

# 10<sup>th</sup> Symposium on **FUNCTIONAL COATINGS** AND **SURFACE ENGINEERING**

## Final program and Book of abstracts

## JUNE 2-5 MONTREAL •













## Organizers of the FCSE-2024 Symposium

#### MEETING CHAIRS

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Regroupement Québécois sur les Matériaux de Pointe (RQMP): <u>www.rqmp.ca</u> AVS Science and Technology of Materials, Interfaces, and Processing: <u>www.avs.org</u> Society of Vacuum Coaters: <u>www.svc.org</u> The International Union for Vacuum Science, Technique and Applications (IUVSTA): <u>www.iuvsta.org</u> Prima Québec: <u>www.prima.ca</u>

#### HOSTING INSTITUTIONS

Polytechnique Montréal: <u>www.polymtl.ca</u> Université de Montréal: <u>www.umontreal.ca</u>

#### Dear Participants,

We are very pleased to welcome you at the 10<sup>th</sup> Symposium on Functional Coatings and Surface Engineering, FCSE-2024, organized by the Regroupement québécois sur les matériaux de pointe (Quebec Consortium on Advanced Materials - RQMP) and the St. Lawrence Chapter of the AVS Science and Technology of Materials, Interfaces and Processing in collaboration with the Society of Vacuum Coaters (SVC), The International Union for Vacuum Science, Technique and Applications (IUVSTA), and Prima Québec, and hosted by Polytechnique Montréal and Université de Montréal between June 2 and 5, 2024.

The technical program of this Symposium reflects recent most significant progress and trends in the area of functional thin films, coatings and surface engineering. It focuses on the latest advances in film fabrication processes, the synthesis of new nanostructured materials, the fabrication of new thin film devices and coating systems, the surface interactions and process control, as well as on the environmental impact, life cycle analysis and sustainability. All these aspects represent the bases of new applications and trends in fields that cover the spectrum from optics and optoelectronics, through biomedical and automotive, to energy, aerospace and outer space, manufacturing, and other industries and products, too numerous to mention them all.

The rich technical and educational programs include invited lectures, oral and poster presentations, vendor and sponsor presentations, short courses, and workshops. The Symposium has been designed to encourage student participation, and to contribute to networking and to the exchange of scientific and technical information in these fast-evolving fields.

Finally, we wish to thank all those who contributed to the organization and to the technical quality of this Symposium, to our invited speakers and presenters, and particularly, to our sponsors who supported it financially. We wish that all the participants will experience a stimulating and productive FCSE-2024 meeting and enjoy their stay in Montreal.

Ludvik Martinu and Jolanta E. Klemberg-Sapieha, Symposium Chairs

Montreal, June 2, 2024





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	Sunday, J			4 SYMPOSIUM SC Monday, June 3		E AT A GLANCE lesday, June 4		dnesday, June 5
Campus MIL Université de Montréal			Campus MIL Université de Montréal, Room A-1502.1			Poly	technique Montréal Main building	
Educational program I				Technical program			Educational program II	
	Short cou	irses	Regis	tration: Atrium B-140	Registr	ation: Atrium B-140	Hands-on workshops Registration: B-415	
8:30	Bre	akfast	8:30	Opening ceremony	Session	4: High entropy films	8:30	Breakfast
			Session 1	: Plasma-based processes	8:40	JW Lee	9:00	PART 1
			8:50	A. Anders	9:10	P. Steyer	Works	shop A: Room B-405
	A	В	9:20	S. Muhl	9:20	S. Alidokht		cal characterization
	Plasma deposition	Stress	9:30	S. Reuter	9:30	P. Mayrhofer		shop B: Room B-401 nical characterization
9	A.	G.	10:00	Break	10:00	Break		shop C: Room B-429 Surface analysis
- 12	Anders	Abadias	Session 2	: Hard protective coatings	Sessi	on 5: Optical films	10:30	Break
			10:30	I. Petrov	10:30	C. Menoni		Workshops
	Room	Room	11:00	K. Thomas	11:00	P. Bhattacharya	10:45	A, B and C
	A-3541	A-3551	11:10	J. Nohava	11:10	W. Skene	- 12:00	
			11:20	M. Javidani M. Olivares-Luna	11:20	R. El Abdi		PART I continued
			11:30 11:40	J. Schneider	11:30 11:40	B. Abdel Samad G. Abadias		Continued
12				Lunch		Lunch		Lunch and
- 13	Lunch and	l discussions	12:10	Exhibit Posters	12:10 -	Exhibit Posters and Awards	12:00	discussions
			13:30	Atrium B-140	13:40	Atrium B-140		
			Sessi	on 3: Bio-related appl.	Sessior	6: Characterization		
			13:30	S. Carvalho	13:40	G. Greczynski		
			14:00	A. Ibrahim	14:10 14:20	T. vom Braucke J. Nikitina		
			14:10	B. Baloukas	14:30	R. Liu	13:00	PART II
					14:40	E. Familsatarasian	-	Hands-on
13	Co	urses			14:50	W. Gajewski	16:30	workshops
17		tinued	14:20	Exhibit	15:00	Break		in the lab
			14:20	Posters Refreshments	Session	7: FCSE perspectives		
			16:30		15:30	F. Schuster		
				Atrium B-140	16:00	P. Immich		
					16:10 16:20	F. Papa L. Josephson		
			16:30	Evening Lecture C. Herrmann	16:30	C. Stoessel		ı
			17:20	Life cycle engineering for a circular economy	17:00	Closing remarks and Visit of the facilities		
	<u>I</u>		18:00	Conference dinner Location: PolyMTL – Lassonde Building		, lot of the facilities		

## FCSE-2024 Symposium program

#### **KEY TO SESSION NUMBERS:**

<b>S</b> 1	Plasma-based processes
S2	Hard protective coatings
S3	Bio-related, energy and other applications
S4	High entropy films
S5	Optical films
<b>S</b> 6	Advanced characterization
<b>S</b> 7	FCSE perspectives

## Sunday, June 2, 2024

	Cunady, Sunc 2, 2024
Locatio	ORT COURSES on: MIL Campus – Université de Montréal ation: Atrium B-140 / Short courses: Rooms A-3541 and A-3551
8:00 - 9:00	Welcome Desk Opens – Atrium B-140
8:30 - 9:00	Continental breakfast
	Short course A – Room A-3541
	Plasma deposition of thin films and related processing of materials
9:00	A. Anders Leibniz Institute of Surface Engineering, Leipzig, Germany
12:00	Short course B – Room A-3551
	Stress evolution during thin film growth by physical vapor deposition
	<b>G. Abadias</b> <i>CNRS-Université de Poitiers, Poitier, France</i>
12:00 - 13:00	Lunch (included) and discussions – Atrium B-140
13:00  17:00	Continuation of the short courses

## Monday Morning, June 3, 2024

#### **ORAL PRESENTATIONS**

11:00

Location: MIL Campus – Université de Montréal Registration: Atrium B-140 / Presentations: A-1502.1

8:30
 Welcome address, acknowledgements, and introductory remarks
 8:50

#### Session 1: Plasma-based processes

Moderator: C. H. Stoessel, StoesselConsulting / SputterTek LLC, Palo Alto, CA, USA

8:50  9:20	S1-1       – Invited         Atomic scale heating in plasma deposition processes       A. Anders         Leibniz Institute of Surface Engineering, Leipzig, Germany
9:20 - 9:30	S1-2         What is the temperature of a target during DC magnetron sputtering?         S. Muhl, J. Cruz, A. Garzon         Instituto de Investigaciones en Materiales, UNAM, Mexico City, Mexico
9:30  10:00	S1-3       – Invited         Advanced laser diagnostics on reactive plasmas at interfaces       S. Reuter         Polytechnique Montréal, Montreal, QC, Canada
10:00 - 10:30	Break
	Session 2: Hard protective coatings rator: JW. Lee, Ming Chi University of Technology (MCUT), Taiwan
10:30	<b>S2-1</b> – <u>Invited</u> Low-temperature synthesis of dense, hard, stress-free ceramic coatings using metal-ion irradiation

**I. Petrov<sup>1,2</sup>**, L. Hultman<sup>1</sup>, J. Greene<sup>1,2</sup>, G. Greczynski<sup>1</sup> <sup>1</sup> Thin Film Physics Division, Department of Physics (IFM), Linköping University, Linköping, Sweden <sup>2</sup> Materials Research Laboratory, University of Illinois, Urbana, IL, USA

## Monday Morning, June 3, 2024 - continued

#### **ORAL PRESENTATIONS**

Location: MIL Campus – Université de Montréal Presentations: Room A-1502.1

11:00 - 11:10	S2-2 Steered high-power-density plasma sputtering as an alternative to HiPIMS K. Thomas <sup>1</sup> , F. Klimashin <sup>2</sup> , A. Lümkemann <sup>1</sup> , J. Kluson <sup>1</sup> , M. Ucik <sup>1</sup> , M. Jilek <sup>1</sup> , J. Michler <sup>2</sup> , T. Edwards <sup>2</sup> <sup>1</sup> Platit AG, Granges, Switzerland <sup>2</sup> EMPA, Dübendorf, Switzerland
11:10 - 11:20	S2-3 Influence of Al-Ti ratio and bias on the structure and mechanical properties of AlTiN coatings J. Nohava <sup>1</sup> , P. Hausild <sup>2</sup> , J. Kalas <sup>3</sup> , S. Zierler <sup>4</sup> , J. Sondor <sup>3</sup> <sup>1</sup> Anton Paar TriTec SA, Corcelles, Switzerland <sup>2</sup> Czech Technical University in Prague, Prague, Czech Republic <sup>3</sup> Platit, s.r.o. Roznov pod Radhostem, Czech Republic <sup>4</sup> Anton Paar, Graz, Austria
11:20 - 11:30	S2-4 Effect of substrate material on the tribological behaviour of AlTiCrN/AlTiN-coated tool steels M. Muhammed <sup>1</sup> , M. Javidani <sup>1</sup> , T. E. Sadrabadi <sup>1</sup> , M. Heidari <sup>2</sup> , T. Levasseur <sup>2</sup> , M. Jahazi <sup>3</sup> <sup>1</sup> Department of Applied Science, University of Quebec at Chicoutimi, QC, Canada <sup>2</sup> DK SPEC, St-Nicolas, QC, Canada <sup>3</sup> Department of Mechanical Engineering, École de Technologie Supérieure, QC, Canada
11:30 - 11:40	S2-5 Insights on the pulsed-DC powder-pack boriding process: The role of the electric charge on the growth of the boride layer and the semiconductor behavior of the boriding media M. Olivares-Luna <sup>1</sup> , J. L. Rosales-Lopez <sup>1</sup> , L. E. Castillo-Vela <sup>1</sup> , K. D. Chaparro-Pérez <sup>1</sup> , A. M. Delgado-Brito <sup>2</sup> , I. Mejía- Caballero <sup>1</sup> , I. E. Campos-Silva <sup>1</sup> ' Instituto Politécnico Nacional, Grupo Ingeniería de Superficies, SEPI-ESIME, Mexico City, Mexico <sup>2</sup> Tecnológico de Estudios Superiores de Jocotitlán, Jocotitlán, Mexico
11:40 - 12:10	S2-6       – Invited         Thin film materials design & some thoughts on complexity and sustainability       J. M. Schneider         Materials Chemistry, RWTH Aachen University, Aix-la-Chapelle, Germany
12:10 	Lunch, Beginning of Poster Session & Exhibit – Atrium B-140 For details, see below

## Monday Afternoon, June 3, 2024

#### **ORAL PRESENTATIONS**

Location: MIL Campus – Université de Montréal Presentations: Room A-1502.1

#### Session 3: Bio-related, energy and other applications

Moderator: S. Reuter, Polytechnique Montréal, Quebec, Canada

13:30 	S3-1       – Invited         Advancing biomedical applications through plasma surface modification: A promising frontier       S. Carvalho         S. Carvalho       CEMMPRE, Department of Mechanical Engineering, University of Coimbra, Portugal
14:00 	S3-2 Towards a durable thin hydrophobic textile finishing: light-curing process "photopolymerization" for stretch textiles A. Ibrahim, J. Decaens, O. Vermeersch, V. Izquierdo <i>Groupe CTT, Saint-Hyacinthe, QC, Canada</i>
14:10 	S3-3         Smart materials for dynamic glazings - opportunities for energy savings and control         B. Baloukas         Department of Engineering Physics, École Polytechnique de Montréal, Montréal, Québec, H3C 3A7, Canada
14:20  16:30	Poster session & Exhibit Continued – Atrium B-140
16:30  17:20	Evening Lecture – Invited – Room A-1502.1 Holistic life cycle engineering for a sustainable circular economy C. Herrmann Technische Universität Braunschweig and Fraunhofer Institute for Surface Engineering and Thin Films, Braunschweig, Germany
18:00 	Conference Dinner Location: Polytechnique Montreal – Atrium of the Lassonde Building

	Tuesday Morning, June 4, 2024
Locatio	L PRESENTATIONS n: MIL Campus – Université de Montréal ation: Atrium B-140 / Presentations: Room A-1502.1
Moder	Session 4: High entropy films
Widdel	rator: J. M. Schneider, RWTH Aachen University, Germany
8:40  9:10	<b>S4-1</b> – <u>Invited</u> <b>Effect of carbon on the microstructure and properties of TiZrNbTaFeC high entropy alloy carbide coatings</b> JW. Lee <sup>1,2,3,4</sup> , I. Rahmadtulloh <sup>1,5</sup> , BS. Lou <sup>6,7</sup> , CJ. Wang <sup>5</sup> <sup>1</sup> Department of Materials Engineering, Ming Chi University of Technology, New Taipei, Taiwan <sup>2</sup> Center for Plasma and Thin Film Technologies, Ming Chi University of Technology, New Taipei, Taiwan <sup>3</sup> Department of Mechanical Engineering, Chang Gung University, Taoyuan, Taiwan <sup>4</sup> High Entropy Materials Center, National Tsing Hua University, Hsinchu, Taiwan <sup>5</sup> Department of Mechanical Engineering, National Taiwan University of Science and Technology, Taipei Taiwan <sup>6</sup> Chemistry Division, Center for General Education, Chang Gung University, Taoyuan, Taiwan <sup>7</sup> Department of Orthopaedic Surgery, New Taipei Municipal TuCheng Hospital, Chang Gung Memorial Hospital, Taiwan
9:10  9:20	S4-2 Advanced microscopic characterization strategies to better understand dynamics of Zr-Cu-Ag PVD thin film metallic glasses P. Steyer <sup>1</sup> , L. Roiban <sup>1</sup> , S. Dassonneville <sup>1</sup> , A. Borroto <sup>2</sup> JF. Pierson <sup>2</sup> <sup>1</sup> INSA de Lyon, Laboratoire MATEIS, Villeurbanne, France <sup>2</sup> Université de Lorraine, Institut Jean Lamour, Nancy, France
9:20 - 9:30	S4-3         Cold sprayed anti-biofouling coatings based on high entropy alloys         M. Ettelaei, S. Alidokht         Department of Mechanical Engineering, Memorial University of Newfoundland, St. John's, NL, Canada
9:30 - 10:00	S4-4       – Invited         High-entropy Hägg phases; A case study of nitrides, carbides, and diborides       P. H. Mayrhofer         Institute of Materials Science and Technology, TU Wien, Vienna, Austria
10:00 - 10:30	Break

## Tuesday Morning, June 4, 2024 - continued

#### **ORAL PRESENTATIONS**

Location: MIL Campus – Université de Montréal Presentations: Room A-1502.1

#### Session 5: Optical films

Moderator: S. Carvalho, University of Coimbra, Portugal

10:30 - 11:00	S5-1 – Invited         Amorphous oxides mixtures for coatings of gravitational wave detectors         C. S. Menoni <sup>1</sup> , A. Davenport <sup>1</sup> , S. Castro-Lucas <sup>1</sup> , R. Osovsky-Shpilman <sup>1</sup> , S. Bhowmick <sup>1</sup> , A. Markosyan <sup>2</sup> , R. Bassiri <sup>2</sup> , M. Fejer <sup>2</sup> , F. Schiettekatte <sup>3</sup> , M. Chicoine <sup>3</sup> , R. Zhang <sup>4</sup> , J. Jiang <sup>4</sup> , HP. Cheng <sup>4</sup> <i>'Dept. of Electrical and Computer Engineering, Colorado State University, Fort Collins, CO, USA 'Dept. of Electrical and Computer Engineering, Colorado State University, Fort Collins, CO, USA 'Dept. of Electrical and Computer Engineering, Colorado State University, Stanford, CA, USA 'Dept. of Electrical and Computer Engineering, Colorado State University, Stanford, CA, USA 'Dept. of Electrical and Computer Engineering, Colorado State University, Stanford, CA, USA 'Department of Physics, Université de Montréal, Montreal, QC, Canada 'Department of Physics, Northeastern University, Boston, MA, USA</i>
11:00  11:10	S5-2 Design and fabrication of color-generating multilayer thin-film optical filters for silicon solar cells P. Bhattacharyya, C. White, R. Kleiman, P. Mascher Department of Engineering Physics and Centre for Emerging Device Technologies, McMaster University, Hamilton, ON, Canada
11:10 	S5-3 Enabling smart windows with rationally designed coatings M. R. Anthony Raj, G. B. Muthuperumal, W. Skene Université de Montréal, Montreal, QC, Canada
11:20 	S5-4 Protective coatings for optical fiber used in telecommunication networks R. El Abdi, R. L. Pinto Université de Rennes, Institut de Physique de Rennes, Rennes, France
11:30  11:40	S5-5         The effect of cupper layer on AlCIPc thin film         B. Abdel Samad, Z. Kabore         Department of Physics and Astronomy, Université de Moncton, Moncton, N-B, Canada
11:40  12:10	S5-6       – Invited         Real-time growth monitoring of ultrathin Ag layers for use as transparent conductive electrodes       G. Abadias         CNRS-Université de Poitiers, Poitier, France
12:10  13:40	Lunch, Continuation of Poster Session, Exhibit & Announcement of the Poster Awards – Atrium B-140

## Tuesday Afternoon, June 04, 2024

#### **ORAL PRESENTATIONS**

Location: MIL Campus – Université de Montréal Presentations: Room A-1502.1

#### Session 6: Advanced characterization Moderator: I. Petrov, Linköping University, Sweden S6-1 - Invited 13:40 Towards reliable X-ray photoelectron spectroscopy of thin films G. Greczvnski 14:10 Thin Film Physics Division, Department of Physics (IFM), Linköping University, Linköping, Sweden S6-2 14:10 Creating a digital twin and how it helps to speed up your coating development **T. vom Braucke<sup>1</sup>**, N. Bierwisch<sup>2</sup> 14:20 GP Plasma, Medina, OH, USA <sup>2</sup> SIOmec, Ummanz, Germany S6-<u>3</u> 14:20 Investigation of the mechanical properties of sculptured thin films by nanoindentation J. Nikitina, L. Grinevičiūtė 14:30 Department of Laser Technologies, Center for Physical Sciences and Technologies, Vilnius, Lithuania S6-4 14:30 Modeling study of interface fracture toughness of thermal barrier coating at high temperature R. Liu, S. K. Essa 14:40 Department of Mechanical and Aerospace Engineering, Carleton University, Ottawa, ON, Canada S6-5 Giant step bunching and Ehrlich-Schwöbel-barrier in thin heteroepitaxial films of strontium titanate on magnesium oxide 14:40 (100) substrates E. Familsatarian<sup>1</sup>, K. Kohlmann<sup>1</sup>, D. Gückelhorn<sup>1</sup>, A. Sarkissian<sup>2</sup>, E. Carbone<sup>1</sup>, P. Antici<sup>1</sup>, 14:50 A. Ruediger<sup>1</sup> <sup>1</sup> INRS - Énergie, Matériaux et Télécommunications, Montreal, QC, Canada <sup>2</sup> Plasmionique, Varennes, QC, Canada S6-6 14:50 Optimization and application of HiPIMS hafnium oxynitride ( $HfO_xN_y$ ) thin films in MOS structures M. Puzniak<sup>1</sup>, W. Gajewski<sup>1</sup>, R. Mroczynski<sup>2</sup>, M. Zelechowski<sup>1</sup> 15:00 TRUMPF Huettinger Sp. z o.o., Zielonka, Poland <sup>2</sup> Institute of Microelectronics and Optoelectronics, WUM, Warsaw, Poland 15:00 Break 15:30

## Tuesday Afternoon, June 4, 2024 – continued

#### **ORAL PRESENTATIONS**

Location: MIL Campus – Université de Montréal Presentations: Room A-1502.1

#### Session 7: FCSE perspectives

Moderator: G. Abadias, University of Poitiers, France

15:30  16:00	S7-1       – Invited         Thin film technologies for low carbon energies in a Green Deal context       F. Schuster <i>F. Schuster CEA, Paris-Saclay, France</i>
16:00  16:10	<ul> <li>S7-2</li> <li>Taking on the challenge for high-volume coating of metallic plates for hydrogen applications using PVD technology</li> <li>P. Immich, R. Bosch, R. Jacobs, T. Karla, M. Horstink, P. Broekx, K. Fuchigami <i>IHI Hauzer Techno Coating B.V., Venlo, Holland</i></li> </ul>
16:10  16:20	<b>S7-3</b> From Nano to Micro: When ALD meets with PVD to enhance coating performance <b>F. Papa</b> <sup>1</sup> , A. Sharma <sup>2</sup> , S. Tsianikas <sup>3</sup> , X. Maeder <sup>3</sup> , C. Guerra <sup>2</sup> <i>GP Plasma, Medina, OH, USA</i> <sup>2</sup> Swiss Cluster AG, Spiez, Switzerland <sup>3</sup> Empa Thun, Thun, Switzerland
16:20 	S7-4 Progress in laser patterning techniques for efficient mass production of flexible microelectronic devices with sputtered coatings L. Josephson, M. Simmons, M. Kleyn, J. Vlach Intellivation LLC, Loveland, CO, USA
16:30  17:00	S7-5       – Invited         Leveraging "external innovation" to enhance the success of commercializing advances in functional coatings & surface engineering         C. H. Stoessel         StoesselConsulting / SputterTek LLC, Palo Alto, CA, USA
17:00 - 17:15	Closing remarks and Visit of the facilities

## Monday & Tuesday, June 3-4, 2024

#### **POSTER PRESENTATIONS**

Location: MIL Campus – Université de Montréal Posters: Atrium B-140 – Posters will be available during both days

	Posters A: Hard & protective coatings and related applications
A1	Dynamic combinatorial 2D synthesis of materials using PVD-HiPIMS technology N. Chaâbane <sup>1</sup> , JP. Poli <sup>2</sup> , F. Schuster <sup>1</sup> <sup>1</sup> Université Paris-Saclay, CEA, INSTN, Gif Sur Yvette, France <sup>2</sup> Université Paris-Saclay, CEA, DRT, Gif Sur Yvette, France
A2	Different TiAlN coating architecture for enhanced solid particle erosion protection B. Millan-Ramos, P. Renato Avila, S. Brown, L. Martinu, J. E. Klemberg-Sapieha Department of Engineering Physics, Polytechnique Montréal, Montreal, QC, Canada
A3	Characterization of spray formed and vacuum induction melted AlSi D2 cold work tool steel V. Rodríguez <sup>1</sup> , A. Ruiz <sup>1</sup> , V. Nadimpalli <sup>2</sup> , D. Bue <sup>2</sup> <sup>1</sup> Universidad Michoacana de San Nicolás de Hidalgo, Morelia, Michoacán, Mexico <sup>2</sup> Technical University of Denmark, Kongens Lyngby, Denmark
A4	Novel approaches in surface engineering: Enhancing adhesion and stress management through interface design for wear- resistant coating T. Ebrahimi Sadrabadi <sup>1</sup> , M. Javidani <sup>1</sup> , M. Muhammed <sup>1</sup> , M. Jahazi <sup>2</sup> Department of Applied Science, University of Quebec at Chicoutimi, Chicoutimi, QC, Canada Department of Mechanical Engineering, École de Technologie Supérieure, Montreal, QC, Canada
A5	Comparison of tool performance in machining Inconel 718 superalloy Y. Wu <sup>12</sup> , N. Côté <sup>2</sup> , M. Azzi <sup>1</sup> , S. Bélanger <sup>3</sup> , E. Péloquin <sup>3</sup> , L. Martinu <sup>1</sup> , J. Klemberg Sapieha <sup>1</sup> <sup>1</sup> Department of Engineering Physics, Polytechnique Montréal, Montreal, QC, Canada <sup>2</sup> Centre Technologique En Aérospatiale, Longueuil, QC, Canada <sup>3</sup> Optimum-Canada, Mercier, QC, Canada
A6	Mechanical and tribological properties of (CoCrFeNiMn) <sub>1-x</sub> Ti <sub>x</sub> high-entropy thin films synthesized by magnetron sputtering L. Wu, T. Liang, R. Chromik McGill University, Montreal, QC, Canada
A7	Structure and mechanical properties of (Al,B,Cr,Si,Ti)-based thin films A. Kirnbauer <sup>1</sup> , P. Konecny <sup>1</sup> , R. Hahn <sup>2</sup> , S. Kolozsvari <sup>3</sup> , P. Mayrhofer <sup>1</sup> <i><sup>t</sup> TU Wien, Thin Film Materials Science Division, Vienna, Austria</i> <sup>2</sup> TU Wien, Christian Doppler Laboratory for Surface Engineering of high-performance Components, Vienna, Austria <sup>3</sup> Plansee Composite Materials GmbH, Lechbruck am See, Germany

	Monday & Tuesday, June 3-4, 2024 - continued
Locatio	TER PRESENTATIONS n: MIL Campus – Université de Montréal : Atrium B-140 – Posters will be available during both days
A8	Mechanical and tribological properties of (AlCoCrNiSi) <sub>100-x</sub> N <sub>x</sub> thin films <sup>1</sup> Department of Mining and Materials Engineering, McGill University, Montreal, QC, Canada <sup>2</sup> Department of Mechanical Engineering, Faculty of Engineering and Applied Science, Memorial University of Newfoundland, St. John's, NL, Canada
	Posters B: Functional coatings and surface modifications for biomedical, electronic and other applications
B1	<b>Epitaxially grown gold (100) surfaces for oxygen reduction reactions</b> <b>K. Kohlmann<sup>1</sup></b> , D. Guay <sup>1</sup> , A. Sarkissian <sup>2</sup> , C. Schindler <sup>3</sup> , A. Ruediger <sup>1</sup> <sup>1</sup> Centre Énergie, Matériaux, Télécommunications, Institut national de la recherche scientifique, Varennes, QC, Canada <sup>2</sup> Plasmionique Inc., Varennes, QC, Canada <sup>3</sup> Department of Applied Sciences and Mechatronics, Munich University of Applied Sciences, Munich, Germany
B2	Quantifying impact of tension on PLA chains mobility when modifying polymer exclusion nets W. Simon <sup>1</sup> , MJ. Dumont <sup>2</sup> , A. Karthikeyan <sup>3</sup> , J. R. Tavares <sup>1</sup> <sup>1</sup> Polytechnique Montréal, Montreal, QC, Canada <sup>2</sup> Université Laval, Laval, QC, Canada <sup>3</sup> University of Ottawa, Ottawa, ON, Canada
В3	Electrostatic and electrochemical doping of metal-oxides ion-gated transistors J.R. Herrera Garza <sup>1</sup> , L.P. Camargo <sup>2</sup> , R.K. Azari <sup>1</sup> , L.C. da Silva Neres <sup>3</sup> , S. Khaleel <sup>1</sup> , M.S. Barbosa <sup>4</sup> , C. Santato <sup>1</sup> , F. Soavi <sup>5</sup> <sup>1</sup> Department of Engineering Physics, Polytechnique Montréal, Montreal, QC, Canada <sup>2</sup> Chemistry Department, CCE, State University of Londrina (UEL), Londrina, PR, Brazil <sup>3</sup> Institute of Chemistry, São Paulo State University (UNESP), Araquara, SP, Brazil <sup>4</sup> Institute of Chemistry, Federal University of Goias (UFG), GO, Brazil <sup>5</sup> Department of Chemistry "Giacomo Ciamician", Alma Mater Studiorum Universitá di Bologna, Bologna, Italy
B4	Period-doubling bifurcations as route to chaos in resistively switching Hf <sub>0.5</sub> Zr <sub>0.5</sub> O <sub>2</sub> thin films S. Obernberger <sup>1</sup> , K. Kohlmann <sup>1</sup> , A. Sarkissian <sup>2</sup> , P. Antici <sup>1</sup> , C. Schindler <sup>3</sup> , A. Ruediger <sup>1</sup> <sup>1</sup> Centre Énergie, Matériaux, Télécommunications, Institut national de la recherche scientifique, Varennes, QC, Canada <sup>2</sup> Plasmionique Inc., Varennes, QC, Canada <sup>3</sup> Dept. of Applied Sciences and Mechatronics, Munich University of Applied Sciences, Munich, Germany
В5	Charge carrier transport in sepia melanin S. Khaleel, Z. Gao, A. Camus, C. Santato Polytechnique Montréal, Montreal, QC, Canada

#### **POSTER PRESENTATIONS**

Location: MIL Campus – Université de Montréal Posters: Atrium B-140 – Posters will be available during both days

B6	Boron nitride nanotube buckypaper surface functionalization by exposure to planar gliding air plasma discharge O. Mostafa <sup>1</sup> , <b>S. Walker<sup>2</sup></b> , S. Coulombe <sup>2</sup> <sup>1</sup> Department of Mechanical Engineering, McGill University, Montreal, QC, Canada <sup>2</sup> Department of Chemical Engineering, McGill University, Montreal, QC, Canada
B7	Boosting the atmospheric water harvesting of carbon-xerogels S. Alavitabari <sup>1</sup> , D. Brassard <sup>1</sup> , S. Ponton <sup>1</sup> , R. Boudreault <sup>2</sup> , PL. Girard-Lauriaut <sup>3</sup> , J. R. Tavares <sup>1</sup> <sup>(</sup> Chemical Engineering Department, Polytechnique Montréal, Montreal, QC, Canada <sup>2</sup> Awn Nanotech Inc., Dorval, QC, Canada <sup>3</sup> Chemical Engineering Department, McGill University, Montreal, QC, Canada
B8	Release of pest repellents from the surface of a biodegradable polymer D. Klassen <sup>1</sup> , A. Karthikeyan <sup>2</sup> , J. R. Tavares <sup>1</sup> , MJ. Dumont <sup>3</sup> <sup>1</sup> Polytechnique Montréal, Montreal, QC, Canada <sup>2</sup> University of Ottawa, Ottawa, ON, Canada <sup>3</sup> Université de Laval, Laval, QC, Canada
В9	Plasma processes based on aerosols for functional coating deposition M. Féron <sup>1,2</sup> , M. Cavarroc <sup>3</sup> , V. Orlandi <sup>1,2,4</sup> , T. Bourriane <sup>5</sup> , L. Stafford <sup>6</sup> , AF. Mingotaud <sup>7</sup> , M.L. Kahn <sup>2</sup> , R. Clergereaux <sup>1</sup> <sup>1</sup> Laboratoire Plasma et Conversion d'Energie - Laplace, Université de Toulouse, France <sup>2</sup> Laboratoire de Chimie de Coordination - LCC, CNRS, Université de Toulouse, France <sup>3</sup> Safran Tech, Paris, France <sup>4</sup> CNES, Toulouse, France <sup>6</sup> Department of Physics, Université de Montréal, Montreal, QC, Canada <sup>7</sup> Laboratoire de Chimie des colloïdes, polymères & assemblages complexes - SoftMat, Université de Toulouse, France
B10	Nanoparticle collection and in-flight functionalization during femtosecond pulsed laser micromachining G. Zeppetelli, AM. Kietzig, S. Coulombe Department of Chemical Engineering, McGill University, Montreal, QC, Canada
B11	Preparation of hydrocarbon thin-films by injection of pentane aerosols into an atmospheric-pressure DBD using a direct liquid reactor injector A. Yazdanpanah <sup>1</sup> , L. Cacot <sup>1</sup> , M. El Rachidi <sup>1</sup> , R. Clergereaux <sup>2</sup> , M. Kahn <sup>3</sup> , L. Stafford <sup>1</sup> <sup>1</sup> Physics Department, Université de Montréal, Montreal, QC, Canada <sup>2</sup> LAPLACE, Université de Toulouse, CNRS, INPT, UPS, Toulouse, France <sup>3</sup> LCC, CNRS (UPR 8241), Université de Toulouse, France
B12	Development of a multi-walled carbon nanotube filter for detaining immunosuppressive T-Cells and inducing the activation of effector T-Cells G. Di Placido, L. Hein, S. Coulombe <i>McGill University, Montreal, QC, Canada</i>

Monday & Tuesday, June 3-4, 2024 - continued		
POSTER PRESENTATIONS Location: MIL Campus – Université de Montréal Posters: Atrium B-140 – Posters will be available during both days		
B13	Electrophoretic deposition of a strongly adhering multi-walled carbon nanotube coating by addition of a plasma polymer interlay L. Hein <sup>1</sup> , S. Coulombe <sup>1</sup> , R. Cecere <sup>2</sup> , R. Mongrain <sup>1</sup> <sup>'</sup> McGill University, Montreal, QC, Canada	
B14	<sup>2</sup> McGill University Health Center, Montreal, QC, Canada Quantum spin pumping in normal/bearded zigzag graphene nanoribbon H. Tian <sup>1</sup> , <b>S. Wang<sup>2</sup></b> <sup>1</sup> School of Physics and Electronic Engineering, Linyi University, Linyi, China <sup>2</sup> College of Science, Jinling Institute of Technology, Nanjing, China	
B15	Enhanced Photocatalytic Degradation Efficiency of Tetracycline by Band Edge Engineering of Thin Film BiVO <sub>4</sub> /TiO <sub>2</sub> Heterostructure A. Seck <sup>1</sup> , A. Mirzaei <sup>1</sup> , Z. Shayegan <sup>1</sup> , B. D Ngom <sup>2</sup> , D. Ma <sup>1</sup> , M. Chaker <sup>1</sup> <sup>1</sup> Institut National de la Recherche Scientifique (INRS), Centre Énergie Materiaux Télécommunications, 1650, Boulevard Lionel- Boulet, Varennes, Québec, J3X 1P7, Canada <sup>2</sup> Laboratoire de Photonique Quantique, d'Energie et de Nano-Fabrication, Faculté des Sciences et Techniques, Université Cheikh Anta Diop de Dakar (UCAD), Dakar-Fann, Dakar, B.P. 5005 Sénégal	
Posters C: Optical films and energy-related applications		
C1	Stress development in amorphous optical thin films: mechanisms of stress generation and the role of the sputtering parameters P. Avila, B. Baloukas, O. Zabeida, J. Sapieha, L. Martinu Department of Engineering Physics, Polytechnique Montréal, Montreal, QC, Canada	
C2	Synthesis, microstructural, optical, and mechanical properties of SiN <sub>x</sub> thin films deposited by LPCVD and reactive sputtering, and their integration into photonic integrated circuits A. Radi <sup>1</sup> , L. Mehrvar <sup>1</sup> , B. Ahammou <sup>1</sup> , A. Zitouni <sup>1</sup> , B. Le Drogoff <sup>4</sup> , M. Chaker <sup>1</sup> , M. Ménard <sup>2</sup> ' Institut National de la Recherche Scientifique - Énergie, Matériaux et Télécommunications (INRS-EMT), Varennes, QC, Canada <sup>2</sup> Department of Electrical Engineering, École de Technologie Supérieure, Montreal, QC, Canada	
C3	Silver-based transparent conductors with improved optical performance and environmental stability P. Rumsby, B. Baloukas, O. Zabeida, L. Martinu Department of Engineering Physics, Polytechnique Montréal, Montreal, QC, Canada	
C4	Low-loss Al <sub>2</sub> O <sub>3</sub> and SiO <sub>2</sub> thin films for photonics deposited by plasma-assisted reactive magnetron sputtering P. Torab Ahmadi <sup>1</sup> , M. Chesaux <sup>2</sup> , J. Wojcik <sup>2</sup> , D. Deligiannis <sup>2</sup> , P. Mascher <sup>1</sup> , J. D. B. Bradley <sup>1</sup> <sup>1</sup> Department of Engineering Physics and Centre for Emerging Device Technologies, McMaster University, Hamilton, ON, Canada <sup>2</sup> Intlvac Inc., Halton Hills, ON, Canada	
C5	Optical and structural properties of Ag-polymer nanocomposites prepared by combination of gas phase methods Z. Krtouš <sup>1</sup> , P. Pleskunov <sup>1</sup> , T. Kosutova <sup>1</sup> , M. Cieslar <sup>1</sup> , M. Dopita <sup>1</sup> , B. Baloukas <sup>2</sup> , L. Martinu <sup>2</sup> , J. Kousal <sup>1</sup> <sup><i>i</i></sup> Charles University, Prague, Czech Republic <sup>2</sup> Department of Engineering Physics, Polytechnique Montréal, Montreal, QC, Canada	

#### POSTER PRESENTATIONS

Location: MIL Campus – Université de Montréal Posters: Atrium B-140 – Posters will be available during both days

C6	The capabilities to form periodically modulated coatings and their applications for spatial filters and polarizers L. Grineviciute <sup>1</sup> , J. Nikitina <sup>1</sup> , K. Staliunas <sup>2</sup> <sup>1</sup> Center for Physical Sciences and Technology, Vilnius, Lithuania <sup>2</sup> UPC, Dep. de Fisica, Terrassa, Barcelona, Spain
С7	a-Si:H/SiO <sub>2</sub> HR coatings for gravitational wave detection A. Lussier <sup>1</sup> , B. Baloukas <sup>2</sup> , S. Roorda <sup>1</sup> , L. Martinu <sup>2</sup> , F. Schiettekatte <sup>1</sup> <sup>'</sup> Université de Montréal, Montreal, QC, Canada <sup>2</sup> Polytechnique Montréal, Montreal, QC, Canada
C8	Exploring optoelectronic properties of magnetron-sputtered nanoparticles with finite-difference time-domain method P. Pleskunov <sup>1</sup> , Z. Krtouš <sup>2</sup> , M. Protsak <sup>1</sup> , T. Košutová <sup>3</sup> , M. Cieslar <sup>4</sup> , L. Martinu <sup>2</sup> , A. Choukourov <sup>1</sup> <sup>1</sup> Department of Macromolecular Physics, Charles University, Prague, Czech Republic <sup>2</sup> Department of Engineering Physics, Polytechnique Montréal, Montreal, QC, Canada <sup>3</sup> Department of Condensed Matter Physics, Charles University, Prague, Czech Republic <sup>4</sup> Department of Physics of Materials, Charles University, Prague, Czech Republic
С9	Bragg-reflector-enhanced electrochromic devices with adjustable optical performance M. Crouan, B. Baloukas, O. Zabeida, J. Sapieha, L. Martinu Department of Engineering Physics, Polytechnique Montréal, Montreal, QC, Canada
C10	Influence of the deposition pressure on the memory effect of sputtered electrochromic WO <sub>3</sub> thin films B. Faceira <sup>1</sup> , L. Teulé-Gay <sup>1</sup> , HY. Huang <sup>2</sup> , YC. Huang <sup>2</sup> , CL. Dong <sup>2</sup> , M. Maglione <sup>1</sup> , A. Rougier <sup>1</sup> <i>'Univ. Bordeaux, CNRS, Bx INP, ICMCB, Pessac, France</i> <i><sup>2</sup> Research Center for X-ray Science &amp; Department of Physics Tamkang University, Tamsui, Taiwan</i>
C11	Origin and nature of defects in low-emissivity coatings O. Touré, B. Baloukas, O. Zabeida, J. Klemberg-Sapieha, L. Martinu Department of Engineering Physics, Polytechnique Montréal, Montreal, QC, Canada
C12	Transparent flexible electrodes through advanced patterning approaches A. Pajak, MA. Dionne, B. Baloukas, O. Zabeida, J. Klemberg-Sapieha, L. Martinu Department of Engineering Physics, Polytechnique Montréal, Montreal, QC, Canada
	Posters D: Advanced characterization
D1	Atomistic insights into the effect of hydrogen on the structure and mechanical properties of amorphous silicon nitride Y. Ouldhnini, B. Ahammou, K. Kaur Ghuman, M. Chaker Institut National de la Recherche Scientifique (INRS), Varennes, QC, Canada

#### POSTER PRESENTATIONS

Location: MIL Campus – Université de Montréal

Posters: Atrium B-140 – Posters will be available during both days

D2	Exploring the structural and mechanical properties of deposited SiN <sub>x</sub> thin films through molecular dynamics simulations B. Ahammou, Y. Ouldhnini, K. Kaur Ghuman, M. Chaker Institut National de la Recherche Scientifique (INRS), Varennes, QC, Canada	
D3	In plasma ion beam analysis LC. Fortier <sup>1</sup> , M. Chicoine <sup>1</sup> , S. Chouteau <sup>1</sup> , M. Clausse <sup>2</sup> , É. Lalande <sup>1</sup> , A. Lussier <sup>1</sup> , G. Terwagne <sup>2</sup> , S. Roorda <sup>1</sup> , L. Stafford <sup>1</sup> , F. Schiettekatte <sup>1</sup> <sup>1</sup> Department of Physics, Université de Montréal, QC, Canada <sup>2</sup> Department of Physics, Université de Namur, Namur, Belgium	
Posters E: Special posters		
E1	How can sustainability be integrated into the research culture? L. Cacot, M. Boiteux, L. Stafford Université de Montréal, Montreal, QC, Canada	
E2	Central Facilities at Polytechnique Campus of the Thin Film Science and Technology Research Center (GCM): - Laboratory for Surface Analysis of Materials (LASM) - Microfabrication Laboratory (LMF) MH. Bernier, J. Lefebvre, C. Clément Department of Engineering Physics, Polytechnique Montréal, QC, Canada	

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## Wednesday Morning, June 5, 2024

INTERACTIVE WORKSHOPS Location: Polytechnique Montréal, Main Building Registration: B-415		
8:00 - 9:00	Welcome Desk Opens	
8:30 - 9:00	Continental breakfast	
9:00 - 10:30	Workshop A – Room B-405         Spectroscopic ellipsometry: Case and tricks of the trade         N. Hong <sup>1</sup> , B. Baloukas <sup>2</sup> 'J.A. Woollam Co, Inc., Lincoln, NE, USA         Polytechnique Montréal, Montreal, QC, Canada         Workshop B – Room B-401         Tribo-mechanical surface characterization         J. Nohava <sup>1</sup> , M. Reza <sup>1</sup> , S. Brown <sup>2</sup> 'Anton Paar TriTec SA, Corcelles, Switzerland         Polytechnique Montréal, Montreal, QC, Canada         Workshop C – Room B-429         Developing an understanding of surface chemistry - Multi-technique electron spectroscopy-based investigation         J. Lallo <sup>1</sup> , J. Lefebvre <sup>2</sup> 'Thermo Fischer Scientific,         'Polytechnique Montréal, Montreal, QC, Canada	
10:30 - 10:45	Break, coffee and refreshments – Room B-415	
10:45 _ 12:00	Continuation of the workshops	
12:00	Lunch (included) and discussions – Room B-415	

	Wednesday Afternoon, June 5, 2024	
INTERACTIVE WORKSHOPS Location: Polytechnique Montréal, Main Building Registration: Room B-415		
	Workshop A: Hands-on workshop in the laboratory – Spectroscopic ellipsometry Location: Optical characterization laboratory – $5^{th}$ floor	
13:00 	Workshop B: Hands-on workshop in the laboratory – Tribo-mechanical characterization Location: Mechanical testing laboratory – $2^{nd}$ floor	
	Workshop C: Hands-on workshop in the surface characterization laboratory Location: Laboratory for surface analysis of materials $(LASM) - 5^{th}$ floor	

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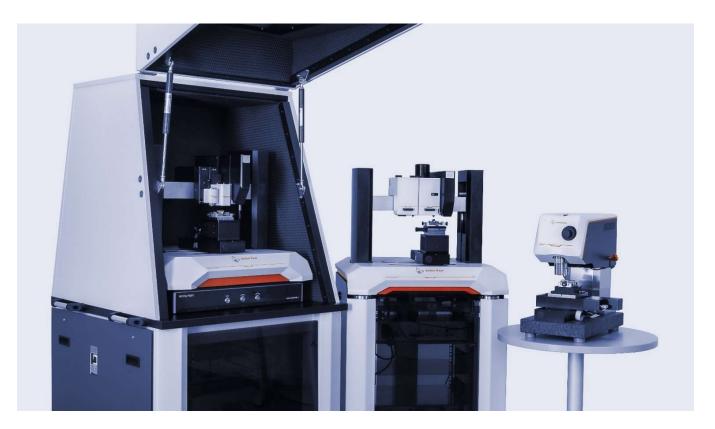
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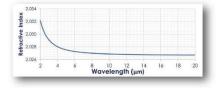
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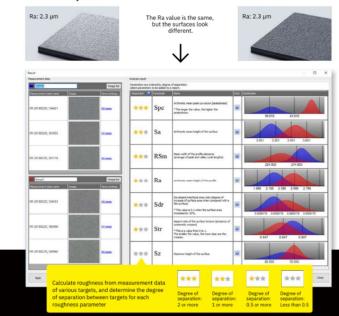
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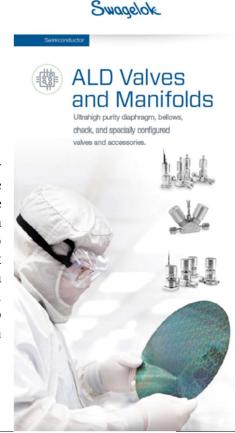


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### Exhibits, June 3-4, 2024

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# FCSE-2024 Symposium abstracts

### **KEY TO SESSION NUMBERS:**

<b>S</b> 1	Plasma-based processes
S2	Hard protective coatings
<b>S</b> 3	Bio-related, energy and other applications
S4	High entropy films
S5	Optical films
S6	Advanced characterization
<b>S</b> 7	FCSE perspectives

### Sunday, June 2, 2024

### SHORT COURSE A

 $9{:}00-12{:}00\ /\ 13{:}00-17{:}00$ 

#### Plasma deposition of thin films and related processing of materials

INSTRUCTOR:

André Anders Leibniz Institute of Surface Engineering, Leipzig, Germany

#### **Course Description**

This course is intended for students, engineers, technicians, and others interested in plasma-assisted deposition of thin film and functional coatings. A good portion of the course is dedicated to the introduction and review the fundamentals of low-temperature plasmas and discharges to produce them. While gas plasmas are often used, emphasis is put on discharges that lead to ionization of plasma with condensable species: metal or metal-containing plasmas, leading to coatings from the plasma phase. In contrast to other courses, the role of plasmas and sheaths (plasma boundaries) will be clearly distinguished and explained. This distinction will be appreciated when examples of processes with plasmas are given, including but not limited to, plasmas made by ion plating, (filtered) cathodic arcs and by high power impulse magnetron sputtering (HiPIMS). After a couple of decades of research, HiPIMS has become an industrially used extension of sputtering technology. With sputtered metals ionized, the microstructure of coatings and resulting properties can be tuned by energetic condensation even when substrates are kept near room temperature. Recent developments of HiPIMS will be discussed, including reactive HiPIMS and so-called "hybrid technology" where one of the components is HiPIMS.



André Anders has a joint appointment as the Director and CEO (Direktor und Vorstand) of the Leibniz Institute of Surface Engineering, Leipzig, Germany, and Professor of Applied Physics at the Felix Bloch Institute of Solid State Physics, Leipzig University. He assumed these positions in 2017 after working at Lawrence Berkeley National Laboratory in Berkeley, CA, USA, since 1992, where he still is a Scientist Affiliate. He studied physics in Wroclaw, Poland, Berlin, (East) Germany, and Moscow (Russia, then Soviet Union), to obtain his PhD degree from Humboldt University in Berlin in 1987. André has worked for about 35 years in basic and applied plasma physics and materials sciences. He has authored 3 books and more than 350 peer-reviewed journal papers (h-index 75, over 21,000 citations, Google Scholar 2023). His work was recognized by several awards and election to Fellow level of professional societies including APS, AVS, IEEE, and IoP. Since 2014 he is the Editor-in-Chief of Journal of Applied Physics published by AIP Publishing, Melville, NY.

### Sunday, June 2, 2024

### SHORT COURSE B

9:00 - 12:00 / 13:00 - 17:00

#### Stress evolution during thin film growth by physical vapor deposition

INSTRUCTOR: **Grégory Abadias** *CNRS-Université de Poitiers, Poitier, France* 

#### **Course Description**

Thin films produced by physical vapor deposition (PVD) techniques are usually under a stressed state, due to the mechanical constraint imposed macroscopically by the substrate on which they are deposited. Several factors are affecting the resulting stress state, which can be either tensile or compressive, with magnitude up to several GPa. The understanding and control of stress development in thin films is essential, especially for nanoscale systems, to ensure device integrity.

This short course will provide an overview on how film stress develops during growth, how it is affected by the main PVD process parameters, and how to mitigate it. The course will be structured around the following objectives:

- Describe the different stress sources in PVD thin films.
- Identify the links between growth stages and intrinsic stress evolution during polycrystalline film growth.
- Provide the basic concepts and underlying atomistic and microscopic mechanisms at the origin of stress generation and relaxation.
- Learn about stress measurement methods (wafer curvature, XRD) and their limitations.
- Understand the influence of microstructure (grain size, texture) and main process parameters (working pressure, bias voltage, vapor flux, substrate temperature) on the stress development.
- Discuss the role of energetic species, involved during magnetron sputtering, HiPIMS or ion-beam assisted deposition, on defect incorporation and compressive stress build-up.
- Gain knowledge on stress manipulation strategies to control and engineer stress for specific applications.



**Gregory Abadias** is Professor at the Physics Department of the University of Poitiers, France. He received his Ph.D. degree in materials science in 1998 at National Polytechnic Institute of Grenoble (INPG), and he is currently group leader of thin films activities at CNRS Pprime Institute (https://pprime.fr/en/home-pprime/) in Poitiers. He conducts research on a range of topics related to nanoscale thin films, including mechanical, electrical and optical properties of metallic, nitride or oxide systems as well as hard and protective coatings in the form of nanocomposites or multilayers. His current research interests focus on the understanding of thin film growth dynamics using real-time and in situ diagnostics as well as computational modelling, with main emphasis on growth manipulation strategies to control morphology and stress development in sputter-deposited metal layers. He is co-authors of more than 160 papers in peer-review journals and one book chapter on stress in PVD thin films. He was member-elected to the Scientific Council of the Physics Institute of CNRS (2019-23), as well as French representative of the Surface Engineering Division of IUVSTA for 2022-25 triennium. He has been involved in the organization of several symposia or workshops at international

conferences (ICMCTF, EMRS) and serves as Editor of Surface and Coatings Technology journal since 2016.

### ORAL PRESENTATIONS

#### Session 1 – Plasma-based processes

MODERATOR: C. H. Stoessel StoesselConsulting / SputterTek LLC, Palo Alto, CA, USA

## $8:50 \text{ S1-1} - \underline{\text{Invited}} - \text{Atomic scale heating in plasma deposition processes}$

#### A. Anders

#### Leibniz Institute of Surface Engineering, Leipzig, Germany

Deposition from the plasma phase implies the supply of energy to the growing film, namely, each of the condensing atoms and ions brings kinetic and potential energy to exactly the surface locations where the film grows. This is especially effective if growth occurs by the supply of multiply charged ions. In this contribution, the concept of atomic scale heating is explained and illustrated for the case of (V, Al)N films.



André Anders has a joint appointment as the Director and CEO (Direktor und Vorstand) of the Leibniz Institute of Surface Engineering, Leipzig, Germany, and Professor of Applied Physics at the Felix Bloch Institute of Solid State Physics, Leipzig University. He assumed these positions in 2017 after working at Lawrence Berkeley National Laboratory in

Berkeley, CA, USA, since 1992, where he still is a Scientist Affiliate. He studied physics in Wroclaw, Poland, Berlin, (East) Germany, and Moscow (Russia, then Soviet Union), to obtain his PhD degree from Humboldt University in Berlin in 1987. André has worked for about 35 years in basic and applied plasma physics and materials sciences. He has authored 3 books and more than 350 peer-reviewed journal papers (h-index 75, over 21,000 citations, Google Scholar 2023). His work was recognized by several awards and election to Fellow level of professional societies including APS, AVS, IEEE, and IoP. Since 2014 he is the Editor-in-Chief of Journal of Applied Physics published by AIP Publishing, Melville, NY.

## 9:20 S1-2 – What is the temperature of a target during DC magnetron sputtering?

#### S. Muhl, J. Cruz, A. Garzon

Instituto de Investigaciones en Materiales, UNAM, Mexico City, Mexico The temperature of a 2" diameter water-cooled titanium target was measured during sputtering as a function of the DC plasma power (power densities of 1.0, 2.2 and 4.1 W/cm<sup>2</sup>) and Ar gas pressures of 10 to 60 sccm. The measurements were made using an electrically floating fine, 0.005" wire, type K chromel-alumel thermocouple. Typically, the temperature difference between the centre of the target and inside the racetrack was more than 200  $^{\circ}$ C, the racetrack temperature increased almost linearly with the applied power to a maximum value of ~840  $^{\circ}$ C.

The target temperature was also investigated as a function of the  $N_2$  gas concentration in the Ar gas mixture (1 to 20%), and these measurements were complemented with the analysis of the elemental composition of the deposits prepared under the different conditions.

Finally, comparative radial temperature measurements were made of new Ti and graphite targets.

## 9:30 S1-3 – <u>Invited</u> – Advanced laser diagnostics on reactive plasmas at interfaces

#### S. Reuter

#### Polytechnique Montréal, Montreal, QC, Canada

Non-thermal atmospheric pressure plasmas provide high reactivity at low gas temperatures, making them ideal for coating and functionalization of thermally sensitive surfaces. Focus is currently on cold plasma jets and their potential for plasmabased surface functionalization in industrial and medical applications [1]. By adding precursors to the plasma jet feed gas, functional coatings and surface modifications are created. To achieve desired surface properties of plasma-treated substrates, more detailed knowledge of the plasma processes is needed. The presentation discusses state of the art optical diagnostics for the characterization of plasma jets' reactive species, as well as electric and flow fields [2-4]. Highlighted are the advantages and challenges of ultrafast time resolved laser spectroscopy in combination with electrical diagnostics of cold reactive plasma jets.

[1] Booth, J.-P., Mozetič, M., Nikiforov, A. & Oehr, C., 2022. Foundations of plasma surface functionalization of polymers for industrial and biological applications. PSST 31 103001.

[2] Schäfer, J., Foest, R., Reuter, S., Kewitz, T., Sperka, J. & Weltmann, K. D., 2012. Laser schlieren deflectometry for temperature analysis of filamentary non-thermal atmospheric pressure plasma. Rev Sci Instrum, 83, 103506.

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Stephan Reuter is full professor for plasma physics and spectroscopy at the Engineering Physics Department of Polytechnique Montréal and TransMedTech chair for plasma medicine. Following his PhD at University Duisburg-Essen in Germany, he first was research fellow at the center for plasma physics at Queen's University

Belfast, UK and then established and led the "plasmatis" physics research group for plasma medicine at the Leibniz Institute INP Greifswald, Germany. From 2017 to 2018, he was Feodor-Lynen Fellow at Princeton University. He is alumnus of the Alexander von Humboldt Foundation.

### Monday 10:30 - 12:10 am, June 3, 2024

### ORAL PRESENTATIONS

#### Session 2 – Hard protective coatings

MODERATOR: J.-W. Lee Ming Chi University of Technology (MCUT), Taiwan

# 10:30 S2-1 - Invited - Low-temperature synthesis of dense, hard, stress-free ceramic coatings using metal-ion irradiation

I. Petrov<sup>1,2</sup>, L. Hultman<sup>1</sup>, J. Greene<sup>1,2</sup>, G. Greczynski<sup>1</sup>

<sup>1</sup> Thin Film Physics Division, Department of Physics (IFM), Linköping University, Linköping, Sweden <sup>2</sup> Materials Research Laboratory, University of Illinois, Urbana, IL, USA

Ion irradiation is a key tool for controlling epitaxy-tonanostructure, phase content, and physical properties of refractory ceramic thin films grown by magnetron sputtering. Until recently, thin film growth relied on enhancing adatom mobility in the surface region by inert and/or reactive gas ion irradiation to obtain dense layers at low deposition temperatures. Development of high-power pulsed magnetron sputtering (HiPIMS), which provides metal-ion plasmas with tunable degree of ionization, enabled systematic studies of the effects of metal-ion irradiation on properties of refractory ceramic thin films. A motivation for the use of metal-ions stems is that they are film constituents, hence they can provide the benefits of ionmixing without causing the high compressive stresses associated with trapping of gas ions at interstitial sites.

This presentation reviews growth experiments of transition metal nitride model systems including TiAlN, TiSiN, VAlN, TiTaN, TiAlTaN, and TiAlWN [1]. Film synthesis is carried out in a hybrid configuration with one target powered by HiPIMS and other operated in direct current magnetron sputtering (DCMS) mode. A substrate bias potential  $V_s$  is synchronized with the metal-ion-rich portion of the HiPIMS pulses to control the metal-ion energy. The time-resolved mass spectrometry analyses performed at the substrate position enables us to suppress the role of gas ion irradiation and select intense  $M_1^{n^+}$  and  $M_2^{n^+}$  metal-ion fluxes (n = 1, 2) to study the effects on film growth kinetics over a wide range of  $M_1M_2N$  alloy compositions. We establish new and quite different pathways for nanostructure control when using either light or heavy metal ions.

Irradiation with lower-mass metal-ions (Al<sup>+</sup> or Si<sup>+</sup>) results in near-surface implantation with the depth controlled by  $V_s$ amplitude. This enables synthesis of *metastable* ternary cubic Me<sub>1</sub>Me<sub>2</sub>N solid solutions far above the Me<sub>1</sub>N concentration range achieved by DCMS [2]. At the other extreme, bombardment of the growing film surface with pulsed high-mass metal ion fluxes (W<sup>+</sup> or Ta<sup>+</sup>) [3] during hybrid HiPIMS/DCMS high-rate deposition of dilute Ti<sub>1-x</sub>Ta<sub>x</sub>N, Ti<sub>1-x</sub>Al<sub>x</sub>Ta<sub>y</sub>N, and Ti<sub>1-x</sub>  $_{\rm y}$ Al<sub>x</sub>W<sub>y</sub>N alloys provides high fluxes of low energy recoils and results in fully-dense, low-stress, hard and superhard coatings without external substrate heating (temperature  $\leq 130$  °C). In addition to energy savings, this approach dramatically expands the application of such coatings on temperature sensitive substrate.

For cubic-TiAlWN, we recently discovered that Guinier-Preston (GP) zone hardening - previous known from soft light-metal alloys - can operate in a refractory ceramic [4]. The present GP hardening at 1000 °C is by the formation of atomic-plane-thick W populating {111} planes.

[1] G. Greczynski, I. Petrov, J.E. Greene, and L. Hultman, *J. Vac. Sci. Technol. A* 37 (2019) 060801.

[2] G. Greczynski, S. Mráz, J.M. Schneider, L. Hultman, *J. Appl. Phys.* 127 (2020) 180901.

[3] G. Greczynski, L. Hultman I. Petrov, J. Appl. Phys. 123 (2023) 140901.

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**Ivan Petrov** is a Professor of Physics at Linköping University, Sweden. He was a Professor of Materials Science and Principal Research Scientist at the Materials Research Laboratory (1998-2010), and Director of the Center for Microanalysis of Materials at the University of Illinois. Ivan earned his Ph.D. in Physics from the Bulgarian Academy of

Sciences and received a Doctor Honoris Causa Degree from Linköping University, Sweden. He has published over 350 refereed papers cited  $> 22\ 000$  times with H-index of 77. Ivan is an Editor of Surface and Coatings Technology. He is a Fellow and Honorary Member of AVS and received the 2009 Bunshah Award from the ASED, and the 2013 AVS John Thornton award" for his seminal contributions in determining the role of low-energy ion/surface interactions for controlling microstructure evolution during low-temperature growth of transition-metal nitride layers." In 2017 he received the Lifetime Achievement Award from the Taiwan Association for Coatings and Thin Film Technology. He has been elected as Chair of the Surface Engineering Division of IUVSTA 2007-2022.

## 11:00 S2-2 – Steered high-power-density plasma sputtering as an alternative to HiPIMS

**K. Thomas<sup>1</sup>**, F. Klimashin<sup>2</sup>, A. Lümkemann<sup>1</sup>, J. Kluson<sup>1</sup>, M. Ucik<sup>1</sup>, M. Jilek<sup>1</sup>, J. Michler<sup>2</sup>, T. Edwards<sup>2</sup>

<sup>1</sup> Platit AG, Granges, Switzerland <sup>2</sup> EMPA, Dübendorf, Switzerland

Thanks to continued advances in HiPIMS, sputter technology beginning to close the performance gap to cathodic arc evaporation for industrial-scale deposition of hard coatings. This is achieved through temporal compression: the deposition energy is applied in short bursts to realize higher power densities. We demonstrate that spatial compression is a viable alternative approach: the deposition energy can instead be concentrated onto a small target area to achieve similar benefits. Used in conjunction with a rotating cylindrical target and a steered magnet precise control over deposition and unrivaled homogeneity in target wear are feasible.

Steered high-power-density plasma sputtering was used in conjunction with two compositions of AlCr targets to produce AlCrN coatings as well as with a graphite target to deposit a t-aC coating. Peak power density up to 840 W/cm<sup>2</sup> were readily achieved, significantly higher than the 10 to 100 W/cm<sup>2</sup> typical for DC sputtering with stationary magnets and not significantly lower than the 1000+ W/cm<sup>2</sup> offered by HiPIMS systems. The coating hardness, fracture toughness, wear resistance, adhesion to both steel and tungsten carbide substrates, chemical composition, roughness, and other properties were evaluated. Initial results indicate that coatings produced using this technology are comparable with the best coatings available produced using cathodic arc evaporation, conventional sputtering, and HiPIMS.

## 11:10 S2-3 – Influence of Al-Ti ratio and bias on the structure and mechanical properties of AlTiN coatings

J. Nohava<sup>1</sup>, P. Hausild<sup>2</sup>, J. Kalas<sup>3</sup>, S. Zierler<sup>4</sup>, J. Sondor<sup>3</sup>

<sup>1</sup> Anton Paar TriTec SA, Corcelles, Switzerland <sup>2</sup> Czech Technical University in Prague, Prague, Czech Republic

<sup>3</sup> Platit, s.r.o. Roznov pod Radhostem, Czech Republic

<sup>4</sup> Anton Paar, Graz, Austria

AlTiN coatings have been used for enhancing machining performance for several decades and they are now routinely produced by many companies. Nevertheless, their performance is limited in more demanding machining because of their insufficient wear resistance. An ongoing research therefore focuses on improving the mechanical and wear properties of the AlTiN. In our work three ratios of Al:Ti (50:50, 60:40, 67:33) and three levels of bias (40 V, 80 V, 120 V) in arc deposition of AlTiN coating were used and their influence mechanical and wear properties was investigated. It is expected that higher Al content will lead to higher hardness, but it might lead to creation of softer hexagonal phase - which higher deposition bias should suppress. XRD measurements indeed showed that the hexagonal phase was present in the 67:33 coating but it was suppressed by higher bias. Hardness of the coatings increased by ~10% with the 120 V bias for all Al:Ti ratios. Pin-on-disc tribological tests revealed that coefficient of friction (CoF) was ~0.6 for the 50:50 and 67:33 samples. On the 60:40 coating a removal of the coating was indicated by change of CoF to ~0.8. The coating removal was confirmed by SEM observations. The wear resistance was slightly higher for higher bias, irrespective of the Al:Ti ratio. This shows that the deposition bias has bigger impact on the wear performance compared to the Al:Ti ratio. Our study contributes to the understanding of the relations between deposition parameters and mechanical properties of more wear resistant AITiN coatings.

[1] Zhang, Q, Zhengtao W, Yu X. X, Qimin W, Li Ch, and Kwang H K. "Improving the Mechanical and Anti-Wear Properties of AlTiN Coatings by the Hybrid Arc and Sputtering Deposition." Surface and Coatings Technology 378 (2019): 1-8.

# 11:20 S2-4 – Effect of substrate material on the tribological behaviour of AlTiCrN/AlTiN-coated tool steels

M. Muhammed<sup>1</sup>, **M. Javidani<sup>1</sup>**, T. E. Sadrabadi<sup>1</sup>, M. Heidari<sup>2</sup>, T. Levasseur<sup>2</sup>, M. Jahazi<sup>3</sup>

<sup>1</sup> Department of Applied Science, University of Quebec at Chicoutimi, QC, Canada

<sup>2</sup> DK SPEC, St-Nicolas, QC, Canada

<sup>3</sup> Department of Mechanical Engineering, École de Technologie Supérieure, QC, Canada

Understanding the influence of the substrate on the tribological performance of a coated material is very crucial as it provides valuable insights into material selection for optimized service performance. In this study, the effect of substrate material on the tribological behaviour of AlTiCrN/AlTiN-coated tool steels was investigated. Two grades of AISI A8 tool steel (denoted as AISI A8 mod I and II) and AISI W360 tool steels were used as the substrate materials, while the coating deposition was by cathodic arc evaporation physical vapour deposition technique. The wear resistance of the coated substrates was characterized using the ASTM G65 test, while the adhesion strength was assessed using the Daimler-Benz test and optical microscopy. The hardness and roughness of the coatings were evaluated using nanoindentation and profilometry, respectively. Scanning electron microscopy and energy dispersive X-ray techniques were used for microstructural characterization. The results of the investigation revealed that the thickness of the coating was in the order of AISI A8 mod II > AISI A8 mod I > AISI W360. Meanwhile, the wear resistance assessment showed that AISI A8 mod II exhibited superior wear performance while the AISI A8 mod I and AISI W 360 showed comparable wear performance. However, the adhesion strength of all the coated substrates was similar, exhibiting the HF2 failure mode. It could be concluded that the substrate material affects the wear resistance of the coated tool steels.

# 11:30 S2-5 - Insights on the pulsed-DC powder-pack boriding process: The role of the electric charge on the growth of the boride layer and the semiconductor behavior of the boriding media

**M. Olivares-Luna<sup>1</sup>**, J. L. Rosales-Lopez<sup>1</sup>, L. E. Castillo-Vela<sup>1</sup>, K. D. Chaparro-Pérez<sup>1</sup>, A. M. Delgado-Brito<sup>2</sup>, I. Mejía-Caballero<sup>1</sup>, I. E. Campos-Silva<sup>1</sup>

<sup>1</sup> Instituto Politécnico Nacional, Grupo Ingeniería de Superficies, SEPI-ESIME, Mexico City, Mexico <sup>2</sup> Tecnológico de Estudios Superiores de Jocotitlán, Jocotitlán, Mexico

In pursuit of innovating the conventional powder-pack boriding process by introducing an electrical driving force, novel findings regarding the kinetics growth of boride layers produced on an AISI 8620 steel through the pulsed-DC powder-pack boriding process (PDCPB) were obtained. The PDCPB accelerates B diffusion on surface of the specimen, resulting in an augmentation of the growth kinetics around 12 % and 15 % for FeB and Fe<sub>2</sub>B, respectively, compared to those observed in the conventional boriding process. Additionally, the effect of polarity inversion half-cycles on the growth of the FeB-Fe<sub>2</sub>B layer during the PDCPB was studied. The experiments were conducted at temperatures of 850 °C, 900 °C, and 950 °C, with exposure times of 1800 s, 2700 s, and 3600 s, and polarity inversion half-cycles of 30 s and 50 s, maintaining a constant current density of around 177 mA cm<sup>-2</sup>. An estimation of the electric charge (q) using a transfer function considering minimal and maximum temperatures was achieved. It was confirmed that with a symmetrical inversion, q was similar for both 30 s and 50 s polarity inversion half-cycles, indicating no influence on the growth kinetics of the boride layers.

# 11:40 S2-6 – $\underline{Invited}$ – Thin film materials design & some thoughts on complexity and sustainability

#### J. M. Schneider

#### Materials Chemistry, RWTH Aachen University, Aix-la-Chapelle, Germany

Designing the next generation of thermally and chemically stable thin films without utilizing trial and error-based methodologies requires truly predictive computational approaches. Important design criteria for protective thin film materials are, besides phase formation, mechanical behavior as well as thermal - and chemical stability. Examples of predictions thereof showcasing so-called MAB phases [1], transition metal nitrides [2], and transition metal aluminum nitrides [3] and transition metal aluminum diborides [5] which are chemically modified will be presented. Furthermore, the generation of point defects in transition metal aluminum nitrides by ion bombardment is predicted [5,6]. All aforementioned predictions are critically appraised by experimental data. Implications for future design efforts will be discussed also in the context of (chemical and structural) complexity as well as sustainability.

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[2] P. Ondračka, M. Hans, D. Holzapfel, D. Primetzhofer, D. Holec, J. M. Schneider, Ab initio-guided X-ray photoelectron spectroscopy quantification of Ti vacancies in  $Ti_{1-\delta}O_xN_{1-x}$  thin films; *Acta materialia* 230, 117778 (2022), [doi.org/10.1016/j.actamat.2022.117778]

[3] D. M. Holzapfel, D. Music, M. Hans, S. Woof-Goodrich, D. Holec, D. Bogdanovski, M. Arndt, A. O. Eriksson, K. Yalamanchili, D. Primetzhofer, C. H. Liebscher, J. M. Schneider, Enhanced thermal stability of (Ti,Al)N coatings by oxygen incorporation, *Acta Materialia* 218, 117204 (2021), [doi.org/10.1016/j.actamat.2021.117204]

[4] A. H. Navidi Kashani, S. Mráz, D. Holzapfel, M. Hans, L. Löfler, P. Ondračka, D. Primetzhofer, J. M. Schneider, Synthesis and oxidation behavior of  $Ti_{0.35}Al_{0.65}B_y$  (y = 1.7-2.4) coatings, *Surface and coatings technology* 442, 128190 (2022), [doi.org/10.1016/j.surfcoat.2022.128190]

[5] S. Karimi Aghda, D. Music, Y. Unutulmazsoy, H.H. Sua, S. Mráz, M. Hans, D. Primetzhofer, A. Anders, J.M. Schneider, Unravelling the ion-energy-dependent structure evolution and its implications for the elastic properties of (V,Al)N thin films, *Acta Materialia* 214, 117003 (2021), [doi.org/10.1016/j.actamat.2021.117003]

[6] D. Holzapfel, D. Music, S. Mráz, S. Aghda, M. Etter, P. Ondračka, M. Hans, D. Bogdanovski, S. Evertz, L. Patterer, P. Schmidt, A. Schökel, A. O.Eriksson, M. Arndt, D. Primetzhofer, J. Schneider, Influence of ion irradiation-induced defects on phase formation and thermal stability of Ti<sub>0.27</sub>Al<sub>0.21</sub>N<sub>0.52</sub> coatings, *Acta Materialia* 237, 118160 (2022), [doi.org/10.1016/j.actamat.2022.118160]



Jochen M. Schneider, Ph.D., is Professor of Materials Chemistry at RWTH Aachen University, Germany. His research focus is quantum-mechanically guided design of thin films regarding thermal and chemical stability as well as elasticity. He also designs self-reporting materials.

Jochen has been awarded the Sofya Kovalevskaya Prize by the Alexander von Humboldt Foundation for excellence in thin film materials science research in 2001 and was named a Fellow of American Vacuum Society (AVS) in 2013. In 2015 he was appointed as Max Planck Fellow. Also, in 2015 Jochen was named RWTH Fellow. In 2020 he was the Bill Sproul Award and Honorary ICMCTF Lecture Recipient. In 2022 received the Rudolf-Jaeckel-award of the German Vacuum Society to recognize outstanding achievements in vacuum-based sciences. In 2023 he was appointed as Honorary doctor of the Faculty of Science and Technology, Uppsala University, Sweden.

### ORAL PRESENTATIONS

#### Session 3 – Bio-related and other applications

MODERATOR: **S. Reuter** *Polytechnique Montréal, Quebec, Canada* 

# 13:30 S3-1 – $\underline{Invited}$ – Advancing biomedical applications through plasma surface modification: A promising frontier

#### S. Carvalho

*CEMMPRE, Department of Mechanical Engineering, University of Coimbra, Portugal* 

Significant advances have been made in the technology of biomedical coatings and materials. This talk will provide an extensive review of coating types and surface modifications for biomedical applications. In many cases, side by side with traditional properties, like wear and corrosion resistance, biomaterials have to be compatible with body tissues and fluids, possess anti-microbial activity and, in specific cases, provide a good compatibility of the material with the human body (e.g. osseointegration). It is difficult to find a unique material with all these functionalities, reinforcing the importance of surface engineering to supply new functionalities. The topic of this talk is centred on surface modification of materials, traditionally used for biomedical applications, in order to improve their performance for specific cases. Different surface modification methods will be presented and potential applications such as orthopaedic, cardiovascular and urethral stents, biosensors, and dental implants will be discussed. Several case studies of antimicrobial coatings and bioactive surfaces will be presented as well.



**Sandra Carvalho** is Full Professor at the University of Coimbra (UC). She obtained her PhD in Physics in 2004, with a work carried out in Portugal, France, the Netherlands and Germany, in the field of hard PVD coatings.

After PhD, her scientific activity has been focused on the development of coatings

and thin films, as well as surface treatment to enhance the performance of various components. In this regard, she leads a Surface Modification and Functionalization group (http://orcid.org/0000-0002-3643-4973).

Sandra is the scientific coordinator at UC of three Mobilizing Agendas for Business Innovation within the scope of the PRR – Portuguese Recovery and Resilience Facility launched by the European Commission, involving more than 100 members (88

companies and 15 R&D institutions and 5 associations) and an investment for UC of €7 million.

Sandra is member of the European Joint Committee on Plasma and Ion Surface Engineering and member of the Executive Committee of Advanced Surface Engineering Division of the American Vacuum Society (AVS). She is President of the Portuguese Materials Society (SPM) since 2023. Sandra serves as vice-director of the FCTUC, with responsibilities in Research, Innovation, and Knowledge Transfer.

# 14:00 S3-2 – Towards a durable thin hydrophobic textile finishing: light-curing process "photopolymerization" for stretch textiles

A. Ibrahim, J. Decaens, O. Vermeersch, V. Izquierdo

#### Groupe CTT, Saint-Hyacinthe, QC, Canada

Century-old textile processing and finishing techniques have been subject to incremental improvements for several decades. Finishing treatments correspond to the final stages that the fabric undergoes before leaving the factory. They are made to improve already existing properties such as softness, feel or wrinkle resistance. Among the traditional finishing processes in the textile industry, there is, among other things, coating. The majority use of aqueous formulations with mass percentages of water that can exceed 70% justifies the need for heating stages at high temperatures that vary according to the type of fiber. This limits the finish of the stretch supports. One type of drying technology already widely used in the coatings and varnishes, printing and paper industry is UV irradiation drying (photopolymerization). The application of light-curable systems is a fast, environmentally friendly and more energy-efficient alternative to traditional drying or thermal curing processes. In times of rising energy prices and growing ecological awareness, the CTT Group has initiated the project to develop a hydrophobic light-curing coating suitable for stretch supports. A light-curing silicone based formulation has been developed. This solvent-free formulation made it possible to achieve the finish at room temperature in 5 times less time (30 seconds for 2 to 3 minutes usually required thermally). This switch from the thermal process to the photochemical process will ensure a reduction (an estimate based on Quebec-2020 data) of 10x the equivalent of carbon dioxide per kilowatt-hour consumed.

## 14:10 S3-3 – Smart materials for dynamic glazings - opportunities for energy savings and control

#### B. Baloukas

### Department of Engineering Physics, École Polytechnique de Montréal, Montréal, Québec, H3C 3A7, Canada

Energy demands are at an all-time high. While we can continue to increase our energy production, we must also, in tandem, develop and promote means of saving it. For instance, silverbased low-emissivity coatings are a staple in most modern buildings and allow for reduced heating and cooling loads. While beneficial, such coatings are static and unable to adapt to seasonal environmental changes. This is where so-called smart or active materials come into play.

In this talk, an overview of the main smart window requirements will first be given. Will follow an overview of our most recent work on inorganic electrochromic (WO<sub>3</sub>) and thermochromic (VO<sub>2</sub>) materials. While these materials offer great potential, we will finally address their multiple challenges regarding their production, integration, management and LCA.

### Monday 16:30 – 17:20, June 15, 2021

### **EVENING LECTURE**

MIL Campus – Université de Montréal, Room A-1502.1

MODERATOR: L. Martinu Polytechnique Montréal, Quebec, Canada

# 16:30 Holistic life cycle engineering for a sustainable circular economy

#### C. Herrmann

#### Technische Universität Braunschweig and Fraunhofer Institute for Surface Engineering and Thin Films, Brunswick, Germany

Despite significant improvements in the eco-efficiency of individual products and processes, the global environment has witnessed a staggering rise in pollution. To ensure a sustainable future in engineering, it is imperative to align micro-level engineering decisions with macro-level sustainability principles, like the concept of planetary boundaries that recognize the finite capacity of the Earth's climate and ecosystems. This presentation will introduce a methodical approach that aids in pinpointing and prioritizing mitigation strategies as valuable input for life cycle engineering endeavours. Case studies within the field of surface engineering will be showcased to illustrate the practical application of this approach.



Prof. Dr.-Ing. Christoph Herrmann is university professor for Sustainable Manufacturing & Life Cycle Engineering and co-director of IWF, Institute of Machine Production Tools and Technology, Technische Universität Braunschweig as well as director of the Institute Fraunhofer for Surface Engineering and Thin Films IST.

### ORAL PRESENTATIONS

#### Session 4 – High entropy films

MODERATOR: J. M. Schneider *RWTH Aachen University, Germany* 

8:40 S4-1 – <u>Invited</u> – Effect of carbon on the microstructure and properties of TiZrNbTaFeC high entropy alloy carbide coatings

**J.-W. Lee<sup>1,23,4</sup>**, I. Rahmadtulloh<sup>1,5</sup>, B.-S. Lou<sup>6,7</sup>, C.-J. Wang<sup>5</sup>

<sup>1</sup> Department of Materials Engineering, Ming Chi University of Technology, New Taipei, Taiwan

<sup>2</sup> Center for Plasma and Thin Film Technologies, Ming Chi

University of Technology, New Taipei, Taiwan

<sup>3</sup> Department of Mechanical Engineering, Chang Gung

University, Taoyuan, Taiwan

<sup>4</sup> High Entropy Materials Center, National Tsing Hua University, Hsinchu, Taiwan

<sup>5</sup>Department of Mechanical Engineering, National Taiwan

University of Science and Technology, Taipei Taiwan

<sup>6</sup> Chemistry Division, Center for General Education, Chang Gung University, Taoyuan, Taiwan

<sup>7</sup> Department of Orthopaedic Surgery, New Taipei Municipal TuCheng Hospital, Chang Gung Memorial Hospital, Taiwan

Research on high entropy alloys [1] and multicomponent alloys [2] has brought about a new era in materials design, greatly impacting the research and development of new materials. High entropy alloys and multicomponent alloys already present very promising properties, such as high fracture resistance in cryogenic temperatures, high strength at high temperatures, good oxidation resistance, good wear and erosion resistance, etc. Coatings based on high entropy alloy and multicomponent alloy concepts have been widely explored in academia and industry. Several researchers have studied the microstructural and mechanical properties of high entropy alloy carbide coatings and confirmed their low friction, high hardness, and excellent corrosion resistance [3,4]. In this study, TiZrNbTaFeC high entropy alloy carbide (HEAC) coatings were fabricated using different acetylene (C<sub>2</sub>H<sub>2</sub>) gas flow ratios through the superimposed high power impulse magnetron sputtering (HiPIMS) and medium frequency (MF) sputtering system. The phase structure of HEAC coatings was explored by XRD and TEM. The FE-EPMA and FE-SEM were used to analyze the chemical compositions and microstructures of HEACs. The nanoindenter, scratch tester, and pin-on-disk wear tester were employed to study the hardness, adhesion, and wear resistance, respectively. The corrosion resistance of HEAC coatings was evaluated by the potentiodynamic polarization test in a 3.5%

NaCl aqueous solution at room temperature. It showed that the tribological performance and corrosion resistance of TiZrNbTaFeC HEAC coatings were improved by increasing carbon contents. Effects of carbon content on the phase, microstructure, hardness, adhesion, pin-on-disk tribological performance, and corrosion resistance of TiZrNbTaFeC coatings were explored in this work.

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**Jyh-Wei Lee** is a Distinguished Professor at the Department of Materials Engineering at the Ming Chi University of Technology (MCUT), Taiwan, and a Joint Appointment Professor, at the Department of Mechanical Engineering at Chang Gung University, Taiwan. He has been the Director of the Center for Plasma and Thin Film Technologies (CPTFT) since 2021

and the Director of the International Ph.D. Program in Plasma and Thin Film Technology, MCUT, since 2023. Prof. Lee is the Chair of the AVS-Taiwan Chapter and a member of the Editorial Board of Surface & Coatings Technology, Applied Surface Science Advances, and China Surface Engineering. He is the AVS ASED Program Committee member. Prof. Lee is the Program Chair of ICMCTF2023 and General Chair of ICMCTF2024. He also serves as an International Program Committee Member, Symposium Chair, and Session Chair of several International Conferences, such as ICMCTF2015-2019, AEPSE2017-2023, ISSP2019, TACT2015-2023, PSE2022, PSE2024, etc. He was the 10<sup>th</sup> President of the Taiwan Association for Coating and Thin Film Technology (TACT), Taiwan from 2018 to 2019. Prof. Lee was the Dean of the College of Engineering, Tungnan University (TNU), Taiwan, from 2007 to 2010, and Director of the Research Center for Micro/Nanotechnologies, TNU, from 2005 to 2010.

His research focuses on developing plasma-based thin film technologies to enhance the properties and performance of functional thin films and coatings used for cutting tools, molding dies, surgical instruments, optical, antibacterial, and pollution treatments. He also investigates the nanocomposite and nanolaminated nitride, carbonitride and boronitride hard coatings for tribological applications, corrosion, and oxidation protection in related industries. Recently, he has worked on the research and development of high entropy alloy thin films and thin film metallic glass materials, which can be applied in the corrosion resistance, high-temperature, and biomedical fields. Prof. Lee is skilled in high power impulse magnetron sputtering (HIPIMS), pulsed DC magnetron sputtering, cathodic arc evaporation deposition and plasma electrolytic oxidation techniques, plasma diagnosis and feedback control, nanoindentation, AFM and related nanomechanical testing methods. Prof. Lee has some research on cold atmospheric plasma applications in medicine and health care. He also studied the chromizing and aluminizing processes for the Fe, Ni, and Cobased alloys to prolong their surface life at high temperatures in the past twenty years.

Prof. Lee is the PI and Co-PI of more than 30 projects from the Taiwan government and industries, with a total budget of around 7.0 million US\$ in the past four years. He holds 13 patents and has published 205 SCI journal papers and over 30 keynote/invited lectures in the field of PVD and related surface engineering technologies. The H-index of his published paper is 42. He is also listed in the World's Top 2% Scientists published by Stanford University from 2020 to 2022.

# 9:10 S4-2 – Advanced microscopic characterization strategies to better understand dynamics of Zr-Cu-Ag PVD thin film metallic glasses

**P. Steyer<sup>1</sup>**, L. Roiban<sup>1</sup>, S. Dassonneville<sup>1</sup>, A. Borroto<sup>2</sup>J.-F. Pierson<sup>2</sup>

<sup>1</sup> INSA de Lyon, Laboratoire MATEIS, Villeurbanne, France <sup>2</sup> Université de Lorraine, Institut Jean Lamour, Nancy, France

Evolution of nanostructured thin films is closely related to their small scale. Therefore, adapted characterization tools and techniques have to be developed, to highlight such relationships. The talk will focus on advanced surfaces such as thin film metallic glasses (TFMGs).

Metallic glasses (MGs) have been intensively studied since the 60's, for their amorphous structure and associated properties. However, applications of MGs have stayed limited due to the fast quenching imposed to limit the crystallization process, and leading to small pieces of multicomponent materials. The condensation from the vapor phase to form a solid film in PVD process is another way to design metallic glasses. TFMGs indeed may show, for instance, particular interest in terms of physicochemical and bactericide behaviors, coupled with an enhanced ductility [1]. Thermal stability of such amorphous metals nevertheless remains an issue, so that we have adapted a nonconventional in situ technique, high-temperature scanning indentation (HTSI) [2], to monitor the physical changes occurring in ZrCu-TFMGs during heat treatment. Thanks to this high-speed nanoindentation technique, the entire mechanical evolution with temperature was characterized in only a few hours. A complementary study was also done in parallel with the same film exposed to the same thermal conditions, at the TEM scale using specific heating chip. Further interesting antibacterial properties will also be presented, and correlated with Ag additions.

# 9:20 S4-3 – Cold sprayed anti-biofouling coatings based on high entropy alloys

#### M. Ettelaei, S. Alidokht

#### Department of Mechanical Engineering, Memorial University of Newfoundland, St. John's, NL, Canada

Marine structures, including ships and offshore facilities, constantly face environmental challenges such as saltwater exposure, biofouling, and temperature fluctuations. Biofouling, the accumulation of aquatic organisms on these structures, elevates ship hull weight and roughness, resulting in high frictional resistance and increased fuel consumption. Moreover, it causes corrosion in metal structures, posing potential risks to marine equipment integrity and safety. The inadvertent release of biofouling organisms during cleaning or relocation of submerged structures further threatens human health, the aquatic environment, and socio-economic values. Addressing this, the urgent development of eco-friendly coatings to prevent and manage biofouling is imperative. This research aims to pioneer anti-biofouling coatings through cold spray technology. Leveraging high entropy alloys (HEA), these coatings will either inherently possess antifouling properties or serve as matrices for doped antifouling agents. Specifically, this study focuses on exploring cold spray of CoCrFeMnNi (cantor allov) combined with varving copper weight ratios. The link that displays between process, structure, property, and performance in these coatings will be explored and applied to materials and design. The outcome of the proposed research will make marine operations less energy-intensive, safer, and less costly, protect marine life, and contribute to the blue economy.

# $9:30 \text{ S4-4} - \underline{\text{Invited}} - \text{High-entropy Hägg phases; A case study of nitrides, carbides, and diborides}$

#### P. H. Mayrhofer

### Institute of Materials Science and Technology, TU Wien, Vienna, Austria

So-called high-entropy materials often outperform their lowerentropy relatives in various aspects. Compared to metallic highentropy alloys, little is known for high-entropy intermetallics, such as the Hägg phases (which include the nitrides, carbides, and diborides of the transition metals). The term "high-entropy" is often used also for this type of materials if they consist of at least five binaries and the configurational entropy (per formula unit) is  $S \ge 1.5R$ . Since such intermetallics usually consist of two sublattices, one of which is essentially unchanged, the term "high-entropy metal sublattice nitrides", carbides, borides, etc. seems more appropriate and precise. Detailed experimental and computational studies show that single-phased materials of this type can exhibit exceptional strength, thermal stability, and oxidation resistance. Furthermore, all magnetron sputtered thin films with a high-entropy metal sublattice investigated were relatively insensitive to variations in their deposition parameters.



**Paul Mayrhofer** is University Professor of Materials Science at the Institute of Materials Science and Technology, and chairs the Materials Science Division at the University TU Wien, Vienna, since 2012. He received a Dr. in 2001 and habilitated in 2005 in Nanostructured Materials at the University of Leoben. In 2003, 2005, and 2006, Paul Mayrhofer

spent his post-doc years and Erwin-Schrödinger-Fellowship at the University of Illinois at Urbana-Champaign, RTWH Aachen, and Linkoping University. Paul is currently Dean of Academic Affairs for Materials Science, and Mechanical and Industrial Engineering at TU Wien. Editor for Short Communications of Vacuum, and in the Editorial Board of Surface and Coatings Technology.

He has pioneered age hardening within hard ceramic thin films based on ternary nitrides and borides and is fascinated by phase transitions in general. His research activities focus on the

development and characterization of vapor phase deposited nanostructured materials by a combination of computational and experimental material science. He won the prestigious START price of the Austrian Science Fund and served scientific societies in numerous appointed and elected positions. Paul is an elected member of the Austrian Academy of Sciences. He is active in the ASED, where he has served as Division Chair in 2020. He was Editor of the ICMCTF Proceedings in the years 2007, 2008 and 2009, and the Program and General Chair of ICMCTF in 2012 and 2013. He also served as the Chair of the ASED Sessions at the AVS International Symposium and Exhibition (2008–11, 2016–17). Paul is Fellow of AVS for Seminal contributions in the development of vapor phase deposited nanostructured materials and self-hardened protective coatings of ternary nitrides and borides. He has published more than 310 SCI listed papers in the general field of thin film materials science, with >16,500 citations to these (h-index of 69; GS) and holds 13 patents regarding hard coatings.

### Tuesday 10:30 – 12:10 am, June 4, 2024

### ORAL PRESENTATIONS

#### Session 5 – Optical films

MODERATOR: **S. Carvalho** *University of Coimbra, Portugal* 

### $10:30 \text{ S5-1} - \underline{\text{Invited}} - \text{Amorphous oxides mixtures for coatings of gravitational wave detectors}$

**C. S. Menoni**<sup>1</sup>, A. Davenport<sup>1</sup>, S. Castro-Lucas<sup>1</sup>, R. Osovsky-Shpilman<sup>1</sup>, S. Bhowmick<sup>1</sup>, A. Markosyan<sup>2</sup>, R. Bassiri<sup>2</sup>, M. Fejer<sup>2</sup>, F. Schiettekatte<sup>3</sup>, M. Chicoine<sup>3</sup>, R. Zhang<sup>4</sup>, J. Jiang<sup>4</sup>, H.-P. Cheng<sup>4</sup>

<sup>1</sup> Dept. of Electrical and Computer Engineering, Colorado State University, Fort Collins, CO, USA

<sup>2</sup> Gintzon Lab, Stanford University, Stanford, CA, USA

<sup>3</sup> Department of Physics, Université de Montréal, Montreal, *QC*, Canada

<sup>4</sup> Department of Physics, Northeastern University, Boston, MA, USA

The mixing of two or more cations in the ion beam sputtering (IBS) of amorphous oxides provides enormous flexibility to tailor the optical and mechanical properties of the mixture thin films. Cation mixing has been instrumental in coatings for gravitational wave detectors to achieve the lowest possible coating thermal noise. Using as example mixtures of TiO<sub>2</sub> and GeO<sub>2</sub> with Ti content ranging from 0 to 60%, this talk will describe the modifications in the atomic structure and bonding that occur when Ti is added to amorphous GeO2. It will be shown that for a Ti content of up to about 44%, the Ti ions substitute Ge ions in the network forming Ti-O-Ge bonds which are mainly corner-shared. Annealing also promotes this type of structural rearrangement, more significantly at temperatures  $\geq 500^{\circ}$ C and before the onset of crystallization. This type of network organization is paramount to reduce internal friction, as demonstrated in IBS mixtures of 44% TiO2 and 56% GeO2 coatings which have achieved a value of internal friction  $\sim 4x$ lower than state-of-the art 25% TiO2:Ta2O5 used for coatings of gravitational wave detectors. This work brings out a new understanding of the modifications in the atomic structure of TiO<sub>2</sub>:GeO<sub>2</sub> mixtures with composition and upon thermal treatment, which is critical to understand the mechanisms involved in affecting internal friction.



**Dr. Carmen S. Menoni** is University Distinguished Professor in the Department of Electrical and Computer Engineering. She also holds appointments in the department of Chemistry, and the School of Advanced Materials Discovery. Prof. Menoni's group investigates the synthesis of amorphous thin film oxides by sputtering

and uses spectroscopic and other material diagnostics to identify their structural organization at the nanoscale. Through a combination of fundamental understanding of the optical and structural properties of the thin film materials and device engineering, Prof. Menoni research is advancing the state-of-art in interference coatings for gravitational wave detectors and ultra-high intensity lasers. Prof. Menoni is Fellow of the Institute of Electrical & Electronic Engineers (IEEE), the American Physical Society (APS), the Optical Society of America (OSA), the American Association for the Advancement of Science (AAAS) and the International Society for Optics and Photonics (SPIE).

### 11:00 S5-2 – Design and fabrication of color-generating multilayer thin-film optical filters for silicon solar cells

P. Bhattacharyya, C. White, R. Kleiman, P. Mascher

Department of Engineering Physics and Centre for Emerging Device Technologies, McMaster University, Hamilton, ON, Canada

Using electric vehicles can reduce greenhouse gas emissions and their adverse health effects on humans. But we can only utilize their full environmental benefits when charging is done using renewable energy sources with zero or low carbon emissions. Researchers have suggested integrating low-cost, flexible, and thin-film copper indium gallium selenide solar cells directly onto all the upward-facing body parts of electric vehicles. However, this integration comes with an aesthetic drawback. We propose replacing the anti-reflective coating in standard solar cells with a notch filter (a narrow high-reflection region in the visible range along with high transmission for the rest of the solar spectrum) to give a distinct color rendering to solar-charged electric vehicles.

Notch filters can be designed using a rugate filter structure consisting of continuously modulated refractive indices or a repetitive two-material stack of alternating high and low refractive index materials with precise thickness, known as the standard two-material technology (S2MT). We used OptiLayer to simulate our S2MT designs. The gradual evolution optimization technique was used to obtain the structures. We explored three color ranges represented by reference wavelengths of 400 nm, 550 nm, and 632 nm. Detailed analysis of various design parameters and their physical limitations will be presented.

We fabricated our designs using Electron cyclotron resonance plasma-enhanced chemical vapor deposition and Radical Assisted Sputtering with three material pairs. Characterizations were done using variable angle spectroscopic ellipsometry and Cary spectroscopy. A detailed comparison of our simulation and fabrication results will be presented.

## 11:10 S5-3 – Enabling smart windows with rationally designed coatings

#### M. R. Anthony Raj, G. B. Muthuperumal, W. Skene

#### Université de Montréal, Montreal, QC, Canada

Globally, building operations contribute 9 GT yearly of green house gas emissions. Upwards of 20% of these operating emissions are a result of cooling/heating losses that occur through windows. Significant reduction in climate emissions can therefore be had by using smart windows. These are conventional windows with a coating whose optical transmission can be adjusted with an applied potential. Indeed, the NIR region of the solar spectrum that contributes to building warming by radiant heat can be removed with smart windows. As such, smart windows are considered sustainable devices.

The performance requirements of coatings for their use in smart windows include electrochemical reversibility, large optical transmission differences between the bleached and the colored states, and broad optical transmission and large contrast ratios in the NIR region. It will be shown that molecular conjugated organic electrochromes are suitable coatings for smart windows by virtue for their optical and electrochemical properties that meet the key performance requirements. Of importance, the effect of the electronic groups on the NIR broad optical transmission will be demonstrated. The role of the electronic groups on the kinetics of switching between the bleached and colored states with applied potential will also be presented. The performance of the molecular coatings will first be illustrated in solution and carried through to functioning test size smart windows to illustrate the suitable of organic electrochromes as smart coatings.

## 11:20 S5-4 – Protective coatings for optical fiber used in telecommunication networks

#### R. El Abdi, R. L. Pinto

### *Université de Rennes, Institut de Physique de Rennes, Rennes, France*

Optical fibers are key components in telecommunication technologies. Fiber failure makes an irreversible accident which may occur when an external stress is applied on a defect located on fiber surface. While intrinsic defects lead to failure only for large, applied stresses, other heterogeneous defects make a far more serious concern as they lead to the fiber failure of the aged fibers under moderate stress. The fabrication process includes a proof test that eliminates the largest defects.

Polymer coatings are currently applied to optical fibers to prevent the formation of surface defects through scratches and abrasion and to minimize the influence of the pre-existing defects. They also act as a diffusion barrier against the surrounding humidity reaching the glass surface.

In this work, the role of the polymer coating is analysed. Optical fibers with and without polymer coatings were submitted to bending tests in two atmospheres: air and inert atmosphere to measure the humidity influence and the role of polymer coatings on fiber strength.

The used monomode silica fiber has an acrylate coating. This fiber was manufactured using the Plasma activated Chemical Vapor Deposition, the combined coating diameter is  $242 \pm 5$  micrometers, the coating thickness is  $58.5 \pm 0.5$  micrometers.

Dynamic tests for different faceplate velocities were implemented using a two-point bending testing device in order to determine the median strength for coated and stripped fibers from Weibull statistics.

The analysis of the Weibull curves demonstrates the influence of the used atmosphere as well as the role of the polymeric coatings.

## $11{:}30\ \mathrm{S5}{-}5$ – The effect of cupper layer on AlClPc thin film

#### B. Abdel Samad, Z. Kabore

#### Department of Physics and Astronomy, Université de Moncton, Moncton, N-B, Canada

Our research aims to investigate the impact of the thickness of cupper layer on the optical and electrical properties of an organic compound in the context of photovoltaics. Currently, siliconbased photovoltaic cells dominate the market with power conversion rates ranging from 15% to 20%. In contrast, inorganic photovoltaics, despite their potential advantages, face obstacles with a power conversion rate of around 10%.

The goal of our study is to identify optimal parameters for achieving transparent cells while enhancing conversion efficiencies. This involves working with materials that exhibit excellent optical properties, including maximum absorption and transmittance of the solar spectrum, as well as favorable electrical properties such as good conductivity and a substantial carrier density.

Our work focused on developing a transparent photovoltaic cell. Optimizing the performance of this cell is crucial, paving the way for new applications like integration into building facades or screens. The significance of this project lies in its potential to address global energy needs while preserving ecological interests.

# 11:40 S5-6 - <u>Invited</u> - Real-time growth monitoring of ultrathin Ag layers for use as transparent conductive electrodes

#### G. Abadias

#### CNRS-Université de Poitiers, Poitier, France

Noble-metal layers, with nominal thickness ~10 nm or below, are ubiquitous in a wide range of plasmonic devices and other optoelectronic applications. Silver (Ag) is by far the material of choice for a number of key technological areas, such as in smart windows for architectural glazing, selective infrared thermal emitters for radiative cooling or transparent conductive electrodes (TCEs) for flexible photovoltaics or flat panel displays. However, the growth of Ag on weakly interacting substrates (e.g. oxides) proceeds in a 3D fashion. At present, there is much interest in producing ultrathin Ag layers as potential TCE alternative to indium tin oxide, which suffers from high cost, poor sustainability, and is prone to cracking upon bending. Strategies to produce fully continuous, ultrathin and ultra-smooth Ag layers without compromising their electrical conductivity have lately been deployed. Among them, the use of gaseous additives, such as N<sub>2</sub> or O<sub>2</sub>, or template layers appears to be an efficient route to improve Ag wetting and favor a 2D growth morphology [1-3]. However, understanding the entire evolutionary growth regime requires the implementation of in situ and real-time diagnostics.

In the present work, the impact of  $N_2$  or Ge addition on the morphological and structural evolution of ultrathin Ag layers is investigated by coupling complementary in situ and real-time diagnostics. Lab-scale studies include wafer curvature, surface differential reflectance spectroscopy and electrical resistivity to determine morphological transition thicknesses such as percolation threshold and onset of continuous film formation [4]. These results are further comprehended using real-time X-ray synchrotron studies (SIXS beamline at SOLEIL) in which the grazing incidence diffraction and small-angle scattering signals are simultaneously recorded, together with stress evolution. This enables us to explore the influence of Ge and  $N_2$  on island shape, texture and stress development, as well as relaxation mechanisms during growth interruptions.

In the case of  $Ag/N_2$  system, we additionally compared the growth morphology of Ag layers obtained by evaporation (ebeam) and sputter-deposition (dcMS and Hipims) processes. These deposition methods enabled us to span a wide range of growth conditions with respect to energies of film-forming and plasma species, as well as  $N_2$  dissociation rates, with the aim to obtain a mechanistic interpretation of the role of nitrogen.



**Gregory Abadias** is Professor at the Physics Department of the University of Poitiers, France. He received his Ph.D. degree in materials science in 1998 at National Polytechnic Institute of Grenoble (INPG), and he is currently group leader of thin films activities at CNRS Pprime Institute (<u>https://pprime.fr/en/home-pprime/</u>) in Poitiers. He conducts research on a range of

topics related to nanoscale thin films, including mechanical, electrical and optical properties of metallic, nitride or oxide systems as well as hard and protective coatings in the form of nanocomposites or multilayers. His current research interests focus on the understanding of thin film growth dynamics using real-time and in situ diagnostics as well as computational modelling, with main emphasis on growth manipulation strategies to control morphology and stress development in sputter-deposited metal layers. He is co-authors of more than 160 papers in peer-review journals and one book chapter on stress in PVD thin films. He was member-elected to the Scientific Council of the Physics Institute of CNRS (2019-23), as well as French representative of the Surface Engineering Division of IUVSTA for 2022-25 triennium. He has been involved in the organization of several symposia or workshops at international conferences (ICMCTF, EMRS) and serves as Editor of Surface and Coatings Technology journal since 2016.

### Tuesday 13:40 - 15:00, June 4, 2024

### ORAL PRESENTATIONS

Session 6 – Advanced Characterization

MODERATOR: I. Petrov Linköping University, Sweden

## 13:40 S6-1 – <u>Invited</u> – Towards reliable X-ray photoelectron spectroscopy of thin films

#### G. Greczynski

Thin Film Physics Division, Department of Physics (IFM), Linköping University, Linköping, Sweden

Raising concern within the surface science community about decreasing quality of X-ray photoelectron spectroscopy papers [1], motivates efforts that would lead to an improved reliability of reported results. One of the major issues is related to an unreliable charge referencing of the binding energy scale [2, 3]. Experiments conducted in our laboratory on large sets of thin film samples demonstrated spectacular failure of commonly used referencing methods based on the C 1s peak of adventitious carbon [2, 4] and the Ar 2p peak of implanted Ar [5]. When applied, both techniques generate a large spread in reported binding energy values that often exceed involved chemical shifts. Based on the model experiments, preformed on alumina layers, that can be repeated for all sorts of thin film insulators, a solution to the binding energy reference problem is proposed for reliable assessment of chemical bonding. Examples illustrating the above issues along with best practices will be discussed during the talk.

[1] G.H. Major, T. G. Avval, B. Moeini, G. Pinto, D. Shah, V. Jain, et al. J. Vac. Sci. Technol. A 38, 061204 (2020)

[2] G. Greczynski and L. Hultman, Angew. Chem. Int. Ed. 59 (2020) 5002

[3] G. Greczynski and L. Hultman, *Progress in Materials Science* 107 (2020) 100591

[4] G. Greczynski, O.V. Pshyk, and L. Hultman, *Science Advances* 9 (2023) eadi3192

[5] G. Greczynski and L. Hultman, Applied Surface Science 635 (2023) 157598

**Grzegorz (Greg) Greczynski** is a Professor in the Department of Physics, Linköping University (LiU) and the head of the Fundamental Science of Thin Films Group. Greczynski received his PhD degree in surface science of organic materials in 2001 and has an eight-year industrial track record. In 2018 he was nominated Fellow of the American Vacuum Society for "seminal contributions to nondestructive X-ray photoelectron spectroscopy (XPS) surface analysis, and the development of novel next-generation HiPIMS metal-ion deposition



techniques". His research interests are presently focused on low-energy ion/surface interactions (including both gas and metal ions) for nanostructure control low-temperature growth during of transition-metal-based nitride, boride, and carbide thin films by physical vapor deposition. Greczynski is also active in the field of XPS, with the aim to enhance the reliability of the technique. He has

published 175 peer-reviewed articles that have been cited more than 10 000 times.

## 14:10 S6-2 – Creating a digital twin and how it helps to speed up your coating development

**T. vom Braucke<sup>1</sup>**, N. Bierwisch<sup>2</sup>

<sup>1</sup> GP Plasma, Medina, OH, USA <sup>2</sup> SIOmec, Ummanz, Germany

sample - we call it a digital twin.

A better understanding of your coating stacks and their behavior in the application is crucial for the optimization of complex engineering systems. In this context, a modeling approach, in conjunction with targeted laboratory and functional tests, is particularly attractive as it can accelerate the coating selection and achieve its goals within the desired application field. Such methodology helps to understand the coating system, including the substrate and all coatings and interfaces. Simulations can find coating limitations and guide the refinement of the coating architecture within a defined framework. A model which will contain as much digital information as possible about your

This work will showcase how the required data can be obtained by analyzing indentation and scratch measurements. SIO developed analytical models which dramatically speed up the simulation and optimization of complex contact conditions. With the help of these models, you can first dimension the relevant experiments. Afterwards you can use the experimental data from the indentation experiments to evaluate the true Young's modulus and yield strength of each coating. By analyzing scratch tests, you can calculate critical values like the tensile stress.

In the second part of this talk we show how the digital twin can help you to find the best coating architecture for a new application by using the gathered digital data. Even if the contact conditions for the new application are not known exactly, you can use the digital simulations to narrow down the applicable samples from your portfolio.

## 14:20 S6-3 – Investigation of the mechanical properties of sculptured thin films by nanoindentation

#### J. Nikitina, L. Grinevičiūtė

#### Department of Laser Technologies, Center for Physical Sciences and Technologies, Vilnius, Lithuania

Oblique angle deposition is a well-known technique for the advanced tailoring of thin films' inner structure. The possibility of engineering the morphology of thin films has garnered significant attention since microstructural sculpturing via dynamic substrate motion offers control over the optical and mechanical characteristics. Common features of sculptured thin films are lower effective refractive indices than of standard dense films, anisotropy and controlled porosity.

In this work, we dive into the detailed analysis of the mechanical properties of sculptured thin films. A systematic study is carried out by comparing the micro-hardness and elastic/plastic behaviour of sculptured thin films with atomic force microscope nanoindentation. Under the test are various dielectric nanocolumnar structures, such as zigzag and square spiral. Deformation tendencies of different microstructures give an insight into their ability to accommodate the deformation under the load. Such a deeper understanding of the mechanical properties of sculptural films allows such coatings to be better and more efficiently combined with dense layers with high internal stresses. Moreover, this work is an intermediate stage of investigation put toward one-step replication of the master stamp (periodic microstructure) by imprinting into the porous sculptured thin films.

# 14:30 S6-4 - Modeling study of interface fracture toughness of thermal barrier coating at high temperature

#### R. Liu, S. K. Essa

#### Department of Mechanical and Aerospace Engineering, Carleton University, Ottawa, ON, Canada

Gas turbine engines operate at high temperatures, in particular, the inlet temperature is continuously increasing for maximum efficiency and power output. Nickel-based superalloys are commonly used for the hot-section components of gas turbine engines, but a thermal barrier coating (TBC) is necessarily deposited on the surfaces of these components to isolate heat from the alloy substrate. In this research, an interface fracture toughness model for thermal barrier coatings (TBCs) is proposed in which model parameters not only include high temperature and exposure period but also take into account mode mixity characteristics. The model is expressed in terms of the Arrhenius-type form showing a temperature-dependent feature and also exhibits a dependence of microcrack density distributed along the coating interface. Two scaling parameters are used in formulating the model, one is introduced to link dislocation Burgers vector to the crack tip opening displacement (CTOD), the other is utilized to describe the crack tip energy release rate associated with the P-N force responsible for dislocation movement. These scaling parameters can be obtained by fitting to the interface fracture toughness data at ambient temperature and the CTOD, respectively. Since the experimentally measured microcrack density exhibits thermal cycle dependent behavior, an attempt is made to explain the experimentally obtained toughness values using the proposed interfacial crack toughness model. The proposed model is applied to a TBC system, determining the model parameters by using the experimental data reported in literature. The interface fracture toughness is determined at selected mode mixity phase angles for the TBC system, showing the temperature dependence relation and the variation with exposure time at a given temperature. The model predicts an increase in fracture toughness with exposure temperature and mode mixity.

#### 14:40 S6-5 – Giant step bunching and Ehrlich-Schwöbelbarrier in thin heteroepitaxial films of strontium titanate on magnesium oxide (100) substrates

**E. Familsatarian<sup>1</sup>**, K. Kohlmann<sup>1</sup>, D. Gückelhorn<sup>1</sup>, A. Sarkissian<sup>2</sup>, E. Carbone<sup>1</sup>, P. Antici<sup>1</sup>, A. Ruediger<sup>1</sup>

<sup>1</sup> INRS - Énergie, Matériaux et Télécommunications, Montreal, QC, Canada

Plasmionique, Varennes, QC, Canada

We reported on the observation of giant step bunching of  $SrTiO_3$ thin films of 15 nm thickness on MgO (100) vicinal surfaces earlier [1]. One additional observation was an increased thickness of the strontium titanate layer near step edges, a phenomenon usually referred to as the Ehrlich-Schwöbel-barrier of reduced diffusion along this region. Conventionally, this barrier is discussed in terms of an interaction between terrace steps for which - so far - no direct evidence has been presented. Here, we discuss the existence of the Ehrlich-Schwöbel-barrier in terms of local surface relaxation and diffusion kinetics as a dynamic process rather than a static one.

[1] A. Hadj Youssef, G. Kolhatkar, I.C. Amaechi, R. Katoch, Y. Gonzalez, A. Merlen, A. Ruediger, "Giant step bunching of SrTiO<sub>3</sub> thin films grown on MgO (100) vicinal surfaces", Applied Surface Science (Elsevier) 570 (2021) 151266.

## 14:50 S6-6 – Optimization and application of HiPIMS hafnium oxynitride (HfO<sub>x</sub>N<sub>y</sub>) thin films in MOS structures

M. Puzniak<sup>1</sup>, W. Gajewski<sup>1</sup>, R. Mroczynski<sup>2</sup>, M. Zelechowski<sup>1</sup>

<sup>1</sup> TRUMPF Huettinger Sp. z o.o., Zielonka, Poland

<sup>2</sup> Institute of Microelectronics and Optoelectronics, WUM, Warsaw, Poland

We report on the process development to improve the electrical parameters of thin hafnium oxynitride layers by the High-Impulse Power Magnetron Sputtering (HiPIMS) method. The optimization procedure was implemented using the Taguchi orthogonal tables and the parameters of examined dielectric films were monitored by optical methods (spectroscopic ellipsometry and refractometry), electrical characterization (C-V and I-V measurements of MOS structures), and structural investigations (AFM, XRD, XPS). The thermal stability of fabricated HfO<sub>x</sub>N<sub>y</sub> layers up to 800 °C was also examined. The HfO<sub>x</sub>N<sub>y</sub> layers formed using optimal HiPIMS process are characterized by improved electrical parameters, which is revealed in lower flat-band voltage (V<sub>fb</sub>) values, the disappearance of frequency dispersion of C-V characteristics, reduced effective charge  $(Q_{eff}/q)$ , and interface traps  $(D_{itmb})$ densities of examined MOS structures. It is worth underlying that the improved electrical properties can correlate with the lower nitrogen content in the layer bulk and at the semiconductor-dielectric interface. Moreover, the superior stability of HfO<sub>x</sub>N<sub>y</sub> layers up to 800 °C was proved, and no deterioration of electrical properties or surface morphology has been noticed. However, a slight increase of crystalline phase in the laver bulk was observed. The HfO<sub>x</sub>N<sub>y</sub> lavers formed using HiPIMS revealed also a higher immunity to thermal treatment as compared to the standard Pulsed Magnetron Sputtering technique. Finally, we applied HiPIMS HfO<sub>x</sub>N<sub>y</sub> films as gate dielectric films in MOSFET devices. The fabricated structures revealed improved electrical properties compared to FET structures based on silicon dioxide (SiO<sub>2</sub>) gate dielectric layers.

### Tuesday 15:30 - 17:00, June 4, 2024

### ORAL PRESENTATIONS

Session 7 – FCSE perspectives

MODERATOR: **G. Abadias** *University of Poitiers, France* 

## $15:30 \text{ S7-1} - \underline{\text{Invited}} - \text{Thin film technologies for low carbon energies in a Green Deal context}$

#### F. Schuster

#### CEA, Paris-Saclay, France

The development of thin-film engineering is absolutely strategic for advanced manufacturing of components that have to operate under extreme environments (nuclear energy, renewables, aeronautics in particular). These components are often exposed to a combination of constraints, thus requiring the design of architectured systems to meet, *in fine*, the multi-functionality expected (diffusion barrier, resistance to oxidation and irradiation, mechanical resistance...).

Thin-film engineering is a field of technology that has made enormous progress in recent years, mainly challenged by the effective improvements demanded by the ever more uncompromising specifications of the microelectronics industry on the one hand, the booming low-carbon energies (in particular photovoltaics, hydrogen economy, as well as future of nuclear industry) and high-performance mechanics, on the other.

These advances concern PVD (Physical Vapor Deposition) technologies, in particular with the deployment of highly ionized plasma generation systems such as HiPIMS (High Power Impulse Magnetron Sputtering), which enable much better control of interface construction and coating microstructures, and, *in fine*, coating properties. These advances also concern CVD (Chemical Vapor Deposition) technologies, in particular thanks to the rich chemistry of organometallic compounds that can be used through the great flexibility of DLI-MOCVD (Direct Liquid Injection Metal Organic Chemical Vapor Deposition).

The field of thin films is also strongly impacted by the coupling between materials science and digital technologies, in particular artificial intelligence. On the one hand, this coupling is enabling the accelerated discovery of coatings, but it is also accelerating the mastery of sovereignty processes.

Since 2006, **Frederic Schuster** has been the Director of the Cross-Disciplinary Program on Material Science & Engineering at CEA. He previously held the position of deputy director of the Institute for Renewable Energies (CEA/Liten) from 2003 to 2006. In parallel, he initiated and managed the European



program Nanosafe on risk management in the field of nanotechnology from 2005 to 2010 and continued to develop a multidisciplinary approach in partnership with Canada, Japan and the US on this issue. He founded the International Conference NANOSAFE (every two years in Minatec, Grenoble, since 2008) on the safe production and use of nanomaterials. He is also the founder of the IMPACT International Chair on Accelerated

Discovery of Materials and Emerging Processes at the National Institute for Nuclear Science and Technology and University of Paris-Saclay. He is also the chairman of the additive manufacturing and circular economy commissions within the French Society of Metallurgy and Materials.

Since June 2022 he is co-director (with CNRS) of the French national initiative on accelerated discovery of materials, the national program DIADEM (DIscovery Acceleration for the Deployment of Emerging Materials).

Frederic Schuster is a CEA international expert in the field of materials science and engineering and especially in surface technology. For 8 years he was in charge of the CEA surface engineering laboratory at CEA Grenoble. Before his experience with CEA, he began his career in industry as manager of surface treatment department in the Arcelor-Mittal group, where he helped industrialize PVD technologies for steel surface functionalization.

Frederic Schuster is graduated from the National Polytechnic Institute of Toulouse. He received an award from the Institute in 1990 for his PhD work on MOCVD technology. He was awarded the RIST prize (young researcher) by the French Society of Metallurgy and Materials for his technology transfer achievements in the industry. In 2018, he received the Grand Award for technological innovation from the French Society for Nuclear Energy for his work on HiPIMS PVD coatings for Enhanced Accident Tolerant Fuels. He is the author of several patents on surface engineering, nanomaterials, and 3D printing and has published numerous articles.

# 16:00 S7-2 – Taking on the challenge for high-volume coating of metallic plates for hydrogen applications using PVD technology

**P. Immich,** R. Bosch, R. Jacobs, T. Karla, M. Horstink, P. Broekx, K. Fuchigami

IHI Hauzer Techno Coating B.V., Venlo, Holland

The hydrogen market is growing rapidly, due to high demand of the industry and mobility sector to decarbonize the production and transport. The industry is developing technical solutions for hydrogen generation and hydrogen-based electricity generation to full fill the needs for mobile and stationary applications. Key components of electrolyzers and fuel cell stacks are e.g. bipolar plates, PTL sheets and CCM's. These components need high quality coatings to enable good catalyst performance, good electrical conductivity and good corrosion properties.

IHI Hauzer is working on this challenge for many years, developing dedicated coatings and machine solutions based on PVD technology for this kind of application field. In the presentation the actual state of the art will be addressed, including the current status of market introduction and our expected further roll-out within the next years. For PVD, the current main challenges related to machine and process solutions for high speed inline coating will also be addressed. We will further address the requests from the market especially the electrolyzer business and give an outlook about possible noble metal free solutions to serve these demands.

## 16:10 S7-3 – From Nano to Micro: When ALD meets with PVD to enhance coating performance

F. Papa<sup>1</sup>, A. Sharma<sup>2</sup>, S. Tsianikas<sup>3</sup>, X. Maeder<sup>3</sup>, C. Guerra<sup>2</sup>

- <sup>1</sup> GP Plasma, Medina, OH, USA
- <sup>2</sup> Swiss Cluster AG, Spiez, Switzerland
- <sup>3</sup> Empa Thun, Thun, Switzerland

Atomic layer deposition (ALD) and Physical Vapor Deposition (PVD) have shaped and progressed a significant number of industrial technologies. These techniques have been mostly growing in their own field of application, but when combined, they become an unparalleled materials factory. This combination offers endless variations of coatings with superior properties.

We will present the incorporation of both techniques in a new way leading to the development of the first system combining ALD and PVD in a compact equipment. The SC-1 can fabricate complex coatings with hundreds of nanolayers from the ALD and PVD materials library. The properties of such multinanolayered coatings are strongly influenced by their interfaces. Carefully engineered coatings translate to lighter and cheaper materials with improved mechanical and thermal properties. We will show a few examples of multinanolayered coatings and their mechanical properties behavior, surpassing the yield strength of existing materials.

One of these examples shows the capabilities of the system, fabricating a  $\sim 2.2 \ \mu m$  thick coating composed by 100 layers of 20 nm of magnetron sputtered aluminum alternating with 100 layers of 1 nm of Al<sub>2</sub>O<sub>3</sub> deposited by ALD. Such coating effectively stabilizes a 20 nm aluminum grain size throughout the cross section of the coating by the introduction of "pinhole free" stable and conformal interfaces of Al<sub>2</sub>O<sub>3</sub>. This translates in a coating that is 2 times harder and stronger than any other aluminum alloy and can maintain 50% of its mechanical behavior at temperatures close to the melting temperature of aluminum. The second example will demonstrate the strengthening mechanisms behind the combination of both techniques by alloying Cu with Al to refine the grain size while the number of interlayers of ALD Al<sub>2</sub>O<sub>3</sub> and its periodicity vary in each coating. The third coating will show the need for ALD

layers to increase plasticity and yield strength in high entropy alloys.

# 16:20 S7-4 – Progress in laser patterning techniques for efficient mass production of flexible microelectronic devices with sputtered coatings

#### L. Josephson, M. Simmons, M. Kleyn, J. Vlach

#### Intellivation LLC, Loveland, CO, USA

Utilizing laser patterning on conductive vacuum-deposited thin films for the mass production of affordable and efficient flexible electronic devices offers adaptability, shortened 2D development cycles, and scalability in manufacturing. Electrical and mechanical properties of sputtered layers make them ideal for flexible electronic applications is sensors, flexible electronics and monitoring devices. The real-time adjustment of device architecture or geometry for optimized performance can be seamlessly achieved through modifications in laser scanning patterns, eliminating the impact on material costs, time, or the need for additional resources like mask fabrication. The success of laser patterning is directly influenced by surface roughness, wherein surface morphology plays a crucial role in the continuity and adhesion of subsequent sputtered thin film layers and their ultimate performance. Integrating laser technology into a roll-toroll system with in-situ quality control facilitates the costeffective, high-volume production of sensors.

#### 16:30 S7-5 <u>Invited</u> – Leveraging "external innovation" to enhance the success of commercializing advances in functional coatings & surface engineering

#### C. H. Stoessel

#### StoesselConsulting / SputterTek LLC, Palo Alto, CA, USA

Corporate implementation of advances in coating and surface science increasingly depends on effectively leveraging innovation that is obtained from external partners. External innovation offers the opportunity to reduce risks, accelerate time-to-market, nimbly react to shifting trends, diversify sources for creativity, and to take advantage of existing technology / market ecosystems. However, it can also pose challenges for corporate intellectual property strategies, stir "not invented here" resentments with internal innovation resources, requires efficient opportunity scouting, prudent due-diligence assessments, and a strategic funding and investment approach. A wholistic commitment throughout the enterprise is required to effectively integrate external innovation into corporate business structures.

In this talk, we will review various external innovation pathways, characterize their strength and weaknesses, explain how academic and tech transfer organizations can play effective "external innovation" roles, and provide guidance how to avoid common pitfalls to leverage external innovation opportunities for successful business growth in technology-driven markets such as coatings and surface engineering.



**Chris H. Stoessel** is a partner and engineering consultant at SputterTek LLC where he advises on innovation management, process engineering and product development in thin films, surface engineering and materials science. He was a Senior Process Development Manager at Eastman Chemical Co.'s Palo Alto Advanced Technology Center (formerly Southwall Technologies

Inc.) in Palo Alto, California. As a member of the Corporate Innovation group, he advised on innovation strategy and managed internal and external innovation projects to develop new deposition processes and products, primarily focused on roll-to-roll coating technologies. He holds a Doctorate in Mechanical Engineering (Materials Science) from the Rheinische Westfälische Technische Hochschule Aachen (Germany) and conducted post-doctoral studies under Rointan Bunshah at UCLA. He has developed thin-film products and deposition processes for a wide range of applications such as tribology, superconducting films, optical coatings (at OCLI/JDS-Uniphase), MEMS, OLED (at DuPont Displays), energy-efficient glazing (at Southwall Technologies/Eastman Chemical Co.), and flexible hybrid electronics (FHE). Chris contributes to several professional organizations in the thin film coating community and is the Program Director for the Society of Vacuum Coaters (SVC).

### POSTER PRESENTATIONS

MIL Campus – Université de Montréal, Atrium B-140

#### Posters A:

# Hard & protective coatings and related applications

## A1 – Dynamic combinatorial 2D synthesis of materials using PVD-HiPIMS technology

N. Chaâbane<sup>1</sup>, J.-P. Poli<sup>2</sup>, F. Schuster<sup>1</sup>

<sup>1</sup> Université Paris-Saclay, CEA, INSTN, Gif Sur Yvette, France <sup>2</sup> Université Paris-Saclay, CEA, DRT, Gif Sur Yvette, France

Autonomous experimentation has emerged as an effective approach to accelerate the pace of materials discovery. Although autonomous synthesis has become widespread in the healthcare field, solution synthesis of hybrid materials and nanoparticles, examples of autonomous tools for physical vapor deposition are still quite rare but extremely important for the sectors lowcarbon energies, frugal digital technology, the environment and health. The Diadem 2D platform allows the dynamic combinatorial synthesis of thin layers of functional coatings with increasingly complex compositions and architectures using PVD-type vacuum deposition technologies, in HiPIMS mode for these different applications.

This flexible and scalable 2D synthesis platform has a system of 4 magnetron cathodes that can work in confocal mode or not (Figure 1a). This multi-cathode system makes it possible to modify the synthesis parameters and therefore to produce a large number of samples under different parametric conditions during the same deposition cycle. It is equipped with an in situ real-time monitoring device using UV-visible optical spectrometry for plasma diagnosis and ex situ high-throughput characterization devices for Raman spectroscopy and X-ray fluorescence. It aims in particular to strongly contribute to the development of a digital twin of HiPIMS technology to both monitor and predict process outcomes such as film thickness, texture and morphology in real time (Figure 1b). The use of an AI tool, developed at the CEA, ExpressIF Materials, will make this equipment completely autonomous.

### A2 – Different TiAlN coating architecture for enhanced solid particle erosion protection

B. Millan-Ramos, P. Renato Avila, S. Brown, L. Martinu, J. E.

Klemberg-Sapieha

#### Department of Engineering Physics, Polytechnique Montréal, Montreal, QC, Canada

Solid particle erosion (SPE) may cause major damage to compressor blades, resulting in significant changes in their aerodynamic performance, followed by an increase in fuel consumption, failure risk, decrease in engine efficiency and service life. In this regard, PVD Ti-based nitride coatings offer a promising solution for SPE protection. Coating architecture should enhance adhesion, mechanical properties, and erosion resistance. In addition, the development of intrinsic stresses during coating deposition must be controlled.

In the present work, two coating architectures were deposited by HiPIMS: a monolithic TiAlN, and a multilayered TiAl/TiAlN coatings, one with sharp interfaces and second featuring a gradient transition between alternating TiAl and TiAlN layers. The addition of metallic TiAl layers in the TiAl/TiAlN coating reduces its hardness and increases its elastic modulus (27 GPa and 340 GPa, respectively) compared to the monolithic TiAlN coating (30 GPa and 287 GPa). Nevertheless, both coatings show very good erosion resistance, with a scar depth lower than 1 µm using the particle speed of 75 m/s at 90°. While both coatings show a columnar structure and are stoichiometric, stress-depth profiles indicate improved management of compressive stresses for the multilayer system compared to the monolithic coating. Additionally, the multilayer system shows superior scratch resistance compared to the monolithic TiAlN. These results indicate that careful design of the coating architecture effectively modulates stress development during deposition, leading to excellent erosion protection and enhanced scratch resistance.

## A3 – Characterization of spray formed and vacuum induction melted AlSi D2 cold work tool steel

V. Rodríguez<sup>1</sup>, A. Ruiz<sup>1</sup>, V. Nadimpalli<sup>2</sup>, D. Bue<sup>2</sup>

<sup>1</sup> Universidad Michoacana de San Nicolás de Hidalgo, Morelia, Michoacán, Mexico

<sup>2</sup> Technical University of Denmark, Kongens Lyngby, Denmark

The spray forming technology is commonly used to process complex alloys in fewer steps than other conventional methods such as conventional casting and powder metallurgy. Its advantage resides in the uniform distribution and homogeneity of the microstructure that results from the solidification process. In this paper, D2 cold work tool steel was considered to analyze the differences in the microstructure and mechanical properties associated with the rapid solidification of the spray-forming process in comparison to its conventionally cast counterpart. Morphological information, such as carbide particle size and distribution as well as phase volume fraction were quantitatively compared through optical microscopy, X-ray diffraction, and scanning electron microscopy. The results indicated that the microstructure of the SF steel exhibited a refined and uniformly distributed carbide phase within the boundaries of equiaxed grains, in contrast to large and interconnected eutectic carbides found in the cast steel. The higher isotropy of the spray-formed steel resulted in improved microhardness, impact toughness, tensile, and compressive properties than that of conventional cast D2 steel.

# A4 – Novel approaches in surface engineering: Enhancing adhesion and stress management through interface design for wear-resistant coating

**T. Ebrahimi Sadrabadi<sup>1</sup>**, M. Javidani<sup>1</sup>, M. Muhammed<sup>1</sup>, M. Jahazi<sup>2</sup>

<sup>1</sup> Department of Applied Science, University of Quebec at

Chicoutimi, Chicoutimi, QC, Canada

<sup>2</sup> Department of Mechanical Engineering, École de Technologie Supérieure, Montreal, QC, Canada

Surface engineering plays a pivotal role in improving the performance and longevity of materials in various industrial applications. This study, based on a comprehensive literature review, introduces innovative techniques in interface design to enhance the adhesion and stress management of wear-resistant coatings, addressing a significant challenge in the field of surface engineering. Traditional methods often struggle to balance the trade-off between high adhesion strength and effective stress management, which is crucial for the durability of coatings under extreme operational conditions. The approach of this review focuses on integrating graded layers and engineered nanocomposites applied to high-performance coatings such as Chromium Nitride (CrN) and Titanium Aluminium Nitride (TiAIN). These durable coatings promise in the aerospace, automotive, and precision tooling industries.

Recent studies in surface engineering have adopted advanced methodologies, conducting thorough testing under diverse mechanical and thermal conditions to closely simulate realworld environments. This comprehensive approach included adhesion strength evaluations, employing scratch testing methods to precisely measure the bond integrity of coatings under stress. Additionally, the distribution and management of stress within these coatings were meticulously analyzed through X-ray diffraction techniques, offering insights into the internal structural dynamics under various load conditions. The outcomes of these investigations have been significant, revealing a marked improvement in both adhesion and stress management. The engineered multi-layered interfaces showcased a superior resistance to wear and delamination, markedly exceeding the durability and resilience of traditional single-layer coatings.

## A5 – Comparison of tool performance in machining Inconel 718 superalloy

**Y. Wu<sup>1,2</sup>,** N. Côté<sup>2</sup>, M. Azzi<sup>1</sup>, S. Bélanger<sup>3</sup>, E. Péloquin<sup>3</sup>, L. Martinu<sup>1</sup>, J. Klemberg Sapieha<sup>1</sup>

<sup>1</sup> Department of Engineering Physics, Polytechnique Montréal, Montreal, QC, Canada <sup>2</sup> Centre Technologique En Aérospatiale, Longueuil, QC, Canada

<sup>3</sup> Optimum-Canada, Mercier, QC, Canada

Inconel 718 superalloy is widely used in the aerospace industry; however, it is recognized as one of the most difficult-to-cut materials. The objective of the present work is to compare the cutting performance of commercially available end-milling tools and provide insights into their performance. All the tools selected for evaluation are recommended for cutting Inconel 718 by their respective manufacturers. These tools uniformly feature 6 flutes and a fixed helix angle. The assessment reveals that an end-milling tool manufactured by Optimum-Canada exhibits the highest performance. This study indicates that cutting Inconel 718 is associated with coating hardness, coating thickness, and tool geometry.

# A6 – Mechanical and tribological properties of $(CoCrFeNiMn)_{1-x}Ti_x$ high-entropy thin films synthesized by magnetron sputtering

L. Wu, T. Liang, R. Chromik

McGill University, Montreal, QC, Canada

High entropy thin films (CoCrFeNiMn)<sub>1-x</sub>Ti<sub>x</sub> (x = 0, 4, 12, 24 in at. %) were deposited by using pulsed direct current magnetron sputtering on silicon wafers. The Cantor alloy and Ti targets were used in the co-sputtering process with various currents being applied. The microstructure, mechanical and tribological properties of the films were studied. The (CoCrFeNiMn)<sub>1-x</sub>Ti<sub>x</sub> films showed a columnar structure, and with the variation of Ti content, there was a trend from FCC crystalline structure (0 at. % Ti) to nearly amorphous (24 at. % Ti). Using nanoindentation, the hardness (H) and reduced elastic modulus (Er) of the films were measured. The highest H (10.0 GPa) was found in crystalline film (4 at. % Ti) and the Er showed a continuous downward trend with the increasing Ti content. The tribological properties of the (CoCrFeNiMn)<sub>1-x</sub>Ti<sub>x</sub> films were evaluated by doing the micro-tribological test under the ambient and dry air conditions. The lower friction coefficients and the wear rates were found in the amorphous films (12 and 24 at. % Ti) under two atmospheres, and the wear mechanisms will be discussed in detail.

## A7 – Structure and mechanical properties of (Al,B,Cr,Si,Ti)-based thin films

**A. Kirnbauer<sup>1</sup>**, P. Konecny<sup>1</sup>, R. Hahn<sup>2</sup>, S. Kolozsvari<sup>3</sup>, P. Mayrhofer<sup>1</sup>

<sup>1</sup> TU Wien, Thin Film Materials Science Division, Vienna, Austria

<sup>2</sup> TU Wien, Christian Doppler Laboratory for Surface

*Engineering of high-performance Components, Vienna, Austria* <sup>3</sup> *Plansee Composite Materials GmbH, Lechbruck am See, Germany* 

High-entropy metal-sublattice ceramics (HESCs) have recently gained particular attraction in the field of materials research due

to their promising properties. Ceramics based on the highentropy concept mostly consist of refractory metals such as Ta, Hf, Zr, W, V etc. These metals are good nitride and carbide formers which is why they are mainly used especially for PVD coatings. Usually, these elements need a lot of energy for production due to their very high melting points and they are rather heavy and expensive. Therefore, we investigate a material system consisting of Al, B, Cr, Si, and Ti which are comparably light and cheap elements, and the production of a corresponding compound target consumes less energy. To get an idea of the properties of coatings based on this material system we investigated "metallic" coatings as well as nitrides and oxides. The coatings were synthesised by magnetron sputtering using a single composite target with an equiatomic composition and different gas mixtures. All the coatings produced show XRD amorphous diffraction patterns without any indication of crystalline phases. Also, SEM images of fracture cross-sections do not show the usually characteristic, columnar growth which further underpins the results obtained by XRD measurements. The hardness and indentation modulus of the coatings range from ~10 to 22 GPa and from ~170 to 260 GPa, respectively, depending on the character of the coating. Furthermore, in-situ cantilever bending tests were done to investigate the fracture toughness of the coating depending on their either "metallic", nitride, or oxide character.

## A8 – Mechanical and tribological properties of $(AlCoCrNiSi)_{100-x}N_x$ thin films

**T. Liang<sup>1</sup>**, S. Alidohkt<sup>2,1</sup>, R. Chromik<sup>1</sup>

<sup>1</sup> Department of Mining and Materials Engineering, McGill University, Montreal, QC, Canada <sup>2</sup> Department of Mechanical Engineering, Faculty of Engineering and Applied Science, Memorial University of Newfoundland, St. John's, NL, Canada

High entropy thin films of (AlCoCrNiSi)<sub>100-x</sub>N<sub>x</sub> were deposited on silicon wafers using a pulsed DC magnetron sputtering technique, with nitrogen gas flow ratios  $(R_N)$  of 0, 0.33, and 0.50. The structure and properties of films were analyzed for elemental composition, surface and cross-sectional morphologies, microstructure, roughness, and mechanical properties. The coatings were primarily composed of an amorphous structure with a minor presence of a BCC structure and exhibited periodic variations in chemical composition from substrate to free surface. An increase in R<sub>N</sub> enhances the crystallinity of the materials. Nanoindentation results showed that the films deposited at  $R_N = 0.50$  displayed the highest hardness (10.7±0.5 GPa) and reduced modulus (176±5 GPa), which were the highest among the films. Microtribology testing was conducted using a 20 µm radius spherical diamond tip under ambient air and normal loads ranging from 0.5 mN to 9 mN. Worn surfaces were characterized using atomic force microscopy (AFM). The coefficient of friction (CoF) was evaluated to investigate the elastic and plastic behaviors of films using Schiffmann's model. The coating without nitrogen displayed a predominant plastic behavior during the initial

cycles, while the coating deposited at  $R_N = 0.33$  demonstrated a more elastic behavior, particularly at lower loads.

#### Posters B:

Functional coatings and surface modifications for biomedical, electronic and other applications

## B1 - Epitaxially grown gold (100) surfaces for oxygen reduction reactions

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<sup>3</sup> Department of Applied Sciences and Mechatronics, Munich University of Applied Sciences, Munich, Germany

Noble metals have long been known to be an excellent basis for electrocatalysts. While the effectivity of catalysts depends on the reaction they are used for, studies have shown that for the oxygen reduction reaction (ORR), Au (100) is the most active face of Au in alkaline media. This work investigates radio frequency (RF) magnetron sputtered epitaxial Au-films on MgO (100) for electrocatalysis. We show that the deposition parameters and their effect on the surface morphology are a key factor to optimize catalytic activity. We explore different methods to improve the adhesion of Au without the use of a transition metal seed layer, including surface treatment and alloying Au with a metal that increases the lattice parameter of Au, thus reducing the lattice mismatch between Au and MgO. The samples are characterized by atomic force microscopy (AFM), X-ray diffraction, and cyclic voltammetry in order to gain insight into the quality of the different surfaces and establish a correlation between the surface topography and electrocatalytic activity.

# B2 – Quantifying impact of tension on PLA chains mobility when modifying polymer exclusion nets

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<sup>1</sup> Polytechnique Montréal, Montreal, QC, Canada

<sup>2</sup> Université Laval, Laval, QC, Canada

<sup>3</sup> University of Ottawa, Ottawa, ON, Canada

To reduce the use of pesticides and fungicides in the agricultural field, biobased hydrophobic exclusion nets have been under research to protect crops from pests. Treatment based on a solvent-induced crystallization process allowed to obtain superhydrophobic PLA yarn. In the process of upscaling treatment, it was found that restricting chain mobility prevented creation of surface topology. Restricting chain mobility was done by putting yarn under tension during treatment, which caused polymer chains to be aligned and stretched. Treatment starts to appear when additional length is given providing the ability for the yarn to shrink. Tuning the amount of slack we give, we found that there is a critical temperature between glass and fusion temperature, where treatment starts. Characterizing chain mobility, we reported that below critical temperature, movement of polymer chains leads to constant shrinkage. However, when above critical temperature, treatment increases chain mobility. Shrinkage growth fits very well a linear law, which can be used to determine minimum slack for treatment to appear.

#### B3 – Electrostatic and electrochemical doping of metaloxides ion-gated transistors

**J.R. Herrera Garza<sup>1</sup>**, L.P. Camargo<sup>2</sup>, R.K. Azari<sup>1</sup>, L.C. da Silva Neres<sup>3</sup>, S. Khaleel<sup>1</sup>, M.S. Barbosa<sup>4</sup>, C. Santato<sup>1</sup>, F. Soavi<sup>5</sup>

<sup>1</sup> Department of Engineering Physics, Polytechnique Montréal, Montreal, QC, Canada

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<sup>3</sup> Institute of Chemistry, São Paulo State University (UNESP), Araquara, SP, Brazil

<sup>4</sup> Institute of Chemistry, Federal University of Goias (UFG), GO, Brazil

<sup>5</sup> Department of Chemistry "Giacomo Ciamician", Alma Mater Studiorum Universitá di Bologna, Bologna, Italy

In ion-gated transistors (IGTs), the semiconducting channel is in direct contact with an ionic gating medium. At the interface, the electronic charge of the semiconducting channel is compensated by ionic charge in the ionic gating medium. The ionic charge forms a layering of ions known as the electrical double layer (EDL). Upon the application of a gating potential, a redistribution of ions at the interface is induced, thereby modulating the electronic conductivity of the semiconducting channel. If the semiconducting channel is impermeable to the ionic gating medium, the electronic conductivity modulation occurs via an electric field effect, akin to metal oxide field-effect transistors. In IGTs, the large electric field induced by the EDL results in surface charge carrier densities of around 10<sup>15</sup> cm<sup>-2</sup> and mobilities of 1 cm<sup>2</sup>  $V^{-1}$  s<sup>-1</sup>, with a low gating potential of around 1 V. If the semiconducting channel is permeable to ions, an electrochemical doping of the channel can be induced, involving complex interactions through the injection of ions into the channel. In this study, we investigate the influence of lithium ions in the electronic conductivity of anatase titanium dioxide, gated in IGT configuration, utilizing the ionic liquid [EMIM] [TFSI], for electrostatic doping, and LiTFSI in [EMIM] [TFSI]. thereby providing the conditions for electrostatic and electrochemical doping [1].

[1] Garza, J. R. H.; Camargo, L. P.; Azari, R. K.; da Silva Neres, L. C.; Khaleel, S.; Barbosa, M. S.; Soavi, F.; Santato, C. *Journal of Materials Chemistry C***2024**.

## B4 – Period-doubling bifurcations as route to chaos in resistively switching $Hf_{0.5}Zr_{0.5}O_2$ thin films

**S. Obernberger<sup>1</sup>**, K. Kohlmann<sup>1</sup>, A. Sarkissian<sup>2</sup>, P. Antici<sup>1</sup>, C. Schindler<sup>3</sup>, A. Ruediger<sup>1</sup>

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With the increasing interest of industry, research, and political decision-makers in growth areas of information technology such as artificial intelligence, quantum computing and quantum cryptography, there is also a growing need for electronic infrastructure. For example, new types of "neuromorphic" memory cells are being developed that can be used as artificial synapses in an artificial neural network due to their "spiketiming-dependent plasticity", which until now have only been simulated inefficiently in computers with von-Neumannarchitecture. We observed period-doubling bifurcations in such (Resistive Random-Access ReRAM Memory) based neuromorphic cells. In this work, RF-magentron sputtered TiN/Hf<sub>0.5</sub>Zr<sub>0.5</sub>O<sub>2</sub> (HZO)/Au capacitors have been fabricated and their switching behavior has been analyzed. We investigate resistive switching of the stacks via the formation and retraction of a conductive filament in HZO, and via the modulation of the tunneling barrier by the tunneling electroresistance effect (TER) to deduce energy dissipative effects leading to a negative feedback-loop in the "spike-timing-dependent plasticity". The negative feedback-loop enables the emergence of bifurcations in the cells switching characteristic. The bifurcations act as a pathway to deterministic chaos in the cells, the detection and control of which intensifies their use as artificial synapses and opens up the implementation as a fast-switching, easily controllable random-number-generator. This access to true randomness is essential not only for machine learning, but also for the quantum technologies mentioned above.

#### B5 – Charge carrier transport in sepia melanin

#### S. Khaleel, Z. Gao, A. Camus, C. Santato

#### Polytechnique Montréal, Montreal, QC, Canada

Sepia melanin, a naturally occurring pigment found in the ink sac of cuttlefish, has garnered significant interest for its intriguing electrical properties and potential as an organic semiconductor material. Sepia melanin exhibits properties of disordered organic semiconductors which display charge transport behavior attributable to a combination of band-like and hopping transport mechanisms. The electrical conduction in Sepia melanin is influenced by its complex hierarchical structure, which consists of melanin nanoparticles selfassembled into granules. These nanoparticles result from variety of arrangements of pi-pi stacked molecules.

Sepia melanin shows promise for organic electronics, energy harvesting, and bioelectronics due to its unique properties like moisture-dependent electrical response and broadband optical absorption. However, its insolubility in common solvents limits its potential. Understanding nanoscale charge transport phenomena could unlock its full potential, given that Sepia melanin granules typically range from 150-200 nm in size.

We focus our investigations on an inter-digitated planar geometry of patterns (inter-electrodes distance ~200-700 nm) as our goal is to detect signals emitted by granules of Sepia melanin. Patterns are fabricated by Electron Beam Lithography.

Preliminary findings indicate that structural disorder affects charge carrier transport in Sepia melanin, highlighting carrier localization and trapping effects. These findings provide opportunities for tailoring charge transport characteristics in devices. A nanoscale study of Sepia melanin granules reveals their remarkable high electrical conductivity.

Work is in progress to study the Electrochemical Impedance Spectroscopy (EIS) response in different atmospheres complemented by current-time measurement to confirm the nature of the charge carriers.

# B6 – Boron nitride nanotube buckypaper surface functionalization by exposure to planar gliding air plasma discharge

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Boron nitride nanotubes (BNNTs) are tubular boron nitride lattices with high thermal and chemical stability theoretically able to withstand reactive plasma environments. BNNTs can be formed into thin sheets (buckypaper) with the potential application as catalyst supports in plasma reactors for gas conversion. To test this, a BNNT buckypaper surface was exposed to a planar gliding air plasma discharge. The samples were treated for 60 min at a flow rate of 2.5 SLPM at atmospheric pressure. A high-voltage amplifier providing a 7 kHz signal with typical peak voltage and current values of 5.4 kV, and 43.9 mA sustained consistent and repetitive gliding discharges. The time-average power was 70 W, leading to a maximum temperature of 483 K measured on the top quartz glass plate. No physical change to the surface was observed under a 100x microscope. Rapid water absorption made contact angle goniometer measurements using 2 µL drops impossible. However, the absorption time decreased from 45.8 s (control) to 24.9 - 2.6 s for plasma treated samples. Faster absorption occurred the further the test was from the ignition point of the gliding discharge. XPS indirectly confirmed the increase in hydrophilicity; atomic oxygen increased from 6.3 to 23.5 -33.3%. Atomic nitrogen decreased from 39.7 to 13.3 - 25.2%. Atomic boron decreased from 51 to 40 - 45%. The boronnitrogen ratio increased from 1.3 to 3.3. The air plasma created nitrogen vacancies in the boron-nitride lattice which were filled with radical oxygen atoms. Argon and nitrogen plasmas effects on the buckypaper will also be assessed.

#### B7 – Boosting the atmospheric water harvesting of carbonxerogels

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Water scarcity is a significant challenge exacerbated by climate change, already affecting more than 1 billion people. While methods like desalination can generate fresh water, they require liquid water, which is not available everywhere. Another resource is atmospheric water, which is accessible without geographic or hydrologic limitations.

Nanoporous carbon sorbents have demonstrated potential for atmospheric water harvesting (AWH). However, currently there is no information available regarding the processing/performance relationship for this new type of AWH material. Here, we developed a carbon xerogel based on resorcinol formaldehyde (RF) resin, combining pyrolysis and physical activation under  $CO_2$  in a single step. This research links the particle size of the RF-xerogel, activation time and temperature to the performance of materials, from maximizing the water uptake to optimizing the daily water yield.

# B8 – Release of pest repellents from the surface of a biodegradable polymer

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Commercial nets made from the biodegradable polymer polylactic acid (PLA) were surface modified through a process known as Dip-Dip-Dry (DDD) to enhance their ability to uptake bioactive compounds, such as pheromones, and decrease the rate at which those compounds desorbed form the surface. The objective was to create a system that could be used to protect crops from pests without the use of harmful pesticides. Both exclusion nets and pheromonal control strategies are currently employed commercially in agriculture to protect crops from insect pests, but they have not been combined in this way before. Furthermore, storing and releasing pheromone directly form a surface is also an unconventional approach that comes with some unique challenges. The pheromone on the nets is exposed to the environment and solutions to issues like wash off by rain as well as pheromone degradation by sunlight had to be investigated. The characteristics of the surfaces created on PLA by the DDD process were studied and it was found that microstructures formed on the more crystalline net fibers differed from those observed on amorphous PLA. Release of volatile compounds, including the aphid alarm pheromone E-beta-farnesene (EBF), was measured on both flat PLA disks and multifilament PLA netting using mass loss. EBF mass loss tests on the nets showed

a release rate of 17.5g/m2•day over a period of 40-45 days after impregnation. This conformed that the time over which the surfaces can store, and release pheromone at biologically relevant levels was substantially extended by DDD.

## B9 – Plasma processes based on aerosols for functional coating deposition

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Thin film deposition garners significant attention due to the diverse functionalities they can reach. For example, nanocomposite thin films, i.e. films with nanoparticles embedded in a matrix, are developing multifunctional properties related to the matrix and the nanoparticles.

Different strategies are developed to form thin films. In dry processes, the use of an aerosol is really innovative [1,2]. Indeed, it enables to produce thin films independently of the liquid composition, e.g. pure liquids, liquid mixtures, liquid solutions (with unstable compounds) or colloidal solutions (with dispersed nanoparticles). For example, the introduction of liquid aerosols into a plasma enable to form various coatings [3]. Nevertheless, a lot of interactions between the plasma and the droplets can be introduced. For example, the evaporation of the liquid phase can affect the plasma physics and, ultimately, the plasma deposition process as well as the structure of the deposited thin film [4]. These phenomena, at the interface between physics and chemistry, are related to the injection method, to the aerosol velocity and to the size and the number of droplets in the aerosol [2].

Here, the presentation aims to review some processes based on aerosols for functional coating deposition.

- [1] M. Mitronika et al., SN Appl. Sci., 3(6), 665, 2021.
- [2] G. Carnide *et al.*, *Coatings*, 13(3), 630, 2023.
- [3] D. Ogawa et al., J. Vac. Sci. Technol. A, 27(2), 342, 2009.
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# B10 – Nanoparticle collection and in-flight functionalization during femtosecond pulsed laser micromachining

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Femtosecond laser ablation is an advanced machining technique where material is ablated from a surface to produce desired structures. This process generates nanoparticles, which in industrial settings become trapped in a fine particle filter. This project focuses on recovering waste by collecting the ejected nanoparticles. The goal is to optimize operating settings for a nanoparticle collector consisting of a rod-shaped electrode contained in a tube that is connected to a suction line. Tunable process parameters are the flowrate in the suction line and the laser machining stage velocity. Three suction flowrates (0, 0.57,and 1.13 m<sup>3</sup>/h) and stage velocities (1, 5, and 10 mm/s) were considered to determine optimal collection parameters for an applied potential of 2.0 kV. Using copper as an initial target; the collection efficiency was determined by comparing the masses of collected and ablated material. We found that the highest stage velocity leads to the best collection efficiency. This result is attributed to the increased distance between irradiated laser spots from subsequent pulses causing less interaction between an incoming pulse and the expanding nanoparticle plume from a previous pulse. Furthermore, the intermediate suction flowrate was optimal as it struck a balance between attracting the plume towards the electrode but not executing too much suction for the nanoparticles not to be collected. The recovery process is validated by comparing the collection of pure metals and alloys. Additionally, a capacitively coupled dielectric barrier discharge plasma source is used for in-flight surface functionalization to produce organic layer coated metal nanoparticles.

#### B11 – Preparation of hydrocarbon thin-films by injection of pentane aerosols into an atmospheric-pressure DBD using a direct liquid reactor injector

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Atmospheric-pressure plasma-enhanced chemical vapor deposition (AP-PECVD) is recognized as an attractive and versatile technique for coating due to its outstanding advantages as a single-step, solvent-free, dry deposition process that can be operated at ambient temperature and pressure. Dielectric Barrier Discharge (DBD) is an atmospheric-pressure plasma process that has proven to be useful in many industrial applications including ozone generation, exhaust gas depollution, plasma medicine, flow control, surface treatment, and thin-film deposition. In this study, we analyze the deposition of a liquid hydrocarbon precursor, pentane, on a silicon substrate using an integrated system of DBD Direct Liquid Reactor Injector (DLRI). The impact of the plasma and injection parameters on deposition efficiency and mechanism is assessed using Fourier Transform Infrared Spectroscopy (FTIR) and Optical Microscopy analyses. The obtained results reveal that the deposition efficiency decreases with increasing gas (N<sub>2</sub>) flow rate in the range of 0.1-1 L/min. Moreover, the deposition mechanism is modified at higher flow rates, as evidenced by the changes in the size of artifacts detected in optical microscopy images. In the range of 2-20 min deposition time, the amount of deposited material increases linearly with time, irrespective of the gas flow rate. Overall, the results indicate that the deposition process is strongly dependent on the injection and plasma parameters. Therefore, these parameters must be carefully adjusted to target specific applications.

# B12 – Development of a multi-walled carbon nanotube filter for detaining immunosuppressive T-Cells and inducing the activation of effector T-Cells

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Cancer is a major public health problem worldwide and the main cause of death in Canada. Effectively treating cancer remains a challenge given its ability to evade and suppress immune responses. Recently, adoptive T-cell transfer (ACT) has gained popularity as a promising cancer immunotherapy that enhances the effectiveness of white blood cells through ex vivo cellular and genetic engineering practices. T-cells are a type of white blood cell that proliferate and differentiate into effector T (T<sub>eff</sub>) cells and memory T  $(T_m)$  cells which play a critical role in killing cancer cells. Regulatory T (T<sub>reg</sub>) cells are immunosuppressive cells that compromise the efficacy of cancer-killing T<sub>eff</sub> cells. Therefore, the goal of this project is to reduce the inhibitory influence of immunosuppressive T-cells and enhance the efficacy of ACT technology by developing a dual-functional filter. This filter aims to detain immunosuppressive T<sub>reg</sub> cells and induce T<sub>eff</sub> cell activation by mechanical forces and nonphysiological agonists. Multi-walled carbon nanotubes (MWCNTs) will be used as the filtrate material and act as a functional coating given their attractive material properties such as high structural integrity, surface area and mechanical performances. To improve the biocompatibility of the MWCNT filters, the environmentally cautious surface modification treatment of ammonia plasma functionalization will be performed to add amine-functional groups on the surface. Target antibodies will then be immobilized on the amine functionalized MWCNT surfaces. Selective enhancement and proliferation of T-cells by passing them through immobilized target antibodies on plasma functionalized MWCNT filters may be a novel method of cancer treatment.

# B13 – Electrophoretic deposition of a strongly adhering multi-walled carbon nanotube coating by addition of a plasma polymer interlay

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Electrophoretic deposition (EPD) is a commonly used technique for coating metallic substrates. While early EPD processes focused on the deposition of ceramic particles, the field has now expanded to depositing advanced materials such as multi-walled carbon nanotubes (MWCNTs). The EPD of MWCNTs has been well researched; however, to produce stable MWCNT suspensions, MWCNTs need to undergo wet chemical treatments or be mixed with surfactants which can lead to coating contamination. In addition, MWCNT deposits often have weak adhesion to the substrate. This work targets these two weaknesses. First, the MWCNTs were functionalized by plasma treatment producing oxygenated MWCNTs (O-MWCNTs). O-MWCNTs were then sonicated in reverse osmosis water to create a stable suspension. Second, an ethane-based plasma polymer was applied on a 316 stainless steel substrate as an interlayer to improve adhesion. O-MWCNT coatings were produced at voltages of 5 - 40 V and deposition times of 1 - 60 min. The deposited coating morphology and chemistry were characterized by scanning electron microscopy and energy dispersive x-ray analysis. Further, they were evaluated by Raman spectroscopy and profilometry. The coatings were homogeneous, free of contamination, and maximum thicknesses of 10 mm were achieved. They were strongly bound to the substrate as confirmed under high-shear stress conditions in a parallel plate liquid flow chamber. This result is supported by the observation of bond formation between the deposited O-MWCNTs and the plasma polymer (cf. Figure). The combination of these properties allows the MWCNT coatings to be further treated or used as-is in a multitude of applications.

# B14 – Quantum spin pumping in normal/bearded zigzag graphene nanoribbon

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Quantum pumping of current is the generation of a DC at zero bias by periodic variation of one or more external system parameters, e.g. the AC field. Quantum pumping contains two opposite photon-assisted processes—photon-absorption and photon-emission processes. The quantum charge and spin pumping in graphene nanoribbons (GNRs) have recently aroused growing attention.

The bearded zigzag GNR is a special kind of GNR, in which an additional atom exists at one edge of the zigzag GNR. A zeroenergy flat band exists in the energy band, which bends upward/downward for the spin-up/down carrier when a local exchange splitting is introduced. The peculiar bending energy bands specify that only one photon-assisted process can occur for a definite spin at low energy.

In this paper, we theoretically investigate the non-adiabatic quantum spin pumping in the zigzag GNR with a local magnetized bearded zigzag GNR inserted between the scattering region and the electrode. It is found that only one spin can enter the electrode, depending on the magnetization direction of the ferromagnetic insulator. The results indicate that spin polarization and a feasible spin separation device can be realized. It is also interesting to find that the direction of the pumped spin current and the phase difference between the two pumping sources is a cosine function rather than the traditional sine function. The calculated results are beneficial for spintronic applications based on GNRs.

# B15 – Enhanced Photocatalytic Degradation Efficiency of Tetracycline by Band Edge Engineering of Thin Film $BiVO_4/TiO_2$ Heterostructure

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The presence of emerging contaminants such as antibiotics in the environment is an increasing health concern due to their role in inducing antibiotic resistance. By utilizing solar energy, visiblelight-driven photocatalysis is a promising technique for degrading toxic contaminants in water. However, designing and fabricating photocatalysts with a strong visible light response, high charge carrier separation efficiency, and high stability remains a significant challenge. In this study, by depositing a thin film of tungsten-doped VO2 (W-VO2) between BiVO4 and TiO<sub>2</sub>, the band alignment and internal electric field (IEF) direction are modified in the ternary heterojunction. As results, under visible irradiation, the kinetic rate constant for tetracycline removal by the BiVO<sub>4</sub>/W-VO<sub>2</sub>/TiO<sub>2</sub> photocatalyst is 225% higher than that of BiVO<sub>4</sub>/TiO<sub>2</sub>, due to the efficient use of charge carriers before recombination. The superior performance of BiVO<sub>4</sub>/W-VO<sub>2</sub>/TiO<sub>2</sub> in charge utilization is further confirmed by photoelectrochemical tests. An improvement in photocurrent density of approximately 145% compared to BiVO<sub>4</sub>/TiO<sub>2</sub> was shown at 1.23 V versus RHE. By employing a pool of characterization tests and advanced analytical method (LC-HR-MS/MS) followed by the Toxicity Estimation Software Tool (T.E.S.T.), it is concluded the band alignment and IEF direction are critical factors for efficient degradation, solution detoxification and the reduction of toxic by-products. The ability of VO<sub>2</sub> to tune band edge ratio opens up new avenues for the design of high-performance heterojunction devices.

### Posters C:

#### Optical films and energy-related applications

#### C1-Stress development in amorphous optical thin films: mechanisms of stress generation and the role of the sputtering parameters

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The control of stresses is one of the key aspects in the development of high-performance optical thin films. Excessive stress development during film deposition can impact its optical and mechanical properties and lead to complete failure. Therefore, thoroughly understanding the mechanisms leading to stress generation and its dependency on processing parameters is fundamental. Recently, comprehensive models for stress generation have been developed for crystalline materials. However, little attention has been devoted to amorphous materials. Seeking to understand the particularities of stress generation in this class of materials, which is highly relevant for optical applications, we deposited model 500-nm-thick SiO<sub>2</sub> and amorphous Si films by RF magnetron sputtering under different conditions of working pressure and deposition rates. The stress development was assessed via in-situ substrate curvature measurements. The nature and the magnitude of the intrinsic stress were found to depend drastically on the gas pressure during the deposition. For instance, a decrease of 0.5 mTorr was sufficient to invert the nature of stress from tensile to compressive in the case of SiO<sub>2</sub> or increase the compressive stress more than two-fold, from -200 MPa to -500 MPa, for an a-Si film. The results show that the intrinsic stresses in amorphous films combine a tensile component arising from pore formation and a compressive component generated from energetic bombardment during film growth. Each of these components can thus be tuned by adjusting the deposition parameters, as demonstrated by a mapping of stress development for each material.

# C2 – Synthesis, microstructural, optical, and mechanical properties of SiN<sub>x</sub> thin films deposited by LPCVD and reactive sputtering, and their integration into photonic integrated circuits

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This study presents a comparative analysis of silicon nitride (SiNx) thin films fabricated using two distinct methods: Low-Pressure Chemical Vapor Deposition (LPCVD) and Reactive Sputtering Deposition (RSD). The LPCVD-produced films demonstrate exceptional uniformity across the 4-inch substrate  $(\pm 0.34\%)$  and exhibit reduced surface roughness (0.16 nm). However, their tensile stress level is high (1 GPa), resulting in the formation of numerous cracks when the thickness exceeds 450 nm. Conversely, sputtered films with similar thickness exhibit lower compressive stress levels (~ 250 MPa) and maintain a crack-free microstructure, albeit with increased roughness (> 1.5 nm) and improved uniformity ( $\pm$  2.6%). Notably, the sputter-deposited films remain crack-free even at thicknesses of up to 800 nm. It is pertinent to mention that both deposition methods maintain optical properties ( $n \sim 2$  at 1.55 μm) suitable for the fabrication of optical waveguides with low propagation losses (<0.4 dB/cm). The results of this comparative study underscore the trade-offs between film microstructure, stress, and optical quality, offering valuable insights for enhancing the performance of optical waveguides.

# C3 – Silver-based transparent conductors with improved optical performance and environmental stability

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Indium-tin oxide is a common material for transparent conductor (TC) applications, but processing limitations and concerns around indium scarcity highlight the need for alternatives. One promising candidate is silver-based TCs, which have been shown to display excellent electrical and optical performance. However, the environmental durability of such coatings is almost never reported, despite that Ag's high susceptibility to corrosion and humidity is a factor of paramount importance in designing functional and sustainable devices. Here, we aim to optimize the durability and antireflective properties of a Agbased TC while maintaining a Haacke figure of merit comparable to other Ag-based TCs in the literature. TCs employing combinations of different seed layers and nitrogen doping levels of the Ag films are tested, and their resulting performances and durability are related to the Ag morphology. We find that excellent performance and outstanding environmental stability can be simultaneously achieved when combining an aluminum-doped zinc oxide seed layer, low concentrations of N<sub>2</sub> doping of the Ag layer, and nickel-chrome nitride protective layers. As a significant improvement can still be observed when the NiCrN<sub>x</sub> layers are removed, we propose a mechanism for the increased durability based on the microstructural changes inherent to the combination of ZnO(AI) and low-concentration  $Ag_{(N)}$ . Finally, we combine these results to create prototype samples with < 0.3% reflection, < 2.5% loss in transmission, sheet resistance of 22.4  $\Omega/\Box$  and high durability, showing minimal changes to the optical or electrical properties following immersion for 20 minutes in a 200 g/L solution of NaCl heated to 50°C.

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# $C4-Low\text{-loss}\ Al_2O_3$ and $SiO_2$ thin films for photonics deposited by plasma-assisted reactive magnetron sputtering

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Oxide-based thin-films play an integral role as optical coatings and light-guiding layers for integrated photonic devices for applications ranging from telecommunications to biomedical imaging. Several methods for depositing optical-quality thinfilms have been employed; however, the fabrication of specific thin-films can pose significant challenges, particularly for industrial-scale production. For instance, the need for hightemperature annealing, which is often necessary to mitigate optical losses, can be undesirable for temperature-sensitive substrates. It can also increase the associated costs and add complexities to the fabrication process. Simplifying the process and reducing the reliance on high-temperature treatments are critical for overcoming these challenges and advancing thin-film technology for broader applications. In this study, plasmaassisted reactive magnetron sputtering (PARMS), is presented as a reliable, straightforward, cost-effective, and wafer-scale compatible technique for depositing high-quality thin-films at low temperatures. Using the PARMS technique, we deposited amorphous Al<sub>2</sub>O<sub>3</sub> and SiO<sub>2</sub>, which are two materials of interest in photonic platforms, for their roles in many passive (e.g., optical waveguides, filters, and resonators) and active (e.g., optical lasers, amplifiers, and modulators) functionalities. We fabricated low-loss thin-films with stoichiometric composition, low surface roughness (R<sub>4</sub>=0.238 nm), and high deposition rates at 150°C. 1.0-µm-thick Al<sub>2</sub>O<sub>3</sub> planar waveguides, deposited with this technique and a deposition rate of 23 nm/min, exhibited optical losses below 1 dB/cm at 638.2-nm wavelength and as low as 0.1 dB/cm in the conventional optical communication band. When employed as a top-cladding layer on silicon nitride strip waveguides, SiO<sub>2</sub> thin-films with similar thickness resulted in negligible excess loss at 1550-nm wavelength.

# C5 – Optical and structural properties of Ag-polymer nanocomposites prepared by combination of gas phase methods

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Metamaterials or metasurfaces based on plasmonic nanoparticles in dielectric matrix represent an emerging topic pushing the limits of standard optical coatings. The usefulness of such materials was demonstrated for absorbers, plasmonic coloration, transparent electrodes, and optical filters. However, derivation of optical properties, i.e., complex refractive index, is still quite a challenging task for such structures, and only the phenomenological approach is adopted for fabrication of optical devices based on these metamaterials.

In our work, we propose a novel approach for the synthesis of Ag-polymer nanocomposites by combining the thermal evaporation of polymer with magnetron sputtering of silver. Such an approach allows the synthesis of homogenous composites with a filling factor varying from 1% up to 80% of silver volume fraction. Moreover, our approach is very reproducible and deposition rates are in range of 10-100 nm per minute. The synthesized composites are holistically investigated from structural, optical, and chemical points of view, with the main emphasis on deriving complex refractive index in a broad range of filling factors by spectroscopic ellipsometry.

The derived optical constants are used for the modelling of the different color Bragg reflectors based on a stack of polymer and composite layers. The predicted thickness and filling factors are subsequently used for the deposition of real Bragg reflectors ranging from blue up to red color.

Reproducible and controllable synthesis of the reflectors verifies derived optical constants of synthetised metamaterials, as well as highlights thermal evaporation of polymer in combination with Ag sputtering.

# C6 – The capabilities to form periodically modulated coatings and their applications for spatial filters and polarizers

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For the formation of interference coatings, the variation of homogeneous films' optical constants is used by combining different materials with high and low refractive indexes. During the glancing angle deposition method, the stationary placed substrate's orientation can be angle-tuned according to the vapor flux in order to form nanostructured anisotropic layers by evaporating amorphous thin films. For various applications, even more complicated 3D structures can be accomplished by depositing layers on periodically patterned substrates, i.e., gratings.

The evolution of optical coatings from one-dimensional to threedimensional periodic structures will be presented. The focus will be on two topics: i) anisotropic coatings for polarization control [1,2] and ii) the possibility to form dielectric structures with periodic modulation of optical constants together with the application of angular filtering of light [3,4]. The investigation of different technologies for the single-layer and multilayer coating deposition on nanostructured surfaces will be reviewed.

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## $C7-a\mbox{-}Si:\mbox{H}\mbox{/}SiO_2$ HR coatings for gravitational wave detection

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In their most sensitive frequency range, current gravitational wave detectors like LIGO are limited by a phenomenon linked to internal mechanical dissipation (IMD) and found in amorphous materials. Indeed, these few-km-long Michelson interferometers feature 34-cm wide Bragg mirrors made of amorphous oxides. Through the dissipation-fluctuation theorem, random fluctuations of the mirror surfaces induce a noise comparable to the shot noise in these instruments. Among the efforts to circumvent this problem for the next generations of detectors, different groups are investigating the possibility of fabricating the Bragg reflectors from amorphous materials possessing the lowest possible IMD such as bilayers of hydrogenated amorphous silicon (*a*-Si:H) and amorphous silica (*a*-SiO<sub>2</sub>), the latter requiring quite high temperature anneal treatments for *a*-Si:H ~ 350 °C.

Amorphous silica  $(SiO_2)$  and *a*-Si have a very high refractive index contrast which has the potential to reduce the total noise in the gravitational wave detectors, but *a*-Si absorption seems too high. *a*-Si:H has a similar structure to *a*-Si but has a much smaller absorption that could be compatible with the high power laser. However, its IMD has never really been studied in its most common range 5-15% [H]. This project aims to investigate how to simultaneously lower the total absorption of the Bragg mirror and lower the IMD of *a*-Si:H. This will be done through the optimization of the deposition conditions and post-treatments such as plasma annealing and forming gas annealing, notably the effect of deuterium and hydrogen.

#### C8 - Exploring optoelectronic properties of magnetronsputtered nanoparticles with finite-difference time-domain method

**P. Pleskunov<sup>1</sup>**, Z. Krtouš<sup>2</sup>, M. Protsak<sup>1</sup>, T. Košutová<sup>3</sup>, M. Cieslar<sup>4</sup>, L. Martinu<sup>2</sup>, A. Choukourov<sup>1</sup>

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Plasmonic nanoparticles (NPs) encompass diverse light-matter interaction regimes and unlock application opportunities in fields of sensing, energy conversion and others. The rapid growth in complexity of nanoplasmonic systems underscores a high demand for efficient and accurate simulation tools. The finite-difference time-domain (FDTD) method, owing to its conceptual simplicity, became the industry standard computational electromagnetic solver used to design image sensors, LEDs and metamaterials. Generally, FDTD is employed when dimensions of domain of interest are comparable to considered wavelength. In this study, we demonstrate applicability of FDTD simulations in modelling the optoelectronic properties of plasmonic NPs and their ensembles, while focusing on magnetron-sputtered metallic (Ag, 30 nm) and transition metal nitride (HfN, 10 nm) NPs. First, absorption and scattering efficiencies of Ag NPs are calculated using a single NP model and compared to the analytical solutions obtained from the Mie theory. Subsequently, the model is extended by incorporating a core-shell structure and integrating the optical constants of HfN and HfO<sub>2</sub> to analyze the NP optical properties and impact of the NP size and level of oxidation. Formation of a 2-nm-thick oxide shell reduces the NP absorption/scattering efficiencies and induces the extinction band red-shift, while variations in the NP size influence the band intensity. Finally, going beyond the single NP model, the HfN NP coating optical spectra are reconstructed by combining FDTD with measured spectroscopic ellipsometry data. This approach reveals the NP coating reflectivity suppression by the coating porosity. As a result, it opens a possibility for modelling complex nanostructured heterogeneous systems.

## C9 – Bragg-reflector-enhanced electrochromic devices with adjustable optical performance

M. Crouan, B. Baloukas, O. Zabeida, J. Sapieha, L. Martinu

#### Department of Engineering Physics, Polytechnique Montréal, Montreal, QC, Canada

Electrochromic (EC) all-solid-state devices (ASSDs) are of great interest across various industrial applications, such as smart glass for buildings, airplane windows, lenses, and mirrors. These devices possess the ability to dynamically change their optical properties, transitioning from a bleached state to a colored state through a redox reaction following the application of a low voltage. Due to the inherent properties of EC materials, ASSDs exhibit significant absorption and transmission modulation and, as a result, a limited capacity for reflection modulation. Yet, achieving a reflection increase upon coloration can offer new functionalities in terms of aesthetics and the development of innovative optical filters. The implementation of EC Bragg mirrors (ECBM) using WO<sub>3</sub> and ITO bilayers in an ASSD hence holds significant promise as a means of reaching a substantial increase in reflection at specific wavelengths during coloration. In this work, we compared a conventional ASSDs with various

ECBM configurations incorporated into an ASSD. Specifically, via a comprehensive optical modeling study, we designed an ASSD which transitions from a transparent anti-reflective state to a mirror-like opaque state within the visible spectrum. The fabricated antireflective ASSD with 2-bilayers of WO<sub>3</sub>/ITO displayed an increase in  $R_{lam}$  from 1.4% in the bleached state to 8.9% in the colored state. By minimizing the constraints on the antireflective properties, we achieved a reflection increase of 19.8% upon coloration, opening new possibilities for dynamic optical interference filters.

### C10 - Influence of the deposition pressure on the memory effect of sputtered electrochromic WO<sub>3</sub> thin films

**B. Faceira<sup>1</sup>**, L. Teulé-Gay<sup>1</sup>, H.-Y. Huang<sup>2</sup>, Y.-C. Huang<sup>2</sup>, C.-L. Dong<sup>2</sup>, M. Maglione<sup>1</sup>, A. Rougier<sup>1</sup>

<sup>1</sup> Univ. Bordeaux, CNRS, Bx INP, ICMCB, Pessac, France

<sup>2</sup> Research Center for X-ray Science & Department of Physics Tamkang University, Tamsui, Taiwan

Electrochromic materials and devices, able to modify reversibly their optical properties caused by a redox reaction in response to an external electrical stimulus are recognized as one of the key green technologies for sustainability and energy savings. WO<sub>3</sub> undergoes coloration upon reduction with insertion of small cations  $(H^{+}, Li^{+})$  associated with a visual switch from colorless to blue. Aiming to reaching zero-energy consumption electrochromic devices, the memory effect property, described as a reversible color persistence while the potential is withdrawn is of particular interest. The influence of the deposition pressure during sputtering on the electrochemical and optical properties of WO<sub>3</sub> films is studied with a focus on their memory effect. It appears that a high deposition pressure favors fast coloration/bleaching kinetics (15.3s/5.2s at 550 nm) but weaken the memory effect. Lowering the deposition pressure allows to enhance the memory effect property until some point where irreversible coloration (reversibility < 24%) of the film is reached during electrochemical cycling. The origin of these discrepancies is studied through the stoichiometry, the local atomic environment, and the morphology of the WO<sub>3</sub> thin films. This study highlights a better understanding of the memory effect property of electrochromic oxides for low-consumption energy electrochromic devices, pointing out morphology as a key parameter [1].

[1] B. Faceira, L. Teulé-Gay, J. Le Hébel, C. Labrugère-Sarroste, F. Ibalot, H.-Y. Huang, Y.-C. Huang, C.-L. Dong, J.-P. Salvetat, M. Maglione, A. Rougier, *Advanced Materials Interfaces* **2023**, *10*, 2300549.

## C11 - Origin and nature of defects in low-emissivity coatings

**O. Touré**, B. Baloukas, O. Zabeida, J. Klemberg-Sapieha, L. Martinu

Department of Engineering Physics, Polytechnique Montréal, Montreal, QC, Canada

Low-emissivity (Low-e) coatings on glass, manufactured to maximize visible light transmission and minimize infrared emissivity via their high infrared reflectance, play an essential role in the reduction of energy consumption in buildings from heating and cooling. In the most frequently used multi-layer designs, metallic (Ag, Au, Cu, etc.) and dielectric (TiO<sub>2</sub>, ZnO,  $SnO_2$ , etc.) layers ensure the expected optical performance, while assisting in the durability, and resistance of the coating to environmental factors such as moisture, oxidation, scratching, etc. However, fabrication steps such as manipulation, cleaning, and storage of the low-e coated glass can create minor surface defects which, fortunately, are most often undetectable by the human eye. However, during the heat treatment (HT) of the glass at high temperatures, required to obtain safer and thermally toughened glass, the added thermal energy paired with the disrupted microstructure from the initial defects can render the latter highly visible. In this work, we analyse the effect of HT on the intensification of defects such as scratches generated under controlled conditions. Degradation mechanisms including Ag agglomeration and corrosion are investigated to develop a general degradation model for surface defects in low-e coatings.

# C12 – Transparent flexible electrodes through advanced patterning approaches

### **A. Pajak, M.-A. Dionne,** B. Baloukas, O. Zabeida, J. Klemberg-Sapieha, L. Martinu

#### Department of Engineering Physics, Polytechnique Montréal, Montreal, QC, Canada

This study addresses the increasing need for advancements in transparent flexible electrodes (TFEs) to facilitate the development of faster and more complex next-generation optoelectronic devices. While tin-doped indium oxide (ITO) is commonly used due to its high luminous transmittance ( $T_{lum}$ ) and low resistivity, its brittleness restricts its application as a flexible conductor. Considering current challenges in existing TFEs, our research focuses on thin film conductors deposited on polymer substrates, matching current state-of-the-art TFEs and introducing improved transparency through nano- and micropatterning. Herein, we propose three such approaches, i.e. electrospinning, nanosphere lithography and UV photolithography, all of which subsequently are used in parallel with magnetron sputtering for depositing various material combinations, e.g. transparent conductive oxides (TCOs) and/or single metallic layers (e.g., Au, Ag, Cu). This procedure leads to the manufacture of conductive nanotrough networks and nano-/micro- meshes of enhanced flexibility. Through optimization, these TFEs can achieve  $T_{lum}$  exceeding 80% and sheet resistance  $(R_S)$  below 50  $\Omega^{-1}$ . Testing for flexibility and compatibility with polymeric substrates further validated the robustness of our approach.

#### Posters D:

#### Advanced Characterization

# D1 - Atomistic insights into the effect of hydrogen on the structure and mechanical properties of amorphous silicon nitride

Y. Ouldhnini, B. Ahammou, K. Kaur Ghuman, M. Chaker

#### Institut National de la Recherche Scientifique (INRS), Varennes, QC, Canada

The mechanical properties of hydrogenated amorphous silicon nitride (a-SiN:H) thin films undergo significant alterations due to the presence of hydrogen. To delve into this behavior, we used molecular dynamics (MD) simulations to explore a-SiN:H with varying hydrogen concentrations. By processing the samples with the melt-quench method, our investigation primarily focused on elucidating the structural properties, including shortand medium-range atomic configurations, correlated with the mechanical responses of a-SiN:H systems with diverse hydrogen amounts. In particular, through pair distributions, angle distributions, and coordination analysis, alongside elastic constants and stress-strain responses, we show that a low hydrogen fraction incorporated into silicon nitride reduces the number of undercoordinated atoms and consequently the concentration of dangling bonds, while high fractions of hydrogen lead to the depolymerization of the film network. These structural changes directly impact the material's strength by reducing a-SiN:H rigidity with increasing hydrogen content. This work elucidates structure-mechanical properties relationships in a-SiN:H through atomistic simulations, providing useful insights for understanding crack initiation and mechanical failures during experimental thin film deposition, especially for the low-pressure chemical vapor deposition technique.

# D2-Exploring the structural and mechanical properties of deposited SiN<sub>x</sub> thin films through molecular dynamics simulations

#### B. Ahammou, Y. Ouldhnini, K. Kaur Ghuman, M. Chaker

#### Institut National de la Recherche Scientifique (INRS), Varennes, QC, Canada

Our study provides a comprehensive analysis of the mechanical properties of deposited silicon nitride  $(SiN_x)$  thin films through molecular dynamics simulations, motivated by  $SiN_x$ 's critical role in enhancing the performance of photonic devices across various applications. We explored the structural and mechanical behaviors of  $SiN_x$  thin films across different stoichiometries and processing conditions. To enhance computational efficiency, our simulations omit hydrogen due to its evaporation at high

temperatures in chemical vapor deposition and its negligible impact on the dynamics of ion bombardment. We focused on the interactions between Si and N, crucial for determining the structural and mechanical properties of SiN<sub>x</sub> films. By employing multibody potentials, our simulations provide insights into the angular dependencies and interactions between atom pairs, thus shedding light on the film's microstructural development without the direct simulation of chemical reactions. Our methodology aims to clarify how microstructural features, such as density variations, influence the films' macroscopic mechanical properties, including intrinsic stress, Young's modulus, and fracture toughness. These insights are vital for understanding the mechanical stability of SiN<sub>x</sub> films in photonic applications. Linking simulation results with experimental characterizations, achievable through X-ray diffraction techniques, nanoindentation, and wafer curvature, is possible. This research not only enhances our comprehension of the growth of SiNx films but also presents a framework for optimizing deposition processes to improve film durability against mechanical failures. Combining simulation with experimental characterizations offers a comprehensive strategy for developing SiN<sub>x</sub> films with specialized properties for photonic applications.

#### D3 – In plasma ion beam analysis

**L.-C. Fortier<sup>1</sup>,** M. Chicoine<sup>1</sup>, S. Chouteau<sup>1</sup>, M. Clausse<sup>2</sup>, É. Lalande<sup>1</sup>, A. Lussier<sup>1</sup>, G. Terwagne<sup>2</sup>, S. Roorda<sup>1</sup>, L. Stafford<sup>1</sup>, F. Schiettekatte<sup>1</sup>

<sup>1</sup> Department of Physics, Université de Montréal, QC, Canada <sup>2</sup> Department of Physics, Université de Namur, Namur, Belgium

We present two experiments where a layer is plasma-etched while monitoring its evolution by *in plasma* ion beam analysis. First, we etch a photoresist with a diffuse  $O_2$  plasma at low pressure. Using a 4.335 MeV He beam, Rutherford Backscattering Spectrometry and Elastic Recoil Detection spectra are acquired every minute during 8 hours. Etching of most elements follows a linear trend, but H desorbs faster at the beginning of the plasma process, which we ascribe to the ion beam-induced desorption. In addition, we observe a thin Mo layer building up at the surface, likely due to the sputtering of an electrode in the plasma source.

Secondly, we study hydrogen etching by a diffuse Ar plasma at low pressure applied to a <100> crystalline Si surface which had been exposed to HF etching expected to leave 14 H/nm<sup>2</sup> bonded to the Si surface at the beginning of the Ar etch. During plasma processing, the H surface concentration is monitored using a resonant nuclear reaction with a <sup>15</sup>N beam at 6.385 MeV. The initial H concentration is H/nm<sup>2</sup> and decreases over a 3-minute timescale to an equilibrium concentration of H/nm<sup>2</sup>. Over the range of experimental conditions investigated, the diffuse Ar plasma is therefore not able to entirely sputter the H from the c-Si surface.

### Posters E:

#### **Special Posters**

### E1 – How can sustainability be integrated into the research culture?

L. Cacot, M. Boiteux, L. Stafford

#### Université de Montréal, Montreal, QC, Canada

In September 2015, UN member states adopted the Sustainable Development Program known as Agenda 2030. This program defines targets to be reached by 2030 to meet the challenges of the current and future environmental crisis.

The UN's Sustainable Development Goals (SDGs) provide a reference framework for operationalizing sustainable development, including adaptation to climate change, improving global health, and reducing social and environmental inequalities. This framework proposes 17 SDGs divided into a number of targets which, taken together, will ensure a more viable future for generations to come.

Universities have a role to play in building a more sustainable future, through knowledge development, education, and knowledge transfer on major societal issues. Furthermore, universities can contribute by adopting sustainable approaches throughout the entire research process, from conceptualization to execution.

Our work builds on these concepts by developing tools for more sustainable scientific research, both in terms of the research object and the way research is carried out in the laboratory. Additionally, our objective is to identify barriers and overlooked areas in research when adopting a sustainable development approach. This works aims to brings researchers together to explore and discuss innovative strategies and best practices for incorporating sustainability into research practices. By recognizing the intrinsic connection between research and sustainability, we can foster interdisciplinary collaboration, enhance knowledge transfer, and accelerate the adoption of sustainable principles across various academic disciplines.

#### E2 – Central Facilities at Polytechnique Campus of the Thin Film Science and Technology Research Center (GCM):

#### M.-H. Bernier, J. Lefebvre, C. Clément

Department of Engineering Physics, Polytechnique Montréal, QC, Canada

- Laboratory for Surface Analysis of Materials (LASM)
- Microfabrication Laboratory (LMF)

### Wednesday, 9:30 - 16:30, June 5, 2024

### WORKSHOP A

 $9{:}00-12{:}00\,/\,13{:}00-16{:}30$ 

#### Spectroscopic ellipsometry: Case and tricks of the trade (sponsored by J.A. Woollam Co., Inc.)

INSTRUCTOR: Nina Hong J.A. Woollam Co., Inc.

Bill Baloukas Polytechnique Montréal, Montréal, QC, Canada

MODERATOR: **Bill Baloukas** *Polytechnique Montréal, Montréal, QC, Canada* 

Spectroscopic ellipsometry (SE) is a proven optical characterization technique for thin film characterization using light polarization. It is primarily used to determine film thickness and material optical properties such as the refractive index and extinction coefficient. Its applications also include the characterization of surface roughness, index gradients, compound compositions, multi-layer stacks, doping concentrations, anisotropy, metamaterials, and multiple other properties associated with the optical response of surfaces. The commercially available wavelength range is now very wide and extends from the vacuum ultra-violet (140 nm) to the terahertz (~3 mm). In addition, the implementation of Mueller matrix SE allows for the characterization of anisotropic samples that may be depolarizing and cross-polarizing.

This one-day workshop will cover the following topics:

- 1. An overview of the fundamentals of SE.
- 2. Standard to advanced applications of SE by a case studies approach including:
  - o SE, from thin films to multilayers.
  - o Obtaining the optical constants in a wide spectral range.
  - o Mueller matrix SE for anisotropic samples.
  - o Other applications such as: *in situ* SE, temperature measurements, composition depth profiles, ellipsometric porosimetry, dynamic measurements, etc.
- 3. Q&A session: Questions sent by the participants 1 week prior to the workshop will be addressed.
- 4. Hands-on laboratory session using RC2-XI and IR-VASE instruments.

During the laboratory session, it will be possible to test a limited number of your own samples. If interested, please contact Bill Baloukas at <u>bill.baloukas@polymtl.ca</u>.

### Wednesday, 9:30 - 16:30, June 5, 2024

### WORKSHOP B

 $9{:}00-12{:}00\,/\,13{:}00-16{:}30$ 

#### Tribo-mechanical surface characterization (sponsored by Anton Paar)

INSTRUCTORS: Jiri Nohava Anton Paar

Mohammad Reza Anton Paar

Stephen Brown Polytechnique Montréal, Montréal, QC, Canada

MODERATORS: **Stephen Brown** *Polytechnique Montréal, Montréal, QC, Canada* 

#### Introduction to Nanoindentation

This presentation introduces the theoretical and practical concepts of instrumented indentation. The participant will discover its origins, its many advantages and its practical applications in a wide range of industrial and academic sectors. The numerous presented examples will illustrate that the properties measured by instrumented indentation extend far beyond the hardness and elastic properties of surfaces.

#### Introduction to Scratch testing

The problems of surface scratches and coating delamination are frequently overlooked or are frequently studied by the use of old and non-repeatable measurement techniques. With the scratch test method, the participant will discover an advanced quantitative technique that enables one to make significant progress in numerous fields of application.

#### Introduction to Tribology

Tribology is commonly defined as the science of friction, lubrication and wear. This presentation will detail the basic concepts of tribology, its specifics, and present numerous examples of applications in fields as varied as medical technologies, food industry, cutting tools and many others.

During the laboratory session, it will be possible to test a limited number of your own samples. If interested, please contact Stephen Brown at <a href="mailto:stephen.brown@polymtl.ca">stephen.brown@polymtl.ca</a>.

### Wednesday, 9:30 - 16:30, June 5, 2024

### WORKSHOP C

 $9{:}00-12{:}00\,/\,13{:}00-16{:}30$ 

# Developing an understanding of surface chemistry – Multi-technique electron spectroscopy-based investigation (sponsored by Thermo Fisher Scientific)

INSTRUCTORS: James Lallo Thermo Fisher Scientific

Josianne Lefebvre Polytechnique Montréal, Montréal, QC, Canada

MODERATOR: Josianne Lefebvre Polytechnique Montréal, Montréal, QC, Canada

Developing an understanding of the surface chemistry of a material is fundamental to optimizing its properties and performance. Whether it be organic, inorganic, or even hybrid materials, from dielectrics to metals, various electron and ion spectroscopic techniques are used to gain insight about the outer layers and adjacent surfaces and interfaces.

X-ray photoelectron spectroscopy (XPS) and ultraviolet photoelectron spectroscopy (UPS) use photon irradiation to initiate electron emission and quantitatively identify chemical groups and occupied states in the valence band, respectively. Reflected electron energy loss spectroscopy (REELS) uses a source of electrons to probe the electronic structure of a material, including unoccupied states, band gap and even hydrogen content. In a similar fashion, ion scattering spectroscopy (ISS) fires ions at a surface and analyses the energy of these elastically scattered ions to identify atomic species in the outermost layer only. All these techniques are brought together into one instrument to get the most out of an investigation.

This one-day workshop will feature the following:

- Introduction to the basic theories of XPS, UPS, REELS and ISS techniques and their instrumentation.
- Overview of electron spectroscopy applications including micro/optoelectronics, biomedical, optics, aerospace, manufacturing, energy and others.
- Demonstration of XPS data analysis using Thermo Fisher Scientific's Avantage software.
- Hands-on laboratory session using the Thermo Fisher Scientific Escalab Xi system.

During the laboratory session, it will be possible to test a limited number of your own samples. If interested, please contact Josianne Lefebvre at josianne.lefebvre@polymtl.ca.