^{3+}, Er^{3+}) / Yb^{3+} pairs by ion implantation with different fluences and energies. After implantation the films were annealed at 1000 ºC for 20 min and characterized by Rutherford Backscattering spectrometry (RBS), Secondary electron microscopy (SEM), X-ray diffraction and Photoluminescence. For the samples implanted with fluences below $1x10^{16}$ cm^{-2} the annealing produces a redistribution of the RE ions over the entire implanted region with some segregation to the surface. For higher fluences the RE profiles remain unchanged and XRD results indicate some crystallization suggesting the possibility to form $YbAl_3$. SEM reveals the formation of nanostructures dispersed on the surface of the films. These structures display a square shape with a silicon rich round structures at the center. The photoluminescence shows the presence of bright spots and the correlation of the luminescence properties with the nanostructures is being investigated and will be discussed and presented. Also, the results will be compared with in-situ doped samples during the spin coating deposition.

Atomic wall recombination in oxygen-containing plasmas

P. Viegas[1], J. Afonso[1] , J. Silveira[1], A. S. Morillo-Candás[2] , L. Vialetto[3] and V. Guerra[1]

[1] Instituto de Plasmas e Fusão Nuclear, Instituto Superior Técnico, Universidade de Lisboa, Portugal
[2] Laboratoire de Physique des Plasmas (UMR 7648), CNRS, Univ. Paris-Saclay, Sorbonne Université, École Polytechnique, France
[3] Theoretical Electrical Engineering, Faculty of Engineering, Kiel University, Germany
**corresponding author e-mail: pedroarsenioviegas@gmail.com*

Introduction

Heterogeneous surface kinetics plays a role in most plasma processes where surfaces interact either with active discharges or their afterglow. It can affect both the plasma and surface properties. In particular, in oxygen-containing discharges the adsorption and recombination of atomic oxygen on reactor surfaces determine the gas composition, the availability of O for important volume reactions (e.g.: $CO_2 + O \rightarrow CO + O_2$; $CO + O + M \rightarrow CO_2 + M$) and eventually the flux of reactive oxygen species (ROS) towards target surfaces.

In Booth et al. (2019) [1], the wall loss frequencies of O atoms have been measured in the positive column of an oxygen DC glow discharge in a Pyrex tube (borosilicate glass), for several pressures and discharge currents. However, the surface mechanisms determining recombination are not fully known yet. In particular, the increasing recombination with decreasing pressure below 1 Torr (see fig. 1) has not been described to date.

Results and discussion

In this work we employ deterministic and Kinetic Monte Carlo methods [2-4] to simulate the surface kinetics of atomic oxygen in the experimental conditions of Booth et al. (2019) and highlight the relevant mechanisms.

The newly developed model describes the experimental dependence of the atomic oxygen recombination probability on pressure, current, gas temperature and wall temperature, and allows to identify the most important recombination mechanisms for each operating condition. Moreover, this work demonstrates that the plasma has important effects on the surface at low pressures. This is due to fast particles that produce new chemisorption sites on the surface, where O atom recombination can take place without an energy barrier [5]. Figure 1 shows the effect of these sites on the atomic oxygen surface recombination frequency below 1 Torr, with a remarkable agreement with the experimental measurements.

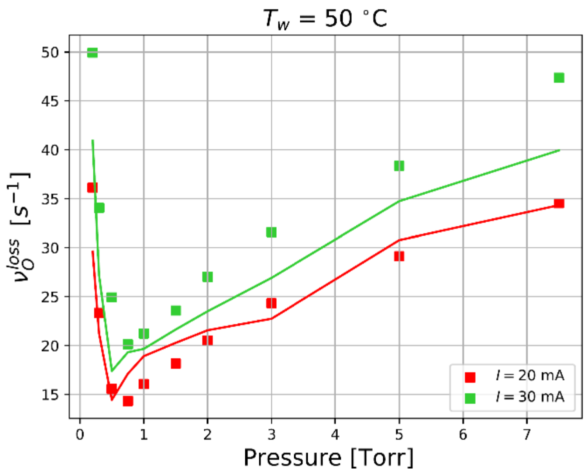


Figure 1 - Loss frequency as function of pressure, for a wall temperature of 50 ºC and discharge currents of 20 mA and 30 mA. Results from experiments [1] (square symbols) and simulations employing the deterministic method (full lines).

Acknowledgements
This work was partially supported by the Portuguese FCT-Fundação para a Ciência e a Tecnologia, under projects UIDB/50010/2020, UIDP/50010/2020 and PTDC/FISPLA/1616/2021 (PARADiSE).

References
[1] Booth *et al., Plasma Sources Sci. Technol.* **28** (2019) 055005
[2] Guerra, *IEEE Transactions on Plasma Science* **35** (2007) 1397
[3] Guerra and Marinov, *Plasma Sources Sci. Technol.* **25** (2016) 045001
[4] Marinov *et al., Plasma Process. Polym.* **14** (2017) 1600175
[5] Schwartzentruber *et al., AIAA International Space Planes and Hypersonic Systems and Technologies Conference* (2015) 3567

The Impact of High-Performance Transparent Substrates on Bifacial Solar Cells Performance

A. F. Violas [1,2,3 *], E. J. Ribeiro [1,3], P. Rebola [1,4], A. J. N. Oliveira [1,2,3], R. F. Alexandre [1], J. P. Teixeira [1], Paulo A. Fernandes [1,5], Pedro M. P. Salomé [1,3]

[1] *INL – International Iberian Nanotechnology Laboratory, Avenida Mestre José Veiga, 4715-330 Braga, Portugal*
[2] *i3N, Departamento de Física, Universidade de Aveiro, Campus Universitário de Santiago, 3810-193 Aveiro, Portugal*
[3] *Departamento de Física da Universidade de Aveiro, Campus Universitário de Santiago, 3810-193 Aveiro, Portugal*
[4] *Departamento de Ciências dos Materiais da Universidade Nova de Lisboa, Nova School of Science and Technology, 2829-516 Caparica, Portugal*
[5] *CIETI, Departamento de Física, Instituto Superior de Engenharia do Porto, Instituto Politécnico do Porto, Porto 4200-072, Portugal*
**corresponding author e-mail: andre.violas@inl.int*

Photovoltaics (PV) is currently one of the mainstream renewable sources of energy, ultimately because it is the cheapest way to produce electricity in most of the world [1]. Unfortunately, PV is not without drawbacks and current technologies still require large amounts of critical raw materials. Therefore, accounting for such concern, bifacial PV devices allow harvesting more energy, which stems from light absorption from both cell contacts, with the same, or even less, amount of raw materials as standard devices. There is still untapped potential in exploring rear contact architectures in $Cu(In,Ga)Se_2$ (CIGS) based solar cells, as the standard one does not allow for bifacial devices and the main alternatives do not fully exploit the CIGS performance potential. Therefore, this work focused on developing high performance transparent substrates (HPTS) to tackle the electrical performance concerns of commonly used transparent substrates and additionally provide enhanced optical behavior, while using industrially scalable nanofabrication processes. A set of different HPTS were developed through nanoimprint lithography (NIL) and/or an additional metal solid-state dewetting step. It includes a dielectric passivation strategy with nanoscale point contacts which despite its potential [2] still need optimization studies. Au plasmonic nanoparticles (NPs) and dielectric photonic crystals were also developed and optimized to boost the cell optical performance by increasing the optical path length [3], and consist on periodic features with lateral dimension values between 100 and 450 nm. Such HPTS may provide for a significant enhanced cell performance as hinted by the diffuse reflectance increase shown in Fig. 1. Electrical simulations show bifacial solar cells with HPTS with a 285 % relative increase performance in power conversion efficiency compared to standard transparent substrates, from improved electrical and optical properties as shown in Fig. 2. Therefore, it is evident the potential of HPTS to unlock the bifacial devices' performance.

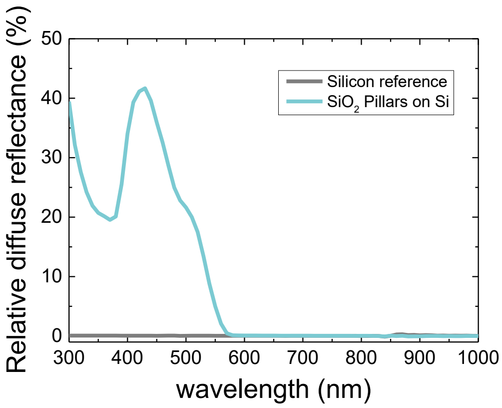


Fig. 1: Relative diffuse reflectance spectra for SiO_2 nano-pillars photonic crystals on Si compared with bare Si reference.

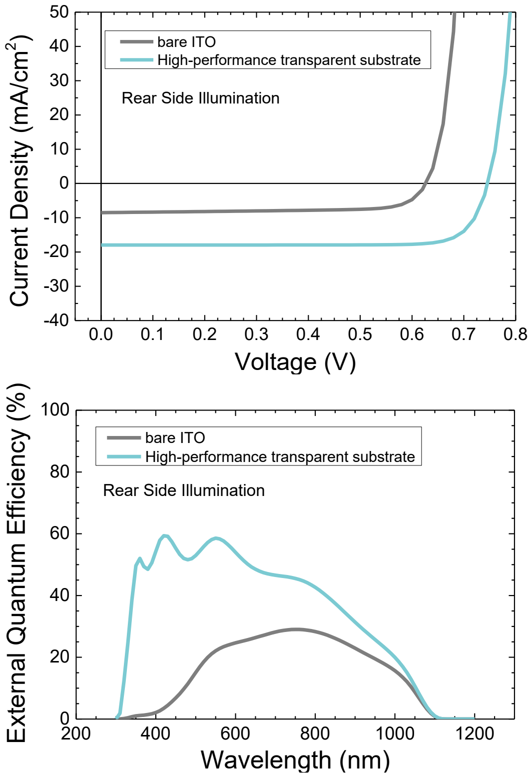


Fig. 2: Current density – Voltage (left) and External quantum efficiency (right) simulated curves for illumination through the rear contact, for the ITO reference cell and a high-performance transparent substrate.

References

[1] IEA (2020), Projected Costs of Generating Electricity 2020, IEA, Paris https://www.iea.org/reports/projected-costs-of-generating-electricity-2020, License: CC BY 4.0

[2] P. M. P. Salomé *et al.*, "Passivation of Interfaces in Thin Film Solar Cells: Understanding the Effects of a Nanostructured Rear Point Contact Layer," *Adv. Mater. Interfaces*, vol. 5, no. 2, pp. 1–10, 2017, doi: 10.1002/admi.201701101.

[3] A. J. N. Oliveira, J. P. Teixeira, D. Ramos, P. A. Fernandes, and P. M. P. Salomé, "Exploiting the Optical Limits of Thin Film Solar Cells: A Review on Light Management Strategies in Cu(In,Ga)Se_2," *Adv. Photonics Res.*, p. 2100190, 2022, doi: 10.1002/adpr.202100190.

Fabrication and Optimization of Intrinsic/Doped a-Si:H Layers for High-Efficiency HIT Solar Cells

Ghulam Abbas[1], Alexandr Zamchiy[1], Pedro Ferreira[1], Manuel Mendes[1], Hugo Águas[1]

[1] *CENIMAT|i3N, Department of Materials Science, NOVA School of Science and Technology, Campus de Caparica, NOVA University of Lisbon, 2829-516 Caparica, Portugal*
**corresponding author e-mail: g.abbas@campus.fct.unl.pt*

Silicon heterojunction (SHJ) photovoltaic (PV) cells, also known as heterostructures with intrinsic thin layers (HIT) technology, have emerged as a promising solution for high-efficiency solar cells. These cells have garnered significant attention due to their superior power-conversion efficiency [1]. Moreover, their potential for large-scale production makes them highly suitable for practical applications on various substrates [2]. In this research, we fabricated HIT solar cells using Plasma Enhanced Chemical Vapor Deposition (PECVD). These HIT solar cells are composed of a thin crystalline silicon (c-Si) wafer surrounded by ultra-thin amorphous silicon (a-Si:H) layers, which are deposited using PECVD. 10nm intrinsic amorphous silicon layers (i-a-Si:H) are used to passivate the c-Si, and p- and n-type a-Si:H layers with 20 nm deposited over the i-a-Si:H to complete the heterojunction. Film quality assessed through their optical and electrical properties were widely studied. Figure 1 shows the effect of trimethylborane (TMB) dopant gas concentration relative to silane during the deposition of (p)a-Si:H films by PECVD using 51% to 55% hydrogen dilution on the activation energy and film conductivity. Film conductivity increases to an optimum value with 2% dopant concentration of TMB (at 51 % hydrogen dilution). During (n) a-Si:H films studies, we deposited several films with different PH_3 concentration relative to silane and 70.1% hydrogen dilution. We got maximum conductivity and minimum activation energy at 0.7% Phosphine (PH_3) dopant gas concentration as shown in figure 2. Activation energy follows inverse trends than conductivity as expected. A comprehensive analysis for several deposition temperatures, pressures and gas flows has been done and fabricated uniform films with better morphology and controlled band gap energies. Transparent conductive oxide (TCO) and Al contacts were deposited on the doped layers by magnetron sputtering and resistive evaporation, respectively. The combination of high-performance c-Si wafers and precise deposition techniques leads to improved power-conversion efficiency and practicality for large-scale production. This advancement holds great promise for the future of photovoltaics and renewable energy applications.

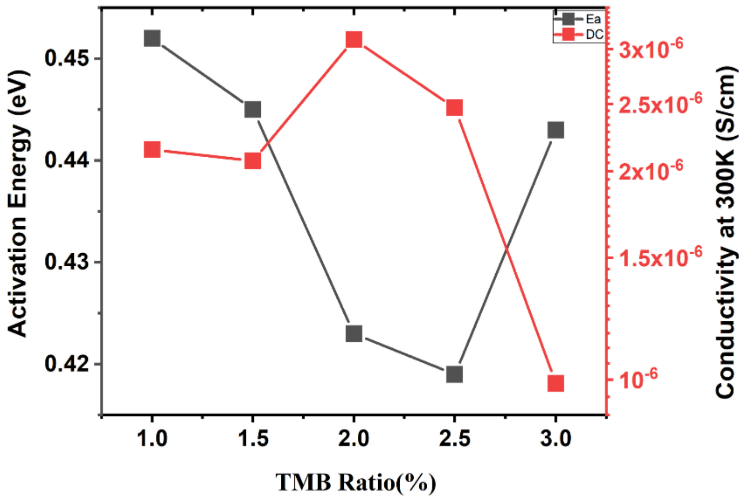


Figure 1 Effect of dopant gas concentration on activation energy and dark conductivity of (p) a-Si:H films at 300 K temperature.

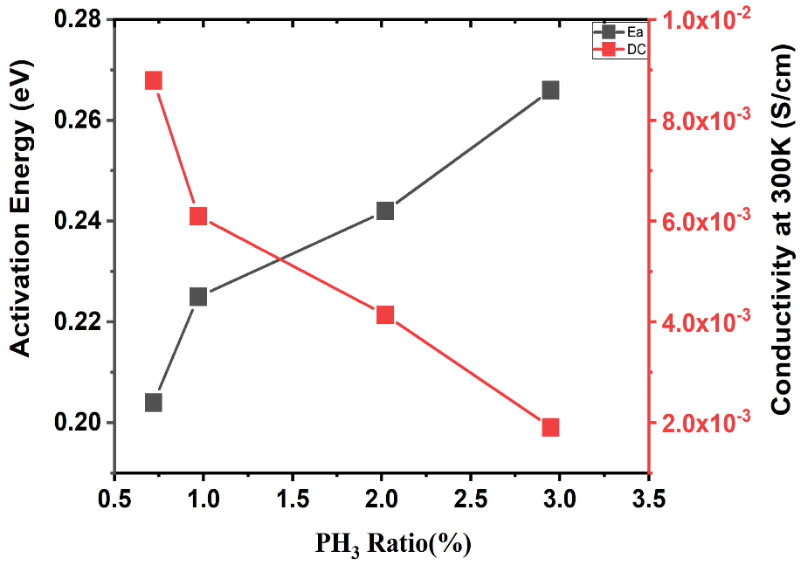


Figure 2 Effect of dopant gas concentration on activation energy and dark conductivity of (n) a-Si:H films at 300 K temperature.

References

[1] Lin, Hao, et al. "Silicon heterojunction solar cells with up to 26.81% efficiency achieved by electrically optimized nanocrystalline-silicon hole contact layers." *Nature Energy* (2023): 1-11.
[2] Águas, Hugo, et al. "Thin film silicon photovoltaic cells on paper for flexible indoor applications." *Advanced Functional Materials* 25.23 (2015): 3592-3598.

Bacterial adhesion on sputter-deposited a-C:H:N coatings for Orthodontics

A. Fróis[1,2,3], R. Francisco[4], P. V. Morais[4], C. S. Louro[1*]

[1] *University of Coimbra, CEMMPRE, ARISE, Department of Mechanical Engineering, Rua Luis Reis Santos, 3030-177 Coimbra, Portugal*
[2] *University of Coimbra, Faculty of Medicine, Biophysics Institute; Coimbra Institute for Clinical and Biomedical Research/Centre for Innovative Biomedicine and Biotechnology (iCBR/CIBB), 3000- 548 Coimbra, Portugal*
[3] *University of Coimbra, Area of Environment Genetics and Oncobiology (CIMAGO), 3000-548 Coimbra, Portugal*
[4] *University of Coimbra, CEMMPRE, ARISE, Department of Life Sciences, Faculty of Sciences and Technology, University of Coimbra, Calçada Martim de Freitas, 3000-456 Coimbra, Portugal*
**corresponding author e-mail: cristina.louro@dem.uc.pt*

Among the under-development strategies to improve the intraoral corrosion resistance of orthodontic alloys, the use of protective coatings stands out. Multiple physical and chemical technologies are employed to synthesize polymeric, metallic, ceramic, and composite coatings onto orthodontic components, some already commercially available [1]. However, the literature shows an evident lack of optimal solutions.
Carbon-based coatings are appealing for such applications, namely the hydrogenated amorphous carbon (a-C:H) group, which can be doped with several metallic and non-metallic elements, still preserving the amorphous structure. The major advantages of these coatings include its outstanding chemical inertness, well-known biocompatibility, and low coefficient of friction [2]. Nevertheless, the oral cavity is quite complex due to the highly variable physicochemical parameters and the presence of plaque-forming microorganisms. In fact, over 700 species of bacteria and numerous fungi and viruses were identified so far [3]. Bacteria adhere on the metallic surface of orthodontic appliances and promote a characteristic corrosion type - the Microbiologically Induced Corrosion (MIC) [3,4] - which must be addressed when designing a coating for dental applications. The present research work aims to assess the influence of nitrogen addition in a-C:H coatings ($N < 10$ at.%) in the bacterial adhesion. For this purpose, a-C:H and a-C:H:N coatings were deposited on medical grade SS 316L substrates by reactive magnetron sputtering from a graphite target, by introducing CH_4 and N_2 into the Ar plasma. The *in vitro* bacterial adhesion was evaluated with three representative strains: *Staphylococcus aureus* UCCCB115, *Bacillus subtilis* UCCCB117 and *Pseudomonas aeruginosa* UCCCB116. The ability to colonize the C-rich surface was evaluated by microstructure and surface morphology coupled with colony forming units. The best results were obtained for *Bacillus subtilis*: the adhesion of this bacterial strain decreased with increasing N content. This surface engineering approach encourages further research for mitigating MIC.

Acknowledgements and Funding
This work was supported by national funds through FCT - Fundação para a Ciência e a Tecnologia, under the projects UIDB/00285/2020 and LA/P/0112/2020, and through the PhD Grant SFRH/BD/143905/2019 attributed to A. Fróis.

References

[1] Arango S, Peláez-Vargas A, García C. Coating and Surface Treatments on Orthodontic Metallic Materials. Coatings 2013;3:1–15. https://doi.org/10.3390/coatings3010001.
[2] Carvalho I, Rodrigues L, Lima MJ, Carvalho S, Cruz SMA. Overview on the Antimicrobial Activity and Biocompatibility of Sputtered Carbon-Based Coatings. Processes 2021;9:1428. https://doi.org/10.3390/pr9081428.

[3] Mystkowska J, Niemirowicz-Laskowska K, Łysik D, Tokajuk G, Dąbrowski JR, Bucki R. The role of oral cavity biofilm on metallic biomaterial surface destruction–corrosion and friction aspects. Int J Mol Sci 2018;19. https://doi.org/10.3390/ijms19030743.

[4] Fróis A, Mendes AR, Pereira SA, Louro CS. Metal Release and Surface Degradation of Fixed Orthodontic Appliances during the Dental Levelling and Aligning Phase: A 12-Week Study. Coatings 2022;12:554. https://doi.org/10.3390/coatings12050554.

Traceability of Hydrogen Leak Detectors

Orlando Ferreira[1], Orlando M.N.D. Teodoro[1]

[1] *Center of Physics and Technological Research*
Nova School of Science and Technology, Caparica, Portugal
**corresponding author: o.ferreira@campus.fct.unl.pt*

Gas mixtures of hydrogen in nitrogen (5% + 95%) are commonly used as tracer gas in leak testing of, for example, automotive hoses, vacuum parts and gas compressors, in the same way as helium. By other hand, the forthcoming introduction of hydrogen in the gas grid, brings extra health & safety requirements of the leak test campaigns performed by the gas operators. In all these applications, it is important to provide a quantitative measurement of the hydrogen leak rate, so proper actions may be taken. Every time a quantity is measured, traceability to SI units should be provided. The simplest way to calibrate an ultra-low flow rate (small leak) is using reference leaks. These are small portable devices which provide a known flow rate and can be calibrated in laboratory.
In this communication, the process of manufacture and calibration of hydrogen reference leaks, with leak rates ranging between 10^{-6} and 10^{-4} mbar.L/s are described. These leaks have the potential to be used in the calibration of hydrogen leak detectors in the future. Two distinct permeation designs have been used with promising results. The process of calibrating leak detectors with these type of leaks will also be discussed.
This work was done in the frame of the European project "Metrology support for decarbonization of the gas grid" in which the portuguese Laboratory for Vacuum Technology and Metrology (METROVAC) is engaged.

Experimental and numerical study of the reaction pathways in low-pressure CO_2-CH_4 glow discharges

Edmond Baratte[2], Tiago Silva[1], Olivier Guaitella[2], Vasco Guerra[1]

[1]*Instituto de Plasmas e Fusão Nuclear, Instituto Superior Técnico, Universidade de Lisboa, 1049-001 Lisboa, Portugal*
[2] *LPP, Ecole Polytechnique, UPMC, Université Paris Sud-11, CNRS, Palaiseau, France.*
**corresponding author: tiago.p.silva@tecnico.ulisboa.pt*

The growing increase of CO_2 emissions calls for green technologies capable to accelerate the transition towards a more sustainable and resilient world. This transition requires the development of storage solutions in which the excess of renewable power is used to convert feedstock of pollutant gases such as CO_2 into chemical fuels. In this context, non-thermal plasmas have gained much attention regarding CO_2 decomposition due to their potential to activate CO_2 at reduced energy cost, while exciting CO_2 vibrations that efficiently contribute to overcome the dissociation barrier. Plasma technology could then serve as vehicle to transform electricity into chemistry, while using the excess of wind of solar power to convert feedstock of CO_2 into fuels.
In this talk, we give an overview of recent research in the field of converting relevant feedstock into value added products using plasma-assisted reactors. The specific case in which valuable products are produced in CO_2-CH_4 plasmas is analysed in detail. More specifically, while combining experimental and modelling investigations, we explore physical and chemical mechanisms involved in CO_2-CH_4 plasmas and discuss which processes contribute for molecular conversion. The modelling studies conducted in this work (taking into account the LisbOn KInetics (LoKI) simulation tool [1]) were based on the coupling of the electron Boltzmann equation with a system of rate balance equations, specifically developed for the description of CO_2-CH_4 chemistry. The experimental work was performed in CO_2-CH_4 glow discharges, sustained at low pressure conditions (between 1 and 7 Torr) with coupled OES-based techniques and FTIR spectroscopy. These diagnostics were essentially used to determine densities of molecules of interest and gas temperature in the reactor [2]

References

[1] A. Tejero-del-Caz et al, The LisbOn Kinetics Boltzmann solver, Plasma Sources Sci. Technol. 28 (2019) 043001. https://nprime.tecnico.ulisboa.pt/loki/index.html
[2] E. Baratte, C. A. G. Soto, T. Silva, V. Guerra, V. I. Parvulescu and O. Guaitella, CO_2/CH_4 glow discharge plasma. Part I: Experimental and numerical study of the reaction pathways, Submitted to *Plasma Sources Sci. Technol.* (2023).

.

Acknowledgments

This work was partially supported by the Portuguese FCT-Fundação para a Ciência e a Tecnologia, under projects UIDB/50010/2020, UIDP/50010/2020, PTDC/FIS-PLA/1616/2021, EXPL/FIS-PLA/0076/2021