

Séminaire de l'école doctorale C2MP

Le cosmos : Les secrets de l'infini



26 juin 2025

Auditorium de l'ENIM à Metz

8h30 - 17h30

9 mini-conférences

2 sessions posters

Conférences plénières

Dr Benjamin Magnelli :

CEA Paris

11h40 - 12h40

Pr Alain Blanchard :

Université Toulouse III

14h00 - 15h00

« La cosmologie : Les secrets de l'infini »

Bonjour à toutes et à tous,

Bienvenue au séminaire de l'école doctorale C2MP. Cette journée sera articulée autour de conférences plénières et de contributions de doctorants (mini-conférences et séances posters) qui vous permettront de découvrir leurs travaux ainsi que la diversité de la recherche présente au sein de l'école. Cette année, le thème de la cosmologie sera mis en avant. Pour cela, deux conférences sont données par Benjamin Magnelli (CEA) et Alain Blanchard (Université de Toulouse 3).

Nous vous souhaitons une excellente journée.

Claire Hugon, présidente du comité d'organisation du séminaire C2MP 2025



Planning

CO: Contribution Orale, CP: Conférence Plénière

Jeudi 26 juin 2025, Auditorium, ENIM

8:30–8:45	Accueil		
8:45–9:00	Accueil par le directeur de C2MP, Jean-Marc Raulot		
9:00–9:20	CO	ABBAS Doha LCP-A2MC	"Nanoparticules de magnésium : une alternative biocompatible et durable à l'or pour les applications plasmoniques avancées"
9:20–9:40	CO	ZIOUANI Charaf-Eddine LEM3	"Rupture des interfaces dans les circuits imprimés : caractérisation expérimentale et simulations numériques"
9:40–10:00	CO	SINGH Harjinder IJL	"Signaux d'accumulation de spin importants dans les expériences magnéto-optiques"
10:00–11:00	Pause café et session Poster		
11:00–11:20	CO	FEZRAOUI Abdelhak LCPME	"Specific Cr(VI) Removal through Colloidal Nanoparticles: Unraveling the Complex Interactions in Mg/Al LDH Anionic Exchange"
11:20–11:40	CO	EGOME NANA Stéphanie Laure LPCT	"Orbitales de type-gaussiennes complexes pour les états du continuum à deux centres"
11:40–12:40	CP	MAGNELLI Benjamin CEA	"Le télescope spatial James Webb : Un nouveau regard sur la formation des galaxies à l'aube de l'univers"
12:40–14:00	Repas		
14:00–15:00	CP	BLANCHARD Alain Université Toulouse III Paul Sabatier, IRAP	"Le Big Bang 2.0"
15:00–15:20	CO	Corentin BOULOGNE CRM2	"Combinaison de différentes méthodes RMN pour l'étude structurale et dynamique d'hydrogels supramoléculaires"
15:20–16:20	Session Poster avec jus de fruit et petits gâteaux		
16:20–16:40	CO	SINGH Ashutosh GIT	"Modelling and simulation of 3D microstructure evolution in selective laser melting by means of an Efficient cellular automaton model"
16:40–17:00	CO	PAZ Luis IJL	"Charbon actif végétal pour la désulfuration du biogaz"
17:00–17:15	Remise des Prix Posters et Conclusion		

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Séminaire de l'ED C2MP

Appel à participation (french version)

« La cosmologie : Les secrets de l'infini »

Bonjour à toutes et tous,

Comme chaque année, l'École Doctorale C2MP organise son séminaire annuel. Les deux conférences plénières de cette session 2025 porteront sur la cosmologie et l'astrophysique.

Le séminaire se déroulera le jeudi 26 juin 2025 à partir de 8h30 sur le site de l'Ecole Nationale des Ingénieurs de Metz (ENIM) du technopole de Metz, 1 route d'Ars Laquenexy 57070 Metz, dans l'auditorium. Pour les doctorants : inscription obligatoire via la plateforme ADUM.

Ouverture de l'appel à contribution : jeudi 24 avril 2025.

Ce séminaire sera animé par des mini-conférences de doctorants ainsi que 2 conférences plénières. La première, d'Alain Blanchard professeur d'astrophysique à l'université Toulouse III Paul Sabatier et chercheur à l'IRAP (Institut de Recherche en Astrophysique et Planétologie) et la seconde de Benjamin Magnelli, astrophysicien au CEA, (travaillant sur l'âge des galaxies grâce au télescope James Webb), toutes deux sur la thématique de " la cosmologie ". Un repas gratuit est également prévu pour le déjeuner, il est nécessaire d'être inscrit au séminaire pour en bénéficier. Le programme de la journée sera mis à jour sur la page ADUM du séminaire.

Vous êtes invités à soumettre un abstract sur votre thématique de recherche (**pas nécessairement la cosmologie**) pour une présentation orale ou une présentation poster. La soumission des résumés se fera via la plateforme ADUM. Avant la date limite de soumission, votre inscription au séminaire peut être modifiée dans votre espace personnel ADUM dans la section " Séminaire C2MP ". N'hésitez pas à faire vos résumés et à préparer vos interventions/supports en anglais afin que le plus grand nombre puisse comprendre vos travaux.

Nous vous rappelons qu'il est obligatoire au cours des 3 ans de thèse de présenter vos travaux au moins une fois lors du séminaire annuel de l'École Doctorale sous forme de communication orale (2,5 crédits) ou d'un poster (1,5 crédit). La participation au séminaire vous octroie également 1 crédit et permet de valider le module " Séminaire C2MP ". Trois prix d'une valeur de 100€ seront décernés au cours de la journée.

Transport : Un bus sera mis en place pour les doctorants et directeurs de thèse Nancéiens participants au séminaire. Rendez-vous le matin à 7h en face de l'entrée 2A de la Faculté des Sciences (FST) à Vandœuvre-lès-Nancy (plan sur le site de l'école doctorale) et le retour en bus aura lieu à 17h30 devant l'ENIM pour une arrivée à la FST à 18h30.

N'hésitez pas à vous inscrire pour cette conférence ! Pour les doctorants du comité d'organisation du séminaire annuel de l'ED C2MP 2025, la présidente, Claire Hugon (claire.hugon@univ-lorraine.fr)

Appel à participation (english version)

« **The cosmos : Secrets of the infini** » Dear all,

As every year, the C2MP Doctoral School is organising its annual seminar. The two plenary lectures of this 2025 session will focus on The Cosmos : Secrets of the Infinite.

The seminar will take place on Thursday 26 June 2025 from 8.30 am on the site of the National School of Engineers of Metz (ENIM) of the Metz technopole, 1 route d'Ars Laquenexy 57070 Metz, in the auditorium..

For doctoral students: compulsory registration via the ADUM platform.

Call for papers opens: Thursday 24th April 2025.

This seminar will feature mini-conferences by doctoral students as well as 2 plenary lectures. The first, by Alain Blanchard, professor of astrophysics at the University of Toulouse III Paul Sabatier and researcher at IRAP (Institute for Research in Astrophysics and Planetology) and the second by Benjamin Magnelli, astrophysicist at the CEA, (working on the age of galaxies using the James Webb telescope), both on the theme of 'cosmology and astrophysics'. A free lunch will also be provided, but you need to be registered for the seminar to take advantage of this. The program will be updated on the seminar's ADUM page.

You are invited to submit an abstract on your research topic (not necessarily cosmology domain) for an oral presentation or a poster. Abstracts will be submitted via the ADUM platform. Before the deadline, your submission can be modified in your personal space ADUM in the section "Séminaire C2MP". Please do not hesitate to write your abstracts and prepare your presentations/supports in English so that as many people as possible can understand your work. We remind you that it is compulsory during the 3 years of your thesis to present your work at least once at the Doctoral School's annual seminar in the form of an oral presentation (2.5 credits) or a poster (1.5 credit). Participation in the seminar also gives you 1 credit and enables you to validate the "C2MP Seminar" module. Three prizes will be awarded during the day.

Transport: A bus will be provided for doctoral students and thesis directors from Nancy who are taking part in the seminar. Meet at 7am in front of entrance 2A of the Faculty of Sciences (FST) in Vandœuvre-lès-Nancy (map on the doctoral school website) in the morning and at 5.30pm in front of entrance of ENIM, returning to Metz at 6.30pm.

Don't hesitate to register for this 2025 edition! On behalf of the doctoral students on the C2MP Doctoral School 2025 annual seminar organising committee, the president of organising committee, Claire HugonDear all,

Communication orale: liste des résumés

Conférences Plénières

Titre/Title:

Le télescope spatial James Webb : Un nouveau regard sur la formation des galaxies à l'aube de l'univers

Auteurs : **Benjamin MAGNELLI**

Benjamin Magnelli étudie la formation et l'évolution des galaxies à travers l'utilisation de grands échantillons multi-longueurs d'ondes. En s'appuyant tout particulièrement sur les observations des champs profonds des satellites Spitzer et Herschel et plus récemment de l'interféromètre ALMA, il étudie l'activité de formation d'étoiles des galaxies lointaines, leur contenu en gaz moléculaire et les propriétés de leur milieu interstellaire. Ses études, cruciales pour contraindre les modèles de formation et d'évolution des galaxies, ont permis de mesurer l'activité de formation d'étoiles de l'univers au cours des dix derniers milliards d'années, d'estimer l'importance relative des mécanismes internes et externes aux galaxies dans leur croissance; et de mieux comprendre l'origine des galaxies les plus lointaines et extrêmes de l'univers, les galaxies dites submillimétriques.

Astrophysicien, équipe Cosmologie et Évolution des Galaxies, Institut de recherche sur les lois fondamentales de l'Univers, Département d'Astrophysique / CEA, France

Résumé/Abstract :

Titre/Title:
Le Big Bang 2.0

Auteurs : *Alain BLANCHARD*

Professeur d'astrophysique à l'université Toulouse III Paul Sabatier et chercheur à l'IRAP (Institut de Recherche en Astrophysique et Planétologie) à l'Observation Midi-Pyrénées de Toulouse (OMP), France

Résumé/Abstract :

Au cours du vingtième siècle la cosmologie est devenue une science à part entière avec l'élaboration du modèle du Big Bang. Basée sur la physique moderne, la mise en évidence de l'expansion de l'Univers, l'abondance des éléments légers, l'existence d'un rayonnement, le fond diffus cosmologique, aux propriétés caractéristiques ont rapidement rendu ce modèle incontournable. Mais de nouvelles questions ont rapidement émergé dont la réponse ne peut se trouver au sein de la physique connue. Les progrès dans ce domaine n'en ont pas moins été spectaculaires. Dès les années 1990, les nouvelles observations du fond cosmologique ont permis d'étudier une physique qui se situe bien au delà des énergies accessibles aux laboratoires terrestres. Cette possibilité a ouvert un champ nouveau d'exploration scientifique riche en avancées plus que jamais en cours.

Conférences des doctorantes et des doctorants

Oral O1

Titre/Title:

Nanoparticules de magnésium : une alternative biocompatible et durable à l'or pour les applications plasmoniques avancées

Magnesium Nanoparticles: A Biocompatible and Sustainable Alternative to Gold for Advanced Plasmonic Applications

Auteurs : Doha Abbas¹, Aotmane En Naciri¹, Montassar Bouzouraa¹, Toni Alhadad¹, Ali Kassem², Alexandre Bouché³, Suzanna Akil¹

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³ Université de Lorraine, CNRS, IJL, F-54000 Nancy, France

Résumé/Abstract :

Magnesium (Mg) is emerging as a promising alternative to noble metals like silver and gold in plasmonic applications, thanks to its abundance, biocompatibility, low cost, and broad plasmonic resonance across the UV-visible-IR spectrum.[1] These characteristics make Mg highly suitable for energy harvesting, sensing, and photocatalysis. However, conventional synthesis of magnesium nanoparticles (MgNPs) often involves hazardous chemicals and complex, energy-intensive procedures.[2] To address these limitations, an eco-friendly, one-step fabrication method based on the self-assembly of poly(methyl methacrylate) (PMMA) doped with an Mg precursor was developed. This process involves spin-coating the mixture onto conductive substrates, forming nanoreactors where MgNPs nucleate and grow under mild conditions without the need for toxic solvents or external reducing agents.[3] The resulting MgNPs are monodispersed and exhibit tunable plasmonic and structural properties, controlled by synthesis parameters. These nanoparticles were successfully applied for the detection of 4,4'-bipyridine (4,4'-BP), achieving notable surface-enhanced Raman scattering (SERS) signal enhancement. Ongoing work explores the integration of MgNPs into hybrid systems with gold or semiconducting ZnO, aiming to further boost plasmonic performance and catalytic activity. This sustainable approach provides a scalable platform for the development of advanced plasmonic nanomaterials with potential applications in environmental monitoring, renewable energy, and next-generation biosensing technologies.

References

[1] J. Asselin, E. R. Hopper, E. Ringe, *Nanoscale* 2021, 13, 20649.

[2] V. Lomonosov, E. R. Hopper, E. Ringe, *Chem. Commun.* 2023, 59, 5603.

[3] S. Akil, R. Omar, D. Kuznetsov, V. Shur, A. En Naciri, S. Jradi, *Nanomaterials* 2021, 11, 1806.

Titre/Title:

Rupture des interfaces dans les circuits imprimés : caractérisation expérimentale et simulations numériques

Fracture of interfaces for Printed Circuit Boards application : Experimental characterization and numerical simulations

Auteurs : Charaf-Eddine ZIOUANI¹, *Gautier GIRARD*¹, *Sébastien MERCIER*¹

¹ Laboratoire d'étude des microstructures et de mécanique des matériaux (LEM3), 7 rue Félix Savart, 57070 Metz, France

Résumé/Abstract :

Dans un contexte de demande croissante en mobilité électrique et en électronique de puissance, la miniaturisation des circuits imprimés (PCBs) pose des défis majeurs en termes de fiabilité et de durabilité. En fonctionnement, les PCBs subissent des contraintes thermiques dues à la fois à la dissipation de chaleur générée par les composants actifs et aux variations de température ambiante. Ces structures multicouches complexes intègrent divers matériaux aux propriétés thermo-mécaniques hétérogènes. En particulier, les incompatibilités entre les coefficients de dilatation thermique (CTE) des matériaux sont à l'origine de contraintes internes susceptibles d'entraîner des phénomènes de délaminage entre couches isolantes ou à l'interface cuivre/substrat. Traditionnellement, l'énergie d'interface cuivre/substrat dans les PCBs est estimée à travers l'essai de pelage, conformément à la norme IPC. Toutefois, le cuivre y subit une forte plasticité, rendant l'interprétation des résultats plus complexe. De nombreux travaux [1] ont ainsi porté sur l'analyse de cet essai en tenant compte du développement de la plasticité dans le film ductile. Plus récemment, les travaux [2] et [3] ont approfondi l'analyse en intégrant un comportement élasto-plastique du cuivre, avec écrouissage (modèle de Voce et/ou cinématique), afin de caractériser l'interface cuivre/substrat. Cependant, cette méthode reste difficilement exploitable pour une évaluation précise du comportement mécanique de l'interface. Pour surmonter ces limites, les essais DCB (Double Cantilever Beam) et ENF (End Notched Flexure) [4], initialement conçus pour des composites épais, ont été adaptés aux structures fines des PCBs, où les épaisseurs des couches de cuivre varient de 17 à 70 μm . Avant la mise en œuvre expérimentale, ces configurations ont été validées par simulation éléments finis (EF), montrant que la dissipation plastique dans les essais DCB et ENF est nettement réduite par rapport à celle observée dans les essais de pelage. Outre l'estimation des taux critiques de restitution d'énergie en mode I et II (GIc et GIIc) ainsi que de la contrainte critique associée, cette approche expérimentale et numérique couplés fournit un cadre pour évaluer les limites de ces méthodes appliquées aux interfaces de circuits imprimés.

References

- [1] [1] Kim K et al. (1988) Elastoplastic analysis of the peel test. International Journal of Solids and Structures 24 :417-435
- [2] E.Simlissi et al.(2019) Elasticplastic analysis of the peel test for ductile thin film pre- senting a saturation of the yield stress. Int J Fract 220 :1-16
- [3] G. Girard et al. (2021) Analysis of the peel test for elastic plastic film with combined kinematic and isotropic hardening. International Journal of Fracture 232 :117-133
- [4] Hongsu Bae et al. (2019), Test and Analysis of Modes I, II and Mixed-Mode I/II Delami- nation for Carbon/Epoxy Composite Laminates, International Journal of Aeronautical and Space sciences 20 :636-652.

Titre/Title:

Signaux d'accumulation de spin importants dans les expériences magnéto-optiques
Large spin accumulation signals in magneto-optical experiments

Auteurs : Harjinder Singh¹, Alberto Anadón¹, Quentin Remy², Michel Hehn¹, Gregory Malinowski² Jon Gorchon³

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² Department of Physics, Freie Universität Berlin, 14195 Berlin, Germany

Résumé/Abstract :

Magneto-optical techniques are powerful and widely used tools that enable the investigation of ultrafast spin dynamics in various magnetic materials [1,2]. Currently, these techniques are becoming one of the emerging tools for studying the accumulation of spin and/or orbital angular momentum in magnetic/non-magnetic materials [3]. In time-resolved magneto-optical experiments, it has long been believed that the signal due to these accumulations was orders of magnitude smaller than the signals due to the magnetization dynamics. Here we show that under certain conditions the accumulation signals can be comparable to or even exceed the signal coming from the magnetization itself during the ultrafast demagnetization. In this case, we experimentally demonstrate how to isolate the accumulation signal, allowing us to better understand the mechanisms at ultrafast timescales.

References

- [1] E. Beaurepaire Physical Review Letters, 1996, 76, 4250.
- [2] G. Malinowski Nature Physics, 2008, 4, 855-858.
- [3] Y.G. Choi Nature, 2023, 619, 52-56.

Titre/Title:

Specific Cr(VI) Removal through Colloidal Nanoparticles: Unraveling the Complex Interactions in Mg/Al LDH Anionic Exchange

Auteurs : **Abdelhak Fezraoui**¹, **Damien Cornu**¹, **Gwladys Steciuk**², **Jaafar Ghanbaja**², **Marc Hébrant**¹

¹ Laboratoire de Chimie Physique et Microbiologie pour les Matériaux et l'Environnement (LCPME), CNRS and Université de Lorraine, UMR7564, 54600, Villers-lès-Nancy, France

² Université de Lorraine, CNRS, IJL, F-54000 Nancy, France

Résumé/Abstract :

Hexavalent chromium (Cr(VI)) is a toxic pollutant requiring efficient removal from industrial effluents. While layered double hydroxides (LDHs) show promise due to their anion exchange properties, the fundamental mechanisms governing Cr(VI) exchange remain poorly understood [1]. This study synthesized Mg/Al-NO₃ LDH nanoparticles via coprecipitation and hydrothermal treatment, then saturated them with Cr(VI). Structural characterization (PXRD, TEM, Raman, FTIR, XPS) revealed that CrO₄²⁻ and Cr₂O₇²⁻ coexist in the interlayer space when dry, but CrO₄²⁻ becomes predominant upon hydration [2]. Ultrafiltration experiments quantitatively evaluated the Cr(VI) recovery efficiency of various competing anions, establishing a clear selectivity hierarchy: HPO₄²⁻ > SO₄²⁻ > CO₃²⁻ » Cl⁻ > NO₂⁻ > NO₃⁻. The findings confirm that outer-sphere complex formation constitutes the primary mechanism at the LDH interface, facilitating potential regeneration through anionic exchange rather than permanent stabilization within the LDH matrix, which enables repeated Cr(VI) adsorption compared to other anions [3]. Thermodynamic exchange constants were calculated, demonstrating significant differences between intercalated divalent anions (K_{ex} values of 5.35, 1.73, and 0.13 for HPO₄²⁻, SO₄²⁻, and CO₃²⁻, respectively) and monovalent anions (K_{ex} values of 2.78 10⁻⁶, 1.32 10⁻⁶, and 0.98 10⁻⁶ for Cl⁻, NO₂⁻, and NO₃⁻, respectively). The observed structural changes accompanying the consecutive 2NO₃⁻ → CrO₄²⁻ → 2NO₃⁻ ion exchange are discussed in terms of thermodynamic constants differences. This work provides essential quantitative insights into the selective Cr(VI) recovery from LDHs.

References

- [1] Brahma, D. et al. (2025). Environmental Science: Water Research & Technology.
- [2] Fezraoui, et al. (2024). Applied Clay Science, 260, 107536.
- [3] Bozorgi, M. et al. (2025). Scientific Reports, 15(1), 1856.

Titre/Title:

**Orbitales de type-gaussiennes complexes pour les états du continuum à deux centres
Use of Complex Gaussian-Type Orbitals expansion for two-center continuum states**

Auteurs : Stéphanie Laure EGOME NANA¹

¹ Institut de Chimie Physique et Matériaux, 1 Bd Dominique François Arago, BP 57070 Metz, France

Résumé/Abstract :

The study of collision processes plays a central role in quantum mechanics, revealing the nature of the interaction between an incident particle and a target. In the case of molecular photoionization, a photon interacts with a target molecule, and an electron is ejected from an initial bound state into a continuum state. An accurate theoretical description of these states is crucial for a correct understanding of the molecular ionization dynamics. Describing molecular continuum states is challenging due to the oscillatory and multicentric nature of their wavefunctions. While molecular bound states are commonly dealt with quantum chemistry methods, for example using Gaussian-type orbitals (GTOs), efficient approaches for continuum states are lacking. For one-center ionization problems, Ammar et al. [1] proposed to use complex GTOs (cGTOs) sets to represent radial functions numerically. This approach has proven accurate over extended radial domains [2] and enables analytical evaluations of matrix elements relevant to ionization processes. In a multicentric framework, continuum states are generally not well mastered. As a contribution to the field, we extend the cGTO approach to handle multiple centers, starting with the two-centers case and apply it to the photoionization of H₂⁺. The molecular ground state is expanded on GTOs while a Two-Center Continuum (TCC) model [3] is represented with cGTOs. With these two expansions, we have obtained a closed-form expression of the scattering amplitude. The numerical implementation of our Gaussian approach is benchmarked with previously published cross sections.

References

- [1] A. Ammar, A. Leclerc and L. U. Ancarani "Fitting continuum wavefunctions with complex Gaussians: Computation of ionization cross sections." J. Comput. Chem. 2020, 41, 2365.
- [2] S. Egame Nana, A. Leclerc and L. U. Ancarani "A complex Gaussian representation of continuum wavefunctions respectful of their asymptotic behaviour." Adv. Quantum. Chem. 2025, 91, (In Press).
- [3] B. Joulakian et al. "Dissociative ionization of H₂⁺ by fast-electron impact: Use of a two-center continuum wave function." Phys. Rev. A 1996, 54, 1473.

Titre/Title:

Combinaison de différentes méthodes RMN pour l'étude structurale et dynamique d'hydrogels supramoléculaires

NMR methods combination for structural and dynamical study of supramolecular hydrogels

Auteurs : **Corentin Boulogne**¹, **Jeremy Morere**², **Paul Hoschtettler**³, **Marie-Christine Averlant-Petit**³, **Emmanuelle Bignon**², **Loïc Stefan**³, **Sabine Bouguet-Bonnet**¹, **Carole Gardiennet**¹

¹ CRM2, BP 70239, Boulevard des Aiguillettes, 54506 Vandoeuvre-lès-Nancy CEDEX, France

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Résumé/Abstract :

Supramolecular hydrogels have been studied for several years for their applications opportunities. We focus here on nucleopeptide-based multicomponent hydrogels. Adjusting the hydrogel mechanical properties to new applications relies on a deeper understanding of the atomic-scale structure and dynamics. In this respect, NMR appears to be the dedicated technique to gather information at the atomic scale of amorphous and neither solid nor liquid samples. We develop here an original methodology combining solid-state, liquid-state, and low field NMR techniques for characterizing supramolecular hydrogels. Solid-state NMR CP-based experiments investigate the gelator network. $T1\rho(1H)$ measurements enables to probe dynamics on the microsecond to millisecond timescale. We assess the efficiency of the relaxation process for different moieties at two temperatures, which is related to the nucleopeptide network organisation and intermolecular contacts that maintains the gel structure. High-Resolution NMR is used for investigating the gelation kinetics and is complemented by FFC-Relaxometry to evaluate the dynamical behaviour of the hydrogel isotropic phase. Dispersion curve analysis highlights the presence of different water populations regarding their correlation times, evolution of which can be followed during the gelation process. The results obtained are supported by Molecular Dynamics simulations, which evidence interactions driving the nucleation steps leading to the gel formation.

Titre/Title:

Modelling and simulation of 3D microstructure evolution in selective laser melting by means of an Efficient cellular automaton model

Auteurs : Ashutosh SINGH^{1,2}, *Luis Antonio Barrales-Mora*¹

¹ Georgia Institute of Technology—CNRS 2958 2 Rue Marconi, 57070, Metz, France

² University of Lorraine, 57070, Metz, France

Résumé/Abstract :

Laser Powder Bed Fusion (LPBF) process is one of the popular additive manufacturing technique for producing metal component with complex geometries and novel material compositions. However, LPBF is characterized by rapid cooling and high thermal gradients. Therefore, components fabricated with LPBF often exhibit unique microstructure which differs from the one obtained by traditional manufacturing techniques. LPBF also offers the possibilities to locally engineer the microstructure of a component, which remains formidable yet rewarding endeavor. In the present work, a novel parallelized 3-d Cellular Automaton (CA) model has been developed to predict the microstructure of the component. The model efficiently manages the computational load posed by the continuous cycles of re-melting and solidification inherent to the LPBF process. The presented CA framework is based on stochastic nucleation mechanism and physics based crystal-grown algorithm. Using the developed model, texture, morphology and grain size of austenitic advanced high-strength steel (AHSS) was simulated and the model was validated by comparing the results with the experimental findings both qualitatively and quantitatively

Titre/Title:

**Charbon actif végétal pour la désulfuration du biogaz
Wood-based activated carbons for biogas desulfurization**

Auteurs : ***Luis Paz***¹, ***Taher Selmi***², ***Vanessa Fierro***¹, ***Alain Celzard***¹

¹ IJL, Université de Lorraine, 27 Rue Philippe Séguin, F-88000, Epinal, France

² Groupe BORDET, Froidvent, F-21290 Leuglay, France

Résumé/Abstract :

This work focuses on the development of a high-performance activated charcoal (AC) derived from wood-based biochar for biogas desulfurization. The process involved multiple stages: physical activation to develop required microporosity, densification using environmentally friendly binders to increase bulk density, and surface functionalization through chemical impregnation to improve H₂S adsorption. The resulting ACs were tested under dynamic conditions simulating biogas desulfurization scenarios. The experimental results demonstrated that our developed ACs achieved competitive H₂S separation capacities, when compared against a set of commercial ACs specifically designed for H₂S removal and tested under identical conditions. To complement the experimental study, a mathematical model was also developed to simulate the adsorption dynamics within the packed bed column. This model provides predictive capability for breakthrough behavior and helps in the design and optimization of adsorption systems. Overall, the study presents a sustainable approach to producing high-performance ACs from biomass, with both experimental validation and theoretical modeling supporting their applicability in biogas purification.

Posters : liste des résumés

Posters

Poster P1

Titre/Title:

Étude atomistique de la stabilité et de la ségrégation des éléments d'addition α et β dans le titane pur

Atomistic Study of the Stability and Segregation of α and β addition Elements in Pure Titanium

Auteurs : Ahcene Amitouche¹, Djafar Iabbaden², Yudong Zhang¹, Jean-Sébastien Lecomte¹, Jean-Marc Raulot¹

¹ Université de Lorraine, CNRS, Arts et Métiers ParisTech, LEM3, F-57000 Metz, France

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Résumé/Abstract :

Titanium is a lightweight and strong metal that is widely used in fields such as aeronautics, medicine, chemical industry and energy. Its ability to resist corrosion, its high strength-to-weight ratio and biocompatibility make it the material of choice for demanding applications. However, the shaping of titanium, especially during machining and casting, is a challenge due to its specific properties, such as low thermal conductivity, high resistance to deformation and tendency to generate excessive heat during machining. Titanium crystallizes in a hexagonal close-packed (hcp) structure at room temperature, which can limit its ductility and complicate its deformation. The addition of additive element can modify the stability of the phases and therefore the mechanical behavior of the alloy as well as its shaping process. The incorporation of hydrogen and oxygen, aluminium ... has a significant impact on plasticity [1]. This phenomenon is complex and depends on several factors, including hydrogen concentration, temperature, and the microstructure of the material. The microstructure depends on the presence of alpha-forming addition elements such as aluminum, boron, carbon, oxygen, and nitrogen that increase the stability range of the α phase, while beta-forming elements such as fully soluble vanadium extend the stability range of the beta phase [2]. The alpha and beta phases of titanium have different crystalline structures, and so are their deformation modes. The yield strength of the beta phase is much higher than that of the alpha phase, distinguishing them as a 'hard' and 'soft' phase respectively. The hexagonal structure exhibits two main deformation mechanisms, slip (five modes) and twinning (four modes). Twinning is a crystallographic deformation that modifies the structure of the crystal without altering its chemical composition and allows the material to deform without fracture. Studies show that cavity nucleation (crack initiation) occurs on microstructural heterogeneities such as grain boundaries or twins [3]. As titanium twinning is a function of the alloy composition and environmental conditions, this work aims to understand the role, on the stability and segregation, of alpha-forming and beta-forming addition elements on the stability of interfaces (grain boundary or twin boundary) in pure titanium by atomistic approaches (molecular dynamics or ab initio).

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Titre/Title:

Résonances plasmoniques infrarouges de nanocristaux de Si dopés par ellipsométrie spectroscopique

Infrared plasmon resonances of doped Si Nanocrystals by Spectroscopic Ellipsometry

Auteurs : *Kevin Dawson Ango Nsa*^{1,2}, *Aotmane En Naciri*¹, *Yann Battie*¹, *Hervé Rinnert*², *Michel Vergnat*², *Laurent Broch*¹, *Montassar Billeh Bouzouraa*¹, *Clavel Berclis Kengne Choumele*², *Mathieu Stoffel*², *Xavier Devaux*²

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Résumé/Abstract :

La résonance plasmonique de surface localisée correspond à des oscillations collectives de porteurs de charge libres (électrons et trous) confinés dans une nanoparticule sous l'effet d'un champ électromagnétique. Les métaux nobles tels que l'or (Au) et l'argent (Ag) ont suscité beaucoup d'intérêt grâce à leur forte concentration en porteurs de charge, qui donne lieu à une résonance plasmonique de surface localisée dans le domaine visible. Cependant, les coûts de production, l'incompatibilité de ces nanostructures avec la technologie CMOS et la volonté d'atteindre le domaine spectral infrarouge avec des structures de taille nanométrique ont conduit les chercheurs à envisager d'autres alternatives. Les nanocristaux de silicium (Si-NC) hyperdopés au phosphore ou au bore se sont révélés être des candidats idéaux pour surmonter les limites des nanostructures de métaux nobles. Ils offrent des applications intéressantes dans un certain nombre de domaines. L'objectif de cette étude est d'évaluer l'effet de la concentration du dopage sur la réponse plasmonique des nanocristaux de silicium hyperdopés au phosphore (Si-NCs:P) en utilisant l'ellipsométrie sur une large gamme spectrale allant de l'ultraviolet à l'infrarouge lointain (250 à 35000 nm). Nous montrons que les mesures ellipsométriques fournissent des informations sur la concentration et la mobilité des porteurs de charge libres ainsi que sur les propriétés plasmoniques des points quantiques de silicium.

Localized surface plasmon resonance corresponds to collective oscillations of free charge carriers (electrons and holes) confined in a nanoparticle under the effect of an electromagnetic field. Noble metals such as gold (Au) and silver (Ag) have attracted great interest thanks to their high charge-carrier concentration, which gives rise to localized surface plasmon resonance in the visible range. However, production costs, the incompatibility of these nanostructures with CMOS technology, and the desire to reach the infrared spectral range with nano-sized structures have led researchers to look at other alternatives. Silicon nanocrystals (Si-NCs) hyperdoped with phosphorus or boron proved to be ideal candidates to overcome the limitations of noble metal nanostructures. They offer interesting applications in several fields. The aim of this study is to evaluate the effect of doping concentration on the plasmonic response of phosphorus-hyperdoped silicon nanocrystals (Si-NCs:P) using ellipsometry over a wide spectral range from ultraviolet to far infrared (250 – 35000 nm). We show that ellipsometric measurements provide informations on the concentration and mobility of free charge carriers as well as the plasmonic properties of silicon quantum dots.

Titre/Title:

Développement de filtres à charbon efficaces pour l'élimination des composés organiques volatils de l'air intérieur

Development of effective carbon filters for volatile organic compounds removal from indoor air

Auteurs : **Monica Aoun**¹, **Alain Celzard**^{1,2}, **France Vanessa Fierro**¹

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Résumé/Abstract :

La qualité de l'air intérieur constitue un enjeu majeur de santé publique et de productivité [1]. Parmi les principaux polluants figurent les composés organiques volatils (COV), notamment les BTEX (benzène, toluène, éthylbenzène et xylènes). Cette étude évalue l'efficacité de charbons actifs (CA) fournis par le Groupe Bordet, et activés par KOH selon trois méthodes: mélange physique (PM), mécanosynthèse (MS) et imprégnation (IMP), afin d'optimiser leur surface spécifique et leur microporosité [2]. Une série de tests de caractérisation a été réalisée afin d'évaluer la composition chimique, les propriétés texturales ainsi que l'hydrophobicité des matériaux. Six échantillons, avec des surfaces SNLDFT de 1250, 1500, 1750, 2000, 2250 et 2500 m²/g, ont été aussi testés pour l'adsorption manométrique du toluène. Les résultats montrent une capacité d'adsorption proportionnelle à l'aire BET ABET, conformément à la littérature, avec un maximum atteint par l'échantillon hydrophobe AC4PM de cette étude (2216 mg/g, ABET = 2865 m²/g). Parallèlement, un banc d'essai a été réalisé pour développer des filtres composites par projection à froid de poudres de CA sur une matrice biosourcée renforcée. Un nouvel outil d'analyse des performances a également été conçu pour simuler les conditions dynamiques réelles d'adsorption sur les filtres composites ainsi synthétisés.

Indoor air quality is a major public health and productivity issue [1]. Among the main pollutants are volatile organic compounds (VOCs), notably BTEX (benzene, toluene, ethylbenzene and xylenes). This study evaluates the efficiency of activated carbons (ACs) supplied by Groupe Bordet, and activated by KOH using three methods: physical mixing (PM), mechanosynthesis (MS) and impregnation (IMP), in order to optimize their specific surface area and microporosity [2]. A series of characterization tests were carried out to evaluate the chemical composition, textural properties and hydrophobicity of the materials. Six samples, with SNLDFT surface areas of 1250, 1500, 1750, 2000, 2250 and 2500 m²/g, were also tested for manometric adsorption of toluene. The results show an adsorption capacity proportional to the BET area ABET, in line with the literature, with a maximum reached by the hydrophobic sample AC4PM in this study (2216 mg/g, ABET = 2865 m²/g). At the same time, a test bench was set up to develop composite filters by cold spraying AC powders onto a reinforced biosourced matrix. A new performance analysis tool was also designed to simulate actual dynamic adsorption conditions on the composite filters thus synthesized.

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Titre/Title:

Analyse des Produits de Décomposition de l'Austénite: Application à la Cuve d'un Réacteur Nucléaire de technologie EPR

Analysis of Austenite Decomposition Products: Application to an EPR Nuclear Reactor Vessel

Auteurs : Nenad Ardeljan^{1,2}, *Lionel Germain*¹, *Thomas Billotte*², *Nathalie Gey*¹

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Résumé/Abstract :

Framatome, through its Le Creusot Forge (FLC) plant, manufactures low-carbon steel components for nuclear reactor vessels. The exceptional size of these components induces complex multi-scale chemical heterogeneities that locally impact microstructure and mechanical properties [1]. This thesis aims to characterize the effect of these heterogeneities on microstructural transformations during heat treatments simulating those applied industrially. The first part of the work focuses on modeling austenitic grain growth kinetics as a function of time and temperature, with the potential identification of stagnation phenomena linked to the presence of precipitates at grain boundaries. The second part studies austenite decomposition products for different cooling conditions and in relation to chemical heterogeneities. A structural definition of the transformation products (ferrite, upper/lower/granular bainite and martensite) will be established on the basis of morphological and crystallographic criteria. The study is based on advanced analysis of phase transformation induced microstructures using EBSD (Electron BackScattered Diffraction) [2] coupled with innovative artificial intelligence approaches [3], crystallographic reconstructions of parent austenite and monitoring of phase transformations by in-situ EBSD at high temperature. Chemical heterogeneities will be analyzed using various complementary techniques: latest-generation EDS/BEX, microprobe and LIBS (laser induced breakdown spectroscopy). The results will be used to draw up a phase transformation diagram under continuous cooling, differentiating between segregated and non-segregated zones, in order to develop a tool for microstructure prediction as a function of the chemical and thermomechanical history of the part. This work is part of a global approach to optimizing the mechanical performance and safety of nuclear components.

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Titre/Title:

Contrôler l'anisotropie dans des systèmes Pt/Co texturés

Anisotropy control in textured Pt/Co systems

Auteurs : Corentin Aulagnet¹, Stéphane Mangin¹, Michel Hehn¹, Eric E. Fullerton²

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Résumé/Abstract :

Le domaine émergent du neuromorphic computing pourrait révolutionner notre façon d'implémenter des réseaux de neurones [1-2]. La spintronique, qui explore le contrôle du spin comme degré de liberté supplémentaire dans l'électronique permet d'envisager des dispositifs, plus rapides, plus efficaces énergétiquement.

Dans ce but, l'étude présentée se concentre sur la modulation de l'anisotropie magnétique dans les systèmes texturés Pt/Co. L'objectif est de contrôler l'anisotropie magnétique dans le plan (IMA) et perpendiculaire (PMA) par l'ingénierie de la texture cristalline des couches minces, notamment via le choix du substrat (MgO(110) ou MgO(111)), la température de dépôt et l'épaisseur des couches.

En étude préliminaire, la qualité de croissance de la première couche de Pt est démontrée avec une transition de (111) vers (110) entre 400°C et 500°C. On montre ensuite, qu'il est possible d'obtenir une transition de l'anisotropie de PMA à IMA avec la température de dépôt. Les résultats montrent enfin qu'une combinaison fine de l'épaisseur de Co/Pt, de la température, et de la texture permet de moduler la IMA et la PMA.

Cela ouvre des perspectives prometteuses pour l'implémentation de neurones spintroniques dans les systèmes de calcul neuromorphique et l'étude de phénomène de transport de spin.

Neuromorphic computing is an emerging field that could revolutionize the implementation of neural networks [1-2]. Spintronics explores the electron spin as an additional degree of freedom in electronics and allows us to imagine new, faster, and more energy-efficient devices.

This study focuses on the control of magnetic anisotropies in textured Pt/Co systems. The goal is to control the in-plane magnetic anisotropy (IMA) and perpendicular magnetic anisotropy (PMA) by carefully engineering the crystalline texture of thin films through an appropriate substrate, deposition temperature, or layer thicknesses.

As a preliminary study, the quality of the Pt seed layer is demonstrated, which shows a transition from (111) to (110) on MgO(110) between 400°C and 500°C. It is then demonstrated that a reorientation of the anisotropy happens from PMA to IMA with the deposition temperature. The results finally show that fine-tuning the thicknesses of a multilayer stack, the deposition temperature, and the texture allows for a modulation between PMA and IMA.

This work opens new perspectives for the implementation of spintronics neurons in neuromorphic computing systems and for studying spin transport phenomena.

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Titre/Title:

OrfL et OrfM : Caractérisation Biochimique et Structurale des Acteurs du Transfert Horizontal de Gènes

OrfL and OrfM: Biochemical and Structural Characterization of Key Players in Horizontal Gene Transfer

Auteurs : *Dunkan Begue*¹, *Hicham Sekkouri-alaoui*¹, *Louise Thiriet*¹, *Thiphaine Dhalleine*², *Aurelien Thureau*³, *France Nicolas Soler*¹, *Nathalie Leblond-Bourget*¹, *Claude Didierjean*¹, *Frederique Favier*¹

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Résumé/Abstract :

Antibiotic resistance poses a critical global health threat, driven by the overuse and misuse of antibiotics, which fosters the selection of resistant bacterial strains. Given the slowdown in new antibiotic discovery, deciphering the underlying mechanisms of resistance is paramount. Horizontal Gene Transfer (HGT) is a major driver in disseminating antibiotic resistance and virulence genes among bacteria. Unlike vertical transmission, HGT enables genetic exchange between spatially proximate cells, facilitating rapid adaptation.

This process involves diverse mobile genetic elements. Extra-chromosomal elements include self-transmissible conjugative plasmids and mobilizable plasmids that rely on other elements for transfer. Intra-chromosomal elements like Integrative and Conjugative Elements (ICEs) and Integrative and Mobilizable Elements (IMEs) also play significant roles, with ICEs being autonomous and IMEs dependent on external machinery.

At this congress, we will present our progress on the biochemical and structural characterization of OrfL and OrfM, two proteins implicated in the HGT of an ICE from *Streptococcus thermophilus*, a crucial model organism for Gram-positive bacterial HGT. Our research investigates the formation of protein complexes involving OrfL and OrfM, and elucidates their interaction mechanisms through various biochemical approaches. Understanding these proteins is critical for developing strategies to combat the spread of antibiotic resistance.

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Titre/Title:

**Comprendre les propriétés d'adsorption des catalystes par atome unique à base de graphène
Understanding adsorption properties on graphene based single atom catalysts**

Auteurs : Théo Bequet¹, *Safouan Ziat*¹, *florian brix*¹, *Emilie Gaudry*¹

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Résumé/Abstract :

Les catalyseurs à atome unique (Single Atom Catalysts, SACs, en anglais) connaissent un essor considérable, puisqu'ils permettent une utilisation optimale des sites métalliques catalytiques en maximisant les performances des sites actifs. Leur développement requiert la connaissance des relations structure-composition-propriétés de ce type de matériau, qui ne peuvent à priori pas être extrapolées directement à partir de celles connues sur les métaux simples.

Dans ce travail, nous nous sommes intéressés à l'énergie d'adsorption de molécules sur des SACs de type graphène dopés avec de l'azote ou du phosphore. Les modèles structuraux ont été élaborés en plaçant un métal de transition en substitution d'un atome de carbone. Les calculs de structure électronique, basés sur la théorie de la fonctionnelle de la densité, ont permis de créer une base de données, qui ont été ensuite analysées par une méthode d'apprentissage supervisé (code SISSO). Cette approche nous a permis de proposer un modèle explicite pour prédire les énergies d'adsorption à partir de la connaissance de descripteurs primaires.

Ces résultats, centrés sur la rationalisation des énergies d'adsorption grâce à des descripteurs simples, constituent une base solide en vue d'aborder la prédiction d'activité et de sélectivité des SACs pour un design de catalyseurs efficaces.

Titre/Title:

Modeling and development of an innovative medical device for cancer drug testing

Auteurs : Cyprien Berthelemy¹, Anthony Biget², Laurent Badie¹, Rainier Hriez², Cécile Lemaitre², Halima Alem¹

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Résumé/Abstract :

Le développement de nouveaux médicaments demande d'examiner l'impact de nombreux paramètres, notamment leur concentration. Cela demande de réaliser de nombreux tests, qui peuvent s'avérer long et coûteux. Il est donc souvent nécessaire de mettre au point des systèmes permettant de réaliser ces tests en parallèle.

Dans le cas des tests étudiant la concentration d'un médicament on utilise des générateurs de gradients de concentration pour permettre cette parallélisation.

Parmi ces derniers les générateurs de gradient dit en « sapin de Noël » et ses variantes sont les plus utilisés, de par leur indépendance à des variations de conditions expérimentales qui permet d'obtenir un gradient de concentration, stable et précis. Mais leur géométrie est basée sur une succession d'étage où l'on passe de n entrées à n+1 sorties ce qui a pour conséquence une grande empreinte spatiale sur une puce microfluidique, ce qui complexifie leur usage. Mettre au point une nouvelle géométrie, permettant d'obtenir ces mêmes avantages tout en maintenant une empreinte spatiale faible serait un grand plus.

Cette nouvelle géométrie est étudiée via simulation numérique sur le logiciel Fluent. Une fois qu'une géométrie optimale est identifiée elle est reproduite expérimentalement afin de valider les données de simulations numériques.

Titre/Title:

Analysis of conformation manifolds for intrinsically disordered proteins

Auteurs : Marina Botnari¹, Nathalie Sibille², Jung-Hsin Lin³, Thérèse Malliavin¹

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Résumé/Abstract :

Determining a protein's functional conformation is one of the greatest challenges in structural biology. Roughly 35–50% of the human proteome does not adopt stable three-dimensional structures. Instead, many proteins are partially (IDRs) or entirely (IDPs) intrinsically disordered. Their inherent flexibility facilitates interactions with multiple partners and participation in various physiological and pathological processes, such as neurodegenerative diseases and cancers¹. However, standard structural techniques fail to capture these proteins' plasticity.

To address this limitation, we propose a computational strategy to explore the local folding of IDPs. First, secondary structure elements are assigned from experimentally derived backbone chemical shifts using $\delta 2d$. To manage the conformational complexity, we employ a threading-augmented interval branch and prune (TAiBP)² method to generate an ensemble of candidate conformations, which are clustered using a self-organizing map (SOM) to select representative structures. After fragment assembly, side chains are added via molecular dynamics simulations using NAMD.

For validation, we apply our method to a set of PED proteins, including the wild-type C-terminal domains of the vasopressin receptor, growth hormone secretagogue receptor type 1a, and B2-adrenergic receptor, along with their phosphomimetic analogues^[3]. Several analyses compare the conformations obtained from the PED proteins with those generated by TAiBP.

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Titre/Title:

Caractérisation de polymères fluorés dans des matrices environnementales par Thermodésorption/Pyrolyse (TD/Py)-DART - Orbitrap MS

Thermodesorption/Pyrolysis (TD/Py)-DART - Orbitrap MS for the characterization of fluoropolymers in environmental matrices

Auteurs : Louise Cadona^{1,2}, Gabriel Gaiffe², Sébastien Schramm², Frédéric Progent¹

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Résumé/Abstract :

Direct Analysis in Real Time (DART) coupled with high-resolution mass spectrometry (HRMS) provides valuable insights into the chemical structure of fluoropolymers, including repeat unit(s), end-groups, and additives. However, DART is primarily effective for small oligomers, as its desorption/ionization efficiency favors the most volatile compounds. Furthermore, it is not well-suited for directly analyzing powdery samples, such as soils contaminated with polymers. To address these limitations, DART can be coupled with a thermodesorption/pyrolysis (TD/Py) device, enabling more comprehensive fluoropolymer characterization and improving sensitivity, particularly in complex environmental matrices.

A sand sample spiked with 2The thermogram revealed two distinct steps: thermal desorption (35–300 °C) and pyrolysis (300–600 °C). The mass spectra displayed ions differing by the number of VDF units, along with various adducts. Different products were observed across temperature program, with pyrolysis yielding more unsaturated compounds. The products detected in the spiked sand matched the most intense signals observed in the bulk sample, allowing the identification of PVDF.

Poster P11

Titre/Title:

Caractérisation physico-chimique des cendres de biomasse pour des applications cimentières
Physico-chemical characterization of biomass ash for cement applications

Auteurs : Tom Charrault¹, *Cécile Diliberto*¹, *Romain Trauchessec*¹

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Résumé/Abstract :

Titre/Title:

**Algorithme explicite pour la simulation du flambement dynamique avec des coques à 7 paramètres
Explicit algorithm for simulating dynamic buckling phenomena using 7-parameter shell elements**

Auteurs : Anh-Khoa Chau¹, *Michaël Brun*¹, *Pascal Ventura*¹, *Hamid Zahrouni*¹

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Résumé/Abstract :

Ce travail propose une stratégie explicite pour la simulation des phénomènes de flambement dynamique à l'aide d'éléments de coque à 7 paramètres [1]. Ces éléments de coque avancés permettent l'utilisation directe de lois de comportement tridimensionnelles sans nécessiter de réduction cinématique ni de condensation, comme c'est le cas dans les formulations classiques de Kirchhoff-Love ou de Reissner-Mindlin. Afin de remédier au verrouillage de Poisson, la formulation à 7 paramètres intègre une méthode de « Enhanced Assumed Strain » (EAS). Cette approche assure une variation linéaire de l'allongement dans la direction de l'épaisseur en imposant une condition d'orthogonalité qui garantit que le champ EAS ne produit aucune énergie de déformation.

L'intégration de cette contrainte dans un schéma explicite pose néanmoins des défis : sa résolution exacte à chaque pas de temps est coûteuse et nuit à la robustesse numérique. Pour y remédier, nous proposons de décaler le calcul du champ EAS au milieu du pas de temps. Cette approche améliore la stabilité, réduit le coût de calcul et reste compatible avec différents modèles de comportement.

La pertinence de l'algorithme explicite proposé est démontrée à travers des cas de flambement dynamique complexes impliquant des matériaux à comportement élasto-plastique.

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Titre/Title:

Simulation numérique du procédé de refusion VAR - Étude de l'impact d'un refroidissement asymétrique

Numerical simulation of the VAR process - Investigation of the impact of asymmetrical cooling.

Auteurs : Alexis Clarissou¹

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Résumé/Abstract :

This article focuses on the application of 3D numerical simulations to investigate the cooling system of a Vacuum Arc Remelting (VAR) furnace, an essential component in the production of high-quality alloys.

The development of the model involves the creation of a 3D simulation using COMSOL Multiphysics to simulate the cooling system dynamics during the VAR process. This model facilitates the computation of heat flows on the crucible walls through thermo-fluidic coupling, providing a detailed representation of the thermal behavior within the cooling system.

To assess the impact of asymmetric cooling in critical cases, one of the four outlets of the cooling system is selectively closed, enabling a focused study on the resultant effects on the cooling process. Through systematic investigation, the article aims to predict the temperature distributions and heat transfer patterns caused by this modification to the cooling system.

The derived heat flows from the 3D simulation serve as a crucial tool to explore the effects of asymmetric cooling on the VAR process. To study those effects, the heat flows are extracted from the 3D model and integrated as boundary conditions into a 2D axisymmetric thermo-mechanical model of the ingot.

COMSOL is a registered trademark of COMSOL AB.

Titre/Title:

**RÉSULTATS PRÉLIMINAIRES POUR L'ENDOMMAGEMENT MACROSCOPIQUE DE LA GELÉE DE WHARTON : UNE ANALYSE ÉLÉMENTS FINIS
PRELIMINARY RESULTS FOR WHARTON'S JELLY MACROSCOPIC DAMAGE PROPERTIES: A FINITE ELEMENT STUDY**

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Résumé/Abstract :

A growing interest has emerged around regenerative medicine since tissue and organ transplantations are no longer the best way to restore body function from diseases, injury or developmental defects due to the shortage of organ donors. Biological materials are preferred for applications in this field. Among them, the Wharton's jelly, a mucous connective tissue that lies inside the umbilical cord stands out from the others due to its potential for creating effective medical devices [1]. Unfortunately, this tissue is poorly described in the literature from a mechanical standpoint [2]. This work is intended to complete the literature's lack of data by proposing a characterization of this tissue's hyperelastic and macroscopic damage properties during tensile tests using a continuum damage mechanics [3] approach coupled with an optimization process and the finite element method.

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Titre/Title:

Effet des surfaces libres sur les champs élastiques des dislocations : application aux dislocations dans le GaN

Effect of free surfaces on dislocation elastic fields: application to threading dislocations in GaN

Auteurs : Fatin El Ajjouri-LEM3¹, *Antoine Guitton*¹, *Vincent Taupin*²

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Résumé/Abstract :

Dislocations are linear crystalline defects that induce long-range elastic fields inside materials. Dislocations can significantly alter the positions of atoms in their neighborhood, enabling their detection through near surface electron diffraction techniques, such as conventional electron backscatter diffraction (EBSD), High-Resolution Electron Backscatter Diffraction (HR-EBSD), or electron channeling contrast imaging (ECCI). In this contribution, we explore the effect of free surfaces on dislocation elastic fields, by comparison with bulk signatures, in order to assess the possible influence of free surfaces on dislocation detection and characterization using near surface electron diffraction techniques. To this end, we employ a field dislocation mechanics (FDM) model numerically approximated by a fast Fourier transform (FFT) algorithm. In addition to strain, rotations and stress fields, the model is further used to generate virtual curvature and associated geometrically necessary dislocation (GND) density maps that can be typically measured in EBSD. We apply the workflow to threading dislocations (TDs) in GaN semiconductor [0001] layers deposited on a Si substrate. Our findings reveal that the elastic fields can differ significantly between the surface and the bulk, which can lead to potential misinterpretation in dislocation characterization. Additionally, the necessary metrics required for the unambiguous characterization and classification of dislocations are established.

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Titre/Title:

Optimisation du procédé spin-coating pour la fabrication de films minces d'oxyde de cuivre à phases Cu₂O et CuO contrôlées

Optimization of the Spin-Coating Process for the Fabrication of Copper Oxide Thin Films with Controlled Cu₂O and CuO Phases

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Résumé/Abstract :

Le développement de matériaux à base d'oxydes métalliques issus d'éléments abondants sur Terre, tels que le cuivre, est essentiel pour les dispositifs optoélectroniques de nouvelle génération, en particulier les cellules solaires à couches minces. Ce travail présente la fabrication et l'optimisation de films minces d'oxyde de cuivre (Cu₂O/CuO) par la technique de spin-coating, une méthode économique et respectueuse de l'environnement, utilisant des précurseurs en solution aqueuse sur substrats en verre. L'étude porte sur le contrôle de la composition de phase Cu₂O /CuO via un recuit post-dépôt, afin d'ajuster les propriétés structurales, optiques et électriques des films pour des applications photovoltaïques. Les films riches en Cu₂O optimisés présentent un gap direct d'environ 2 eV, une conductivité de type p, des mobilités de porteurs comprises entre 17 et 30 cm²·V⁻¹·s⁻¹ et des concentrations de porteurs allant de 8 × 10¹³ à 10¹⁵ cm⁻³, les positionnant comme des couches absorbantes prometteuses pour les cellules solaires tout-oxyde. Les analyses structurales et morphologiques confirment la pureté de phase et l'uniformité des films, tandis que les mesures optiques révèlent une transmittance et un gap modulables via le recuit. Ce travail confirme le potentiel des procédés sol-gel basés sur le spin-coating pour produire des films minces de haute qualité, adaptés aux dispositifs optoélectroniques durables et à faible impact environnemental.

The development of metal-oxide materials based on Earth-abundant elements, such as copper, is key to advancing next-generation optoelectronic devices, particularly thin-film solar cells. This study focuses on the synthesis and optimization of copper oxide thin films via a cost-effective and environmentally sustainable spin-coating technique, using water-based precursors and glass substrates. Emphasis is placed on achieving controlled phase composition between Cu₂O and CuO through careful adjustment of processing parameters, particularly post-deposition annealing. The resulting Cu₂O -rich thin films exhibit a direct bandgap of 2 eV, p-type conductivity, carrier mobility ranging from 17 to 30 cm²·V⁻¹·s⁻¹, and carrier concentrations between 8 × 10¹³ and 10¹⁵ cm⁻³, properties that make them highly suitable as absorber layers in all-oxide solar cells. Structural, optical, and morphological characterizations confirm the successful modulation of the Cu₂O /CuO phase ratio, crucial for device performance. This work highlights the potential of eco-friendly, scalable spin-coating processes for fabricating high-quality copper oxide thin films. The ability to control phase composition directly supports the development of low-cost, sustainable solar cell architectures and broadens the material's applicability to other optoelectronic devices, such as gas sensors and photodetectors, contributing to the future of green energy technologies.

Titre/Title:

Interaction of Unconventional Airy Beams with optically induced Waveguide arrays in nonlinear crystals

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Résumé/Abstract :

Recent studies suggest new physical phenomena resulting from the interaction of unconventional optical beams with nonlinear media. These beams present unique intensity profiles and intriguing nonlinear propagation behaviors in photorefractive crystals, making them strong contenders for all-optical applications. Increasing interest has been directed toward their propagation in discrete periodic media, namely photonic lattices. This study explores the numerical interactions of Airy beams with a strontium barium niobate (SBN) crystal embedded with an optically induced photonic lattice [1]. A key focus is placed on the introduction of defect guides within the lattice, which significantly alter beam dynamics and reveal new regimes of interaction. Beyond the impact of defects, the lattice parameters appear as critical factors, influencing the propagation in terms of both the number and spatial distribution of outputs channels. Under strong nonlinearity and by rightfully tuning the system parameters, a single Airy beam launched into a negative defect site can split into up to 7 well-defined outputs channels with a large input-to-output transverse shift reaching 19 times the beam width. These results underscore the role of the photonic lattice as a versatile platform for beam manipulation.

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Titre/Title:

Modélisation du comportement vibratoire des structures multi-matériaux sur fondation périodique

Modelling the vibratory behaviour of multi-material structures on periodic foundations

Auteurs : Adil ABID¹, Guillaume ROBIN¹, El Moustafa DAYA¹

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Résumé/Abstract :

La modélisation des vibrations des structures multi-matériaux est un sujet essentiel dans l'industrie, tels que l'aéronautique, l'automobile et le génie civil.... En effet, le contrôle et l'amortissement des vibrations de ce type de structures dépendent fortement des conditions aux limites imposées et des lois de comportements des matériaux utilisés. L'objectif principal de ce travail est d'étudier l'effet des appuis répétitifs sur le comportement vibratoire de la structure. Ainsi, notre étude repose sur le développement de modèles analytiques et numériques par éléments finis. Un modèle multicouche de type poutre reposant sur une fondation élastique à forme répétitive a été considéré. Les premières modélisations ont permis d'identifier les effets du nombre des conditions aux limites répétitives sur les fréquences de résonance par la largeur des bandes interdites (band gaps). En particulier, l'ajout d'appuis élastiques le long de la structure a révélé des mécanismes permettant de moduler les modes propres et d'élargir les zones de réduction des vibrations. Ces résultats mettent en lumière le rôle clé du nombre d'appuis élastiques et leurs rigidités sur le contrôle des vibrations. Ce travail constitue une première étape vers l'étude des vibrations de structure multicouches reposant sur fondation élastique et répétitive.

Vibration modelling of multi-material structures is an essential subject in many industries such as aeronautics, automotive and civil engineering.... The control and damping of vibrations of these structure are highly dependent on the boundary conditions imposed and the behaviour laws of the used materials. The main objective of this work is to investigate the effect of repetitive supports on the vibration behaviour of the structure. Our study is therefore based on the development of analytical and numerical models using finite elements. A multi-layer beam-type model resting on a repetitive and elastic foundation is considered. First modelling has identified the effect of repetitive boundary conditions number on resonance frequencies and band gaps size. In particular, the addition of elastic supports along the structure revealed mechanisms for modulating the eigenmodes and widening the vibration reduction zones. These results highlight the key role of the interactions between geometry, materials and the number of supports and their effect on vibration control. This work is a first step to study the vibrations of multi-layer structures on elastic and repetitive foundation.

Mots clefs : Amortissement, vibration, structures multi-matériaux, fondation périodique, Band gaps.

Poster P19

Titre/Title:

Caractérisation des résidus miniers de lithium pour les applications cimentières
Characterization of lithium mining residues for cement applications

Auteurs : Ewen FLOCH¹, *Romain TRAUCHESSEC*¹, *Cécile DILIBERTO*¹, *Omar RODRIGUEZ VILLARREAL*¹

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Résumé/Abstract :

Titre/Title:

Etude structurale sur monocristal de la transition de spin dans Fe(pyrazine)[Fe(CN)₅(NO)]
Single-Crystal Structural Investigation of the Spin-Crossover in Fe(pyrazine)[Fe(CN)₅(NO)]

Auteurs : Dorsaf Gheries¹, Dominik Schaniel¹, Maxime Deutsch¹, Abdelatif Doudouh¹

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Résumé/Abstract :

Les matériaux à transition de spin sont très utiles pour développer des dispositifs intelligents tels que les capteurs, les mémoires de stockage d'informations. Dans cette étude, nous rapportons la synthèse et la caractérisation structurale du complexe de Fe(pyrazine)[Fe(CN)₅(NO)] sous forme de monocristaux. L'analyse par DRX sur monocristal révèle que le composé cristallise dans le groupe d'espace Pm, avec les paramètres de maille: $a = 7,1966(5) \text{ \AA}$, $b = 14,8617(01) \text{ \AA}$, $c = 14,3612(01) \text{ \AA}$ et $\beta = 104,488(2)^\circ$, avec des molécules de pyrazines désordonnées. La transition de spin induite thermiquement a été étudiée en résolvant les structures à l'état haut spin (260 K) et à l'état bas spin (220 K), révélant une diminution de 23 % du volume de l'octaèdre FeN₆ lors de la transition. Ce phénomène de TS est également confirmé par spectroscopie infrarouge (IR) et calorimétrie différentielle à balayage (DSC), qui mettent en évidence des hystérèses thermiques larges d'environ 40 K. Les prochaines études porteront sur l'étude de TS de ce composé sous pression, afin de mieux comprendre l'influence de la pression sur ses propriétés.

Titre/Title:

Caractérisation expérimentale et modélisation micromécanique des effets d'interface sur le comportement mécanique des aciers multiphasés
Experimental characterization and micromechanical modeling of interface effects on the mechanical behavior of dual phase steels

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Résumé/Abstract :

In response to the automotive industry's efforts to reduce greenhouse gas emissions, there is growing demand for high strength steels with both excellent mechanical performance and good formability. Third-generation multiphase steels are promising materials that can reduce vehicle weight without sacrificing safety. ArcelorMittal is actively developing these steels to optimize the balance between strength, ductility, and cost. However, their complex microstructures especially the role of phase interfaces pose significant challenges. This study combines experimental techniques with micromechanical modeling to investigate how microstructural features affect steel performance. Using two-dimensional electron backscatter diffraction (2D-EBSD) and instrumented nanoindentation with a Berkovich tip, we analyze internal length scales and phase boundary effects in Dual-Phase steels, focusing on ferrite-martensite and ferrite-ferrite interactions. These experiments aim to clarify how interphase boundaries influence deformation and strength. To complement this, we propose a new micromechanical model called the Internal Length Mean Field (ILMF) approach. This model integrates geometrically necessary dislocation (GND) densities and interface properties to account for plastic incompatibilities between phases. ILMF is designed to predict local and global mechanical behavior, plasticity, and damage initiation, with a specific focus on interface-driven effects.

Keywords: Dual-Phase steels, Nanoindentation, 2D EBSD, Internal lengths, Dislocation densities, GNDs

Titre/Title:

Comportement tribologique de l'interface outil-pièce Ti-6Al-4V/WC-Co sous des charges de contact et des vitesses extrêmes

Tribological behavior of the Ti-6Al-4V/WC-Co tool-workpiece interface under extreme contact loads and sliding speeds

Auteurs : Najwa Haterbouch¹, Hamid Makich¹, Andrea Cappella¹, Ben Boubaker¹, Mohamed Nouari¹

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Résumé/Abstract :

L'usinage des alliages de titane, en particulier le Ti-6Al-4V, présente d'importants défis en raison de phénomènes sévères de frottement et d'usure, dégradant à la fois les outils de coupe et la qualité de surface des pièces usinées. Cette étude examine le comportement tribologique du Ti-6Al-4V en contact avec le WC-Co sur une large gamme de pressions de contact (16-477 MPa) et de vitesses de glissement (0.5-60 m/s), générant des valeurs de Pression × Vitesse (PV) allant de 8 à 16800 MPa.m/s. Ces conditions sont représentatives des interactions outil/copeau et outil/pièce lors de l'usinage. Deux dispositifs expérimentaux ont été utilisés : un tribomètre pion-sur-disque pour les essais à basses vitesses, et un banc balistique à haute vitesse, permettant de simuler des conditions extrêmes d'usinage. Des mesures des coefficients de frottement et des analyses de surface détaillées ont été réalisées pour évaluer les performances selon les différents régimes. Les résultats ont révélé une usure adhésive dominante à basse vitesse et sous fortes pressions, tandis que les vitesses plus élevées induisent une usure tribo-oxydative et abrasive. Les résultats ont également mis en évidence une dépendance non linéaire du frottement quant à la pression et la vitesse, reflétant la complexité des interactions de contact.

Titre/Title:

Replication of PA-ALD Cobalt Thin Films : Reproducibility of Deposition Processes and Comparative Results

Auteurs : JingYa Huang¹, *Alexandre Bouche*¹, *François Montaigne*¹

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Résumé/Abstract :

Based on a previously reported study [1], this work aims to replicate the deposition of cobalt thin films on silicon oxide substrates using a Plasma-Assisted Atomic Layer Deposition (PA-ALD) system. In addition to following the original deposition conditions, platinum-coated silicon substrates (Si/Pt) were introduced to evaluate the influence of substrate type on film growth. Characterization was performed using X-ray reflectometry (XRR), atomic force microscopy (AFM), and magnetometry. The results indicate partial reproducibility, with noticeable variations in film thickness and surface roughness compared to the original study. Moreover, the choice of substrate was found to significantly affect film uniformity.

References

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Titre/Title:

**Vers l'étude de la structure de bande électronique de Bi₂Te₃ déformé
Toward investigating the electronic band structure of strained Bi₂Te₃**

Auteurs : Romain Jenn¹, Yannick Fagot-Revurat¹, France Geoffroy Kremer¹

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Résumé/Abstract :

L'application d'une déformation mécanique anisotrope sur les matériaux peut modifier leurs propriétés physiques, par exemple en induisant des transitions de phase [1], en les modulant [2] ou en levant des dégénérescences [3]. Pour accéder aux propriétés électroniques des matériaux une technique adaptée est la spectroscopie de photoémission résolue en angle (ARPES) ; néanmoins on ne trouve que peu d'articles pour coupler déformation mécanique et ARPES. Il s'agit donc ici d'expliquer les différentes étapes menant à la déformation des matériaux et à la mesure de leur structure de bande électronique. Une fois présenté et caractérisé le dispositif de mise sous contrainte, la mesure de la déformation du matériau sera expliquée. Les premières mesures de propriétés ex- et in-situ, commentées à l'aide des modélisations, permettent de démontrer la faisabilité du programme de recherche.

Applying an anisotropic mechanical strain on materials can modify their physical properties, for example by driving [1] or tuning [2] phase transitions or by lifting some degeneracies [3]. Angle-resolved photoemission spectroscopy (ARPES) is a well-adapted technique to investigate the electronic properties of materials; despite that only few articles endeavour to use ARPES on mechanically strained samples. This poster aims at explaining the successive steps toward straining materials and measuring their electronic band structure. After having presented the stress cell and characterized it, the strain measurement will be explained. First ex- and in-situ measurements of physical properties, in confrontation to modelling results, enable to justify the feasibility of this experimental program.

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Titre/Title:**Composites de MOF avec des matériaux à base de carbone pour le stockage de l'hydrogène
MOF hybrids with carbon based materials for hydrogen storage**

Auteurs : Laura Jimenez Lopez¹, Rafael Morales Ospino¹, Jimena Castro-Gutiérrez¹, Alain Celzard^{1 2}, Vanessa Fierro¹

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Résumé/Abstract :

Metal-organic frameworks (MOFs) are promising materials for hydrogen storage due to their high surface areas and tunable porosity. This study explores the hybridization of various MOFs-HKUST-1, MIL-101(Cr), MIL-100(Fe), and MOF-5-with carbon-based materials including activated carbon (AC), exfoliated graphite (EG), carbon quantum dots (QDOTs), and graphene oxide (GO). Three synthesis strategies were employed: physical mixing, in situ synthesis, and post-synthetic modification. The resulting hybrid materials were evaluated for hydrogen storage via cryo-adsorption at 77 K and pressures up to 130 bar. Results demonstrate that hybridization improves the volumetric usable hydrogen capacities by enhancing packing density and, in some cases, increasing specific surface area. Notably, cryo-adsorption at 10 bar yields higher storage capacities than simple compression, with gains up to 432%. Additionally, incorporating these materials into tanks for liquid hydrogen storage significantly raises the hydrogen boiling point-from 21 K (empty vessel) to as high as 64 K-thus mitigating boil-off losses. The synthesis route proved critical, with in situ methods yielding the most integrated structures and superior performance. These findings underscore the potential of MOF@carbon hybrids to address key challenges in hydrogen storage and transport

Titre/Title:

Caractérisation mécanique et microstructurale de phases MAX à haute entropie irradié pour la nouvelle génération de réacteurs nucléaires.

Mechanical and microstructural characterizations of irradiated high-entropy MAX phases for the new generation of nuclear reactors.

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Résumé/Abstract :

With an energy density far greater than that of hydrocarbons, nuclear energy is a cornerstone of the European energy mix: 100 grams of uranium produces as much energy as one ton of oil. In this context, research is currently focused on developing a fourth-generation nuclear reactor. Several routes are explored, particularly on new materials selection that respond to reactors specific requirements. In this context MAX phases are interesting candidates. These ceramics, with the general formula M_n+1AX_n (where n ranges from 1 to 4), are composed of a transition metal M (Ti, V, Cr, Zr...) an A element from groups 13 to 16 (Al, Si, P...) and an X element which is carbon and/or nitrogen [1]. MAX phases are distinguished by their unique combination of ceramic-like properties (refractoriness, oxidation resistance, stiffness, low density) and metal-like properties (machinability, thermal and electrical conductivity, high thermal shock resistance and plastic deformation) [2]. Moreover, these ternary compounds exhibit good radiation tolerance, a key criterion for applications in nuclear environments [3]. The design of high-entropy MAX phases, with 3 to 5 elements in M or A sites, could also enhance their microstructural stability in such environments. In order to assess their suitability in nuclear environments where the material resistance to irradiation is critical, this thesis project aims to study the effect of irradiation and induced defects on their microstructure, deformation mechanisms and mechanical properties.

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Titre/Title:

Characterization of 2024 alloy with thick corroded layer: a mock-up of ancient aircraft aluminum alloys

Auteurs : Roua Kaddah¹, Delphine Veys-Renaux¹, François Mirambet², Emmanuel Rocca¹

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Résumé/Abstract :

Since the 1970s, preserving aircraft in aeronautical museums has posed significant challenges, particularly due to the corrosion of aluminum-copper (Al-Cu) alloys. This type of corrosion can lead to lamellar and intergranular corrosion, which weakens the mechanical strength of these materials [1]. To tackle this issue, efforts are being made to develop protective treatments for corroded metal parts.

This study aims to create controlled samples of corroded aluminum alloys that mimic the severe corrosion observed in aging aircraft [2]. Mock-ups of corroded 2024-T3 aluminum alloys were developed using an electrochemical approach. This involved a traditional three-electrode experimental setup in a sodium chloride solution. Electrochemical measurements, including open-circuit potential, polarization curves, and electrochemical impedance spectroscopy, were conducted to analyze thick intergranular corrosion layers that reached depths of over 300 μm . The corrosion layers were further examined using X-ray diffraction and scanning electron microscopy coupled with energy-dispersive X-ray spectroscopy (EDS).

The methods developed in this study will contribute to formulating new treatments for thick corrosion layers on aluminum in future research.

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Titre/Title:

Synthèse en une seule étape par magnétron non réactif de couches minces de γ -CuI pour conducteurs transparents de type p en photovoltaïque

Single-Step Non-reactive Magnetron Synthesis of γ -CuI Thin Films for p-type Transparent Conductors in Photovoltaics

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Résumé/Abstract :

Magnetron sputtering is frequently employed, versatile and scalable thin-film deposition technique to fabricate functional materials. Under vacuum conditions, this technique facilitates the ejection of atoms from a solid target, followed by condensation on a substrate to produce films with tailored properties. In this study, we employed a single step, non-reactive sputtering approach to deposit γ -phase cuprous iodide (CuI) thin films on Si and silica substrate at room temperature using ceramic CuI target. This single-step strategy allows the direct formation of CuI in the presence of Ar gas circumventing the need for intermediate phases or reactive gas environment, ensuring high quality films with control, avoiding complex iodination steps. Our results demonstrate the successful growth of highly transparent and well-crystallized CuI thin films, exhibiting p-type conductivity with a direct optical bandgap of approximately 2.9 eV. The films show strong light transmission in the visible range and the work function values, aligning well with transparent electronics and photovoltaic device requirements. This study highlights the potential of a simplified and efficient sputtering strategy to produce high-performance p-type transparent semiconductors for optoelectronic applications.

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Titre/Title:

Commutation de magnétisation tout optique en un seul coup dans des couches simples d'alliages ferrimagnétiques Co-RE

Single-shot all-optical magnetization switching in ferrimagnetic Co-RE alloys single layers

Auteurs : *Boonthum Kuyangyuen*¹, *Gregory Malinowski*¹, *Jun-Xiao Lin*¹, *Yann Le Guen*¹, *Stephane Mangin*¹, *Julius Hohlfeld*², and *Michel Hehn*¹

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Résumé/Abstract :

Ultrafast all-optical helicity-independent switching (AO-HIS) enables magnetization reversal in nanostructures without any applied magnetic field, with a characteristic timescale of 1 ps to cross zero magnetization. This is the fastest magnetization reversal reported in magnetic materials and is considered crucial for the development of faster, smaller, and energy-efficient data storage technologies. AO-HIS was first demonstrated in the ferrimagnetic alloy $(\text{FeCo})_x\text{Gd}_{1-x}$ [1], where it is attributed to ultrafast laser-induced heating that drives the rare earth (RE) and transition metal (TM) sublattices out of equilibrium. The magnetization reversal results from exchange-driven angular momentum transfer between Gd and Fe/Co atoms. However, achieving AO-HIS in other TM-RE single-layer alloys has proven difficult. In $\text{Co}_{0.75}\text{Tb}_{0.25}$ and $\text{Co}_{0.75}\text{Dy}_{0.25}$, only partial switching was observed and only for initial pulses [2]. In contrast, AO-HIS has been realized in Co/Ho multilayers [3], and by introducing Gd into Co-Tb, Co-Dy, and Co-Ho systems—suggesting Gd plays a key role. This work addresses single-pulse AO-HIS in Co-RE alloy single layers (RE = Tb, Dy, Ho, Er). AO-HIS occurs in Dy- and Ho-based alloys near the magnetic compensation point, while Tb and Er only show demagnetization. Hall cross studies reveal domain-wall-mediated reversal occurring on microsecond timescales. These results challenge current models and deepen our understanding of ultrafast magnetic switching.

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Titre/Title:

Le charbon actif en vedette : est-ce la clé pour de meilleurs capteurs de gaz NO₂ ?

Le charbon actif en vedette : est-ce la clé pour de meilleurs capteurs de gaz NO₂ ?

Auteurs : Proscovia Kyokunzire¹, Jean Zaraket¹, Vanessa Fierro¹, Alain Celzard¹

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Résumé/Abstract :

Gas sensors play a crucial role in detecting harmful environmental gases. This study focuses on optimizing a resistive sensing layer for nitrogen dioxide (NO₂) detection at room temperature (RT = 25 °C), based on commercial activated carbon (AC). NO₂ sensing was assessed over a dynamic concentration range from 1 to 20 ppm. The impact of cycle time, interdigitated electrode gap, NO₂ gas flow rate, synthetic air purge rate and saturation on sensor response has been examined. NO₂ sensing proceeded by adsorption, facilitated by the porosity and high surface area of AC. Sensing capability is reversible, suggesting purely physical adsorption. A response limit close to 65

Titre/Title:

**Recherche de microtreillis résilients inspirés d'analogues en plasticité cristalline
Resilient microtrusses inspired by analogues in bi-crystal plasticity**

Auteurs : Nicolas Lallemand¹, Stéphane Berbenni¹, Justin Dirrenberger², Thiebaud Richeton¹

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Résumé/Abstract :

Additive manufacturing has allowed the development of architected materials in the industry. However, despite their advantages, low density and good energy absorption, the use of cellular materials as structural components is still hindered by concerns toward their mechanical stability and resistance [1]. In particular, highly periodic lattice structures are weakened by localization bands [2], which causes mechanical instabilities and early failure. A framework for improving the mechanical resistance of those lattice metamaterials consists in drawing from an analogy between the macroscopic lattice structures and the crystalline microstructures to derive design guidelines and obtain the desired mechanical response in metamaterials [2]. The introduction of defects like interfaces between different lattice orientations has been shown to hinder localization band similarly to the interaction between grain boundaries and slip bands in polycrystals [2]. The objective is to explore this analogy by applying an approach based on bi-crystallography to design bi-crystal inspired lattice structures. A geometrical analogy is developed by using the crystallographic Coincidence Site Lattice (CSL) theory to obtain various interface morphologies in the bi-crystal inspired structures. This allows to test the influence of specific interfacial connectivity on the mechanical behavior. It opens the possibility to tailor the metamaterial for certain applications.

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Titre/Title:

**Simulation d'instabilités Weibel en plasmas relativistes avec des paires d'électron-positron
Simulation of Weibel instabilities in relativistic plasmas with electron-positron pairs**

Auteurs : *Charles Lanher*¹, *Daniele Del Sarto*¹, *Alain Ghizzo*¹

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Résumé/Abstract :

L'auto-organisation est un mécanisme permettant de créer des structures à grande échelle, comme des galaxies, dans un environnement turbulent. Ce processus reste aujourd'hui mal compris par les scientifiques en raison du transfert non-linéaire d'énergie de champ entre grande et petite échelle. Ce travail de thèse propose de faire avancer les connaissances actuelles de cette physique de plasma relativiste en étudiant la reconnexion magnétique qui se produit dans beaucoup de systèmes d'astrophysique avec de l'auto-organisation. Pour simuler et étudier les instabilités déclenchées durant une reconnexion magnétique, nous avons utilisé le code numérique Particle-in-Cell (PIC) SMILEI [1] dans le mésocentre EXPLOR. Les résultats numériques d'instabilités de type Weibel sont présentés dans ce poster, et nous ont permis d'étudier le processus de chauffage qui est une signature de l'auto-organisation des plasmas. Avec les paramètres des simulations, nous expliquons des conséquences de quelques caractéristiques d'instabilité faisceau-plasma dans les environnements d'astrophysique. Pour finir, ces simulations du code PIC SMILEI nous permettent de trouver un nouveau mécanisme physique (différent de la reconnexion magnétique) qui mène à un processus de chauffage.

The self-organisation is a mechanism permitting to create large-scale structures like galaxies in turbulent environment. This process remains today misunderstood by the scientists because of the non-linear transfer of field energy between large scale and small scale. This thesis work proposes to advance current knowledges of this relativistic plasma physics by studying the magnetic reconnections which occur in many astrophysics systems with self-organisation. To simulate and study the instabilities triggered during a magnetic reconnection, we used the numerical Particle-in-Cell (PIC) SMILEI [1] code in the EXPLOR centre. Numerical results of Weibel-type instabilities are presented in this poster, and they permitted us to study the heating process which is a signature of the plasma self-organisation. With the parameters of the simulations, we explain consequences of some beam-plasma instability characteristics in astrophysical environments. Finally, these simulations of PIC SMILEI code allow us to find a new physical mechanism (different of magnetic reconnection) that leads to a heating process.

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Titre/Title:

EBIC contrast in GaN:C - from electrical signal to crystal

Auteurs : Etienne N. Lavallée¹, *Autriche Antoine Guitton*², *Claire Chisholm*¹

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Résumé/Abstract :

Interest for Gallium Nitride (GaN) based power devices has risen in the last years as a competitor to silicon (Si). In the former material threading dislocations (TD) are more numerous and conflicting observations on their influence on electrical performance and reliability of GaN devices have been made. TDs are widely assumed detrimental for the devices and therefore, their characterization is of utmost interest to understand their role and may lead to chips improvement. Electron Beam Induced Current (EBIC), an in-situ SEM characterization method, provides a mean to pinpoint the local electrical activity of a semiconductor. EBIC enhances leakage identification by separation of electron-hole pairs within an internal Built-in field. Electron Channeling Contrast Imaging (ECCI), a Scanning Electron Microscopy (SEM) technique, provides fast, non-destructive crystal defect characterization of a wide area on a bulk sample. The contrast arising in ECCI allows for defect imaging by mapping the local changes of stress and strain as a variation of the Backscattered Electron (BSE) intensity. A correlative workflow has been developed between both methods. Defects of different nature have been observed responsible for the local electrical activity and not all of them match a dislocation.

Titre/Title:

Identification of conduction mechanisms in ZnMgO thin films via temperature-dependent conductivity and magnesium composition

Auteurs : *Krishna Lone*¹, *Wafae El-Berjali*¹, *Victor Colas*¹, *Sidi Ould Saad Hamady*¹

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Résumé/Abstract :

Zinc magnesium oxide (ZnMgO) is an n-type semiconductor from non-toxic, abundant elements, with a direct band gap tunable from 3.3 to 4.9 eV via Mg content. This study investigates defect states and conduction mechanisms in ZnMgO and ZnO thin films with 4% Mg, grown by ultrasonic spray pyrolysis. Aluminum ohmic contacts (~200 nm) were deposited by thermal evaporation. Conductivity was measured from 40 K to 420 K at fixed Mg concentration. Data analysis revealed three conduction mechanisms: shallow donor activation at high temperatures, and Mott variable range hopping (VRH) plus nearest neighbor hopping (NNH) at low temperatures. Incorporating 4% Mg increases activation energy from 48.3 meV to 69.0 meV and shifts the dominant low-temperature mechanism from VRH in ZnO (density of localized states $\approx 2.3 \cdot 10^{21} \text{ cm}^{-3} \text{ eV}^{-1}$, localization length 1.8 nm) to NNH in ZnMgO (hopping energy 2.8 meV). Optical characterization showed bandgap widening (3.279 to 3.318 eV) and increased Urbach energy, aligning with conduction changes. These findings advance understanding of ZnMgO conduction and inform its development for optoelectronic applications.

Titre/Title:

Exploration de la microstructure des fines et de leur comportement mécanique
Exploring the microstructure of fines and its mechanical behavior

Auteurs : Mengyu Ma¹, *Fares Bennai*¹, *Mahdia Hattab*¹, *Pierre-Yves Hicher*², *François Nicot*³

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Résumé/Abstract :

Les sols argileux présentent un comportement mécanique complexe, fortement influencé par leur microstructure. Les particules de kaolinite sont négativement chargées sur leurs faces, leurs bords sont positivement chargés en milieu à pH faible et négativement chargés en milieu à pH élevé [1]. Ces variations induisent des interactions électrostatiques entre les particules, conduisant à la formation de microstructures variées. Cette étude se concentre sur l'impact des microstructures initiales formées lors de la sédimentation des argiles sur leur comportement mécanique sous compression unidimensionnelle. Pour cela, différentes microstructures initiales ont été générées par sédimentation à pH variable, suivies d'essais œdométriques sur les boues sédimentées. Les échantillons, à différents niveaux de chargement, ont été observés au microscope électronique à balayage (MEB) pour visualiser leur microstructure [2]. Une structure en château de cartes a été observée dans la boue floculée, tandis que des empilements de particules ont été observés dans la boue dispersée. Les essais œdométriques montrent que les échantillons floculés présentent une compressibilité plus élevée. La microstructure floculée évolue progressivement vers celle des échantillons dispersés sous compression unidimensionnelle. Sur le palier de déchargement, le gonflement des échantillons est similaire, ce qui suggère une convergence des microstructures après un chargement œdométrique à 1000 kPa.

Clay soils exhibit complex mechanical behavior, strongly influenced by their microstructure. Kaolinite particles are negatively charged on their faces; their edges are positively charged in low pH environments and negatively charged in high pH environments [1]. These charge variations induce electrostatic interactions between particles, leading to the formation of different microstructures. This study focuses on the impact of initial microstructures formed during sedimentation on the mechanical behavior under one-dimensional compression. To this end, various initial microstructures were generated through sedimentation under different pH conditions, followed by oedometer tests on the sedimented clay suspensions. The samples, at different loading stages, were observed using scanning electron microscopy (SEM) to visualize their microstructure [2]. A card-house like structure was observed in the flocculated clay, while face-to-face particle stacking was observed in the dispersed clay. Oedometer tests show that flocculated samples exhibit higher compressibility. Under one-dimensional compression, the flocculated microstructure progressively evolves toward that of the dispersed samples. During the unloading stage, the swelling behavior of the samples is similar, suggesting a convergence of microstructures after oedometer loading up to 1000 kPa.

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Titre/Title:

**Pérovskites chirales hybrides : des monocristaux aux films minces et aux dispositifs
Hybrid chiral perovskites : from single crystals to thin films and devices**

Auteurs : Samuel Mathieu^{1,2}, Mathieu Stoffel¹, Hervé Rinnert¹, Yuan Lu¹, , Maoxiang Zhu¹, Sébastien Pillet², Abdelatif Doudouh², Emmanuel Wenger²

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Résumé/Abstract :

Hybrid organic inorganic halide perovskites (HOIP) have been extensively studied due to their applications in the field of photovoltaics and light emitting devices. The substitution of either the metal or the halogen enables the tuning of their optical properties for desired applications. Moreover, the introduction of a chiral organic cation in the perovskite structure allows to further modify the properties of the HOIP thanks to the chirality-induced spin selectivity effect (CISS). This opens the route to novel applications in the field of spin-optoelectronics such as the fabrication of spin light emitting diodes (Spin-LEDs). This work combines the skills of two laboratories (CRM2 and IJL) in order to study the structure and physical properties of chiral HOIPs and functionalize these materials into a Spin-LED.

Titre/Title:

A staggered mesh electromagnetic model for investigating slag skin defects in electroslag remelting

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Résumé/Abstract :

Electroslag remelting (ESR) is used to produce high-performance metallic alloys due to its ability to enhance cleanliness, homogeneity, and surface quality. Surface and slag skin defects are rare in ESR and difficult to interpret. This study focuses on a specific defect involving abnormal thickening of the solidified slag layer, which affects and is affected by lateral heat and electrical transfer, disrupting other physical phenomena in the system. The defect compromises ingot quality, especially in critical applications. Industrial data analysis revealed a correlation between the defect and deviations in the electrical current path, underscoring the need for accurate electromagnetic modeling. Existing finite volume models fall short due to their co-located meshes, which prevents proper enforcement of Gauss's laws and lead to high computational costs when resolving thin slag layers. To address this, a new electromagnetic finite-volume model based on the Yee scheme was developed, using staggered meshes to enforce charge conservation and accurate field coupling. Simulations showed that changing the electrical conductivity of the solidified slag layer from 10^{-3} to 5 S/m increased current flow through the layer from 0.1% to 40%. The model accurately resolves thin slag layers, maintains stability, and enables fast, robust analysis for ESR process optimization.

Titre/Title:

Effets de la concentration en graphène sur les propriétés thermique et mécaniques des nanocomposites Elium/Graphène

Effects of Graphene Concentration on the Thermal and Mechanical Properties of Elium/Graphene Nanocomposites

Auteurs : Laurenza Mengue¹, Matadi-Boumbimba¹, Abdelkibir Benelfellah², Lucie Chupin³

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Résumé/Abstract :

Les nanocomposites à base de résine Elium acrylique et de graphène en couches minces (Few-Layer Graphene, FLG) constituent une solution prometteuse pour répondre aux exigences croissantes en matériaux légers, durables et recyclables dans les secteurs du transport et de l'aéronautique. L'influence de faibles concentrations de FLG (0,01 à 0,4 % en masse) sur les propriétés thermique et mécaniques de ces nanocomposites est examinée dans cette étude. La résine Elium acrylique, thermoplastique polymérisable à température ambiante, présente plusieurs avantages en termes de traitement et de recyclabilité, bien que son association avec le graphène reste encore peu explorée. Les nanocomposites ont été caractérisés par DSC, ATG, DMA, ainsi que par des essais de traction et de compression dynamique à différentes vitesses de déformation. Les résultats ont mis en évidence une amélioration significative des propriétés à 0,1 % de FLG, avec un gain de +64,4 % de résistance à la traction et une augmentation de la température de transition vitreuse de 98 °C à 118,2 °C. Des observations MET ont également confirmé une bonne dispersion du FLG et une interface matrice-nanocharges bien adhérente. Ces résultats soulignent le potentiel des nanocomposites Elium/graphène pour des applications structurales à hautes performances, notamment dans les environnements soumis à des contraintes mécaniques et thermiques exigeantes.

Titre/Title:

**Synchronisation de dynamiques spatio-temporelles complexes entre des lasers couplés
Synchronization of complex spatiotemporal dynamics between coupled lasers**

Auteurs : Jules Mercadier¹, Stefan Bittner¹, Marc Sciamanna¹

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Résumé/Abstract :

We report the first experimental demonstration of chaos synchronization between two spatially extended, multimode lasers operating under free-running conditions. Synchronization of complex dynamics has traditionally been studied in systems driven into chaos by external perturbations, motivating our investigation of coupled lasers exhibiting intrinsic multimodal chaos. We observe synchronization when a dominant transverse mode of the master laser becomes spectrally aligned with a mode of the slave, without requiring a perfect matching between the spatial field profiles. Several dynamical regimes are identified, including synchronization of fast chaotic fluctuations and low-frequency mode-hopping, along with transitions between normal and inverse synchronization. These results show that the presence of complex states disordered in space and time does not hinder synchronization, instead, it enables a variety of coupling regimes. Our findings offer new insights into how multimode chaotic lasers can self-organize through weak coupling, highlighting the role of spectral alignment and dominant modes in the emergence of coherent behavior. In addition, since chaos is here achieved without the need for additional optical feedback, the present chaos synchronized system is kept at its simplest level for future information security applications.

Titre/Title:

Caractérisation multi-échelle d'un alliage de rechargement dur chrome-carbone appliqué à la protection balistique

Multi-scale characterization of a high chromium-carbon based hardfacing alloy for ballistic protection applications

Auteurs : **Antoine Monnet**^{1,2}, **Teresa Fras**¹, **Slim Bahi**², **Alexis Rusinek**², **Antoine Guitton**²

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Résumé/Abstract :

Hardfacing process is currently widely used for the protection of materials and structures exposed to complex and severe environments. This technique involves the fusion application of a protective coating onto a surface, significantly enhancing its resistance to wear, corrosion, and other forms of degradation [1,2]. In sectors such as aerospace and automotive, hardfacing extends the lifespan of components and preserves their performance over time. However, its application in the field of ballistic protection remains relatively unexplored, even though research and development of new armor systems are crucial in light of the rapidly evolving current kinetic threats. The use of this technique could not only significantly increase the impact resistance of armor but also maintain the mobility of structures and the cost-effectiveness of deployed solutions [3]. In this context, the work presented here focuses on the analysis of a bilayered passive protection composed of a S355MC steel substrate (C < 0.2% by weight) with a thickness of 8 mm, onto which a material of the same thickness, equivalent to a highly alloyed chromium cast iron (Cr: 27-30% by weight; C: 4-6% by weight), is applied using flux-cored arc welding (FCAW). Impact tests were conducted on several units using a 7.62x51 mm caliber projectile, equivalent to the M61, on the instrumented ballistic testing facility of the Franco-German Research Institute of Saint-Louis (ISL). A comprehensive microstructural analysis of the composite is proposed and linked with target damage during impact. Additionally, a model of the welding deposit used is proposed with a view to the numerical simulation of ballistic tests.

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Titre/Title:

Une stratégie de micropatterning pour évaluer la morphologie et la topographie des cellules endothéliales

Auteurs : ***Daniele Pedroni***¹, ***Demba Ba***¹, ***Laurent Badie***¹, ***Halima Alem***¹, ***Caroline Gaucher***²

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Résumé/Abstract :

Micropatterning via electron-beam lithography provides a powerful tool for endothelial cells alignment and confinement. In this study, we employed this technique to fabricate high-resolution patterns on glass substrates, enabling a controlled cellular microenvironment for fluorescence and atomic force microscopy (AFM) analysis. Human umbilical vein endothelial cells (HUVECs) cultured on patterned glass surfaces exhibited distinct morphological adaptations depending on the geometric constraints. Microscopy observations revealed that cell adhesion, alignment, and spreading were strongly influenced by pattern dimensions, with effective orientation occurring only for inter-line distances of at least 10 μm . Furthermore, alignment was lost over time on patterns with line widths below 20 μm , indicating critical geometric thresholds for maintaining directed cell organization. Complementarily, AFM analysis provided a detailed characterization of the three-dimensional surface topography of cells confined within square micropatterns ranging from 10 to 30 μm . Key roughness parameters-including RMS height, RMS slope (Sdq), kurtosis, and skewness-were extracted, and high-pass filtering allowed for precise separation of local surface roughness from overall cell shape. The results demonstrated a strong correlation between available adhesion area and nanoscale topographical features, revealing how substrate patterning modulates cellular surface properties at multiple scales. By integrating fluorescence and AFM measurements within a single micropatterning-based approach, this study offers a robust and reproducible platform for dissecting the relationship between cell shape, adhesion, and nanometric surface characteristics, advancing our understanding of endothelial cells behavior in controlled microenvironments. Keywords: Micropatterning, microfabrication, gas-phase silanization, fluorescence microscopy, atomic force microscopy, endothelial cells

Titre/Title:

**Étude de textures magnétiques générées par impulsion laser
Magnetic textures generated by laser pulses**

Auteurs : Léo Petitdemange¹, Michel Hehn¹, Grégory Malinowski¹, Daniel Lacour¹

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Résumé/Abstract :

Dans la matière condensée, l'étude des textures magnétique concilie la recherche fondamentale et l'innovation technologique, avec des applications potentielles dans des domaines variés tels que l'informatique, l'énergie et la physique fondamentale. Ces textures complexes peuvent être générées par impulsion laser, favorisant alors l'émergence des systèmes de stockage d'informations ultra-rapide à faible consommation d'énergie. [1] Notre étude s'inspire des travaux de Zhang et al. [2] et est effectuée sur des films minces à anisotropie perpendiculaire. Nos mesures de caractérisations magnétiques montrent qu'en diminuant l'épaisseur d'un film mince de CoFeGd de 8.5 à 7 nm l'état d'aimantation passe d'une configuration magnétique homogène à inhomogène en champ nul. Avant la transition, il est possible de préparer le système dans un état métastable en champ nul. L'utilisation d'une impulsion laser femtoseconde peut alors fournir suffisamment d'énergie localement pour changer la configuration magnétique et générer une texture. Dans ce poster, nous allons présenter nos résultats sur CoFeGd en film mince sur un substrat monocristallin de Si/SiO₂, élaboré par Physical Vapor Deposition sous ultravide à l'Institut Jean Lamour. Après une impulsion laser de 30 fs sur ce matériau, nous avons observé l'apparition d'une texture magnétique puis imagé par une technique de microscopie magnétique récente. [3]

In condensed matter physics, the study of magnetic textures bridges fundamental research and technological innovation, with potential applications in various fields such as computing, energy, and fundamental physics. These complex textures can be generated by laser pulses, fostering the emergence of ultra-fast, low-energy information storage systems. [1] Our study is inspired by the work of Zhang et al. [2] and is conducted on thin films with perpendicular anisotropy. Our magnetic characterization measurements show that by reducing the thickness of a CoFeGd thin film from 8.5 nm to 7 nm, the magnetization state transitions from a homogeneous to an inhomogeneous magnetic configuration in zero field. Before the transition, it is possible to prepare the system in a metastable state in zero field. The use of a femtosecond laser pulse can then provide enough localized energy to change the magnetic configuration and generate a texture. In this poster, we will present our results on CoFeGd thin films deposited on a monocrystalline Si/SiO₂ substrate, fabricated by Physical Vapor Deposition under ultra-high vacuum at the Institut Jean Lamour. After a 30 fs laser pulse on this material, we observed the appearance of a magnetic texture, later imaged using a recent magnetic microscopy technique. [3]

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Titre/Title:

Structure et dynamique des assemblages de nanodisques lipidiques mimétiques de l'apoA-1 en intégrant des données expérimentales et des simulations de dynamique moléculaire.

Structural and dynamics of apoA-1 mimetic peptide lipid nanodisc assemblies by integrating experimental data with molecular dynamics simulations.

Auteurs : Rohith Ravi¹, Mounir Tarek¹

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Résumé/Abstract :

Apolipoprotein A-1 (ApoA-1) is the major protein component of high-density lipoproteins (HDL) and plays a critical role in reverse cholesterol transport (RCT) as well as disease progression. Its structure consists of a series of tandem amphipathic helical domains. Based on this structure and helix theory, amphipathic helical peptides were designed as potential therapeutic tools in biomedical applications¹. In particular, we focus on the 14A, 4F, 4FP4F peptides, which have demonstrated superior therapeutic efficacy in animal models of cardiovascular diseases (CVDs) the leading cause of death worldwide. In each year, more than 17.6 million deaths were attributed to CVDs globally. Despite the significance of peptide-lipid nanodisc assemblies in biomedical therapy, there is still a lack of detailed structural, dynamic, and biophysical characterization of these assemblies. To address this gap, we combined small-angle X-ray scattering (SAXS) and nuclear magnetic resonance (NMR)² spectroscopy with molecular dynamics (MD) simulations to validate our models³. Our study characterizes lipid-peptide and peptide-peptide interactions, which play a crucial role in stabilizing nanodiscs, an essential component in lipid metabolism pathways. Our findings will contribute to the future design and development of ApoA-1 mimetic peptide-lipid nanodisc assemblies for therapeutic applications.

Keywords: All-atom Molecular Dynamics, Nanodiscs, HDL, Apolipoprotein-A1 mimetic peptides, SAXS, Solid-state NMR.

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Titre/Title:

**Intercalation de photosensibilisateurs dans des hydroxydes doubles lamellaires de type Zn₂Al-
pour la dépollution de l'eau**

Intercalation of photosensitizers in Zn₂Al-layered double hydroxides for water remediation

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Résumé/Abstract :

Layered double hydroxides (LDHs), also known as anionic clays, have the general chemical formula $[M_{1-x}^{II}M_x^{III}(OH)_2]^{x+}[(A_{x/n}^{n-}) \cdot yH_2O]^{x-}$. They consist of positively charged metal hydroxide sheets where cations are located at the center of octahedra formed by hydroxides. Solvated anions (Aⁿ⁻) are intercalated between these sheets. The compositional tunability of LDHs, enabled by the flexible selection of cations and intercalated anions (organic or inorganic), makes them highly versatile for various applications, with particular interest in water remediation [1]. In this context, the use of 2D systems, such as films formed either by in situ method or by particle deposition, is attractive as the materials can be recycled and reused. According to the literature, certain organic anions (benzoate, isophthalate, trimesate, etc.) intercalated into Zn₂Al-LDH through direct synthesis have been used as supramolecular photosensitizers, exhibiting photocatalytic properties in the near-infrared region [2]. These could allow the formation of highly reactive singlet oxygen ¹O₂, to initiate the degradation of organic pollutants by oxidation mechanisms [3]. In this work, we investigated the intercalation of various anions (benzoate, terephthalate, and pyromellitate) into Zn₂Al-LDH in two systems: films and suspensions. The LDHs were synthesized using direct coprecipitation, and anion exchange. The arrangement of anions in the interlayer space was investigated as a function of (1) the synthesis method and (2) the system. The intercalation of organic anions in LDH materials was characterized by vibrational spectroscopies (Raman, IR), scanning electron microscopy (SEM) and X-ray diffraction (XRD).

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Titre/Title:

**Composites magnétorhéologiques à inclusions fluides
Magnetorheological composites with fluid inclusions**

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Résumé/Abstract :

Des composites à matrice de polydiméthylsiloxane, intégrant un fluide magnétorhéologique (MRF), ont été élaborés afin de concevoir des matériaux dont les propriétés mécaniques peuvent être modulées par un champ magnétique externe. Leurs performances ont été évaluées en compression statique et cyclique sous champs allant jusqu'à 500 mT, puis comparées à celles d'élastomères magnétorhéologiques (MRE) conventionnel. En l'absence de champ, ces matériaux restent très souples ; sous l'influence du champ magnétique, la réorganisation réversible des particules magnétiques induit un renforcement notable de la raideur et de la dissipation. Un échantillon contenant 13,3 La capacité de ces composites à ajuster finement leurs propriétés mécaniques les rend donc particulièrement adaptés aux actionneurs et aux dispositifs de contrôle vibratoire.

Titre/Title:

Recherche des déclencheurs du clivage et de leurs effets sur la rupture des aciers faiblement alliés.

Investigation of cleavage initiators and their effects on fracture in low-alloy steels.

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Résumé/Abstract :

En tant qu'exploitant de centrales nucléaires, EDF est garant de la sûreté de ses installations. Dans cette optique, l'entreprise cherche à se doter des moyens techniques et scientifiques pour prévoir les propriétés mécaniques des gros composants forgés en aciers faiblement alliés. Cette thèse s'inscrit dans cette démarche en visant à développer un outil prédictif capable d'établir un lien entre les microstructures locales de ces composants et leurs propriétés de rupture. Pour modéliser la rupture par clivage des aciers faiblement alliés, une approche de type " submodel " est mise en œuvre. Il s'agit d'une approche locale de la rupture à l'échelle micromécanique [1], visant à expliquer et quantifier l'aspect statistique de la rupture fragile dans la transition ductile-fragile. Le modèle simule explicitement le comportement du matériau à deux échelles :

— L'échelle Macroscopique modélisant le comportement d'une éprouvette de mécanique de la rupture.

— L'échelle Microscopique modélisant le comportement du matériau à l'échelle de la microstructure. Le clivage y est représenté par un critère de rupture déterministe fondé sur celui de Griffith [2]. Un travail expérimental de synthèse de microstructures basé sur des variations maîtrisées des paramètres métallurgiques des traitements thermiques a permis d'obtenir des variantes microstructurales à confronter au modèle.

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Poster P47

Titre/Title:

Etude de la structure et du magnétisme de nouveaux composés intermétalliques de type R_2MoSi_2C ($R = Y, Gd-Tm, Lu$)

Crystallographic and magnetic study of novel intermetallic compounds R_2MoSi_2C ($R = Y, Gd-Tm, Lu$)

Auteurs : Ibrahima Sarr¹, *Bernard Malaman*¹, *Léopold V.B. Diop*¹, *Anne Vernière*¹

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Résumé/Abstract :

Titre/Title:

Elaboration of LDH films and evaluation of their photoactive properties for antibacterial application

Auteurs : Sushant Sharma¹, Samantha Soulé¹, Fabienne Quilès¹

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Résumé/Abstract :

Layered double hydroxides (LDH) have gained significant attention as promising photoactive materials [1] for antibacterial applications [2]. These two-dimensional hydrotalcite-like materials, with the general formula $[M_{1-x}^{2+}M_x^{3+}(\text{OH})_2]^{x+}[(A^{n-})_{x/n} \cdot \gamma \text{H}_2\text{O}]^{x-}$, consist of anions A^{n-} sandwiched between positive brucite-like sheets containing divalent M^{2+} and trivalent M^{3+} cations. Interestingly, by altering the composition of the octahedrally centered divalent and trivalent cations, these materials can be photoactive either by Reactive Oxygen Species formation or photothermal effect on light irradiation. Developing these LDH in the form of film is ideal for antibacterial assays. The growth of LDH as films [3] favours precise morphological control and easy retention after use. To harness these advantages, we have optimised the synthesis of different LDH films on aluminium-based substrates. Using hydrothermal routes and different precipitants (ammonia, urea), we have obtained LDH films with different compositions ($M^{2+}=\text{Cu/Zn/Co}$). The as-synthesized films are characterized by XRD and vibrational spectroscopies (Infrared and Raman) to confirm the LDH phase and determine the intercalated anions. The film morphology was analyzed by SEM. DRS was used to determine the optical properties. The elementary composition was determined by XPS and EDX Spectroscopy. These films will be evaluated for their photoactive antibacterial assay upon light irradiation both for ROS production and photothermal effect.

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Titre/Title:

Propriétés structurales et magnétiques d'alliages à haute entropie dérivés de composés intermétalliques de type Heusler

Structure and magnetic properties of Heusler-based High Entropy Alloys.

Auteurs : D. Sihom Kwekam¹, G. Lengaigne¹, J. Ledieu¹

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Résumé/Abstract :

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³ Institute of Materials for Electronics and Magnetism, IMEM-CNR, Parma, Italy. High-entropy alloys have been proposed as a new concept for alloy design [1]. They have been mainly investigated for their structural properties, as they can exhibit very high fracture toughness as well as good resistance to oxidation and corrosion. More recently, there have been new interest in their functional properties, including superconductivity, thermoelectricity as well as magnetic properties [2]. In this work, we will present an investigation on new HEAs derived from the Ni₂MnGa Heusler compound, a ferromagnetic shape memory alloy with interesting magnetocaloric properties.

A set of new quaternary HEA compounds have been prepared in the (Ni,Co,Fe,Mn)₃(Sn,Sb,Ga,Si) system by arc-melting or induction furnace followed by post-annealing treatments. Powder X-ray diffraction analysis reveals that some compositions preserve the Fm-3m cubic structure of the ternary parent phase, like in (NiCoFeMn)₃Sn. This pure cubic phase was further investigated by scanning transmission electron microscopy (STEM). The results indicate that a high-entropy intermetallic compound forms, rather than a pure solid solution as in HEA, in which all the transition metal (TM) atoms occupy the TM crystallographic sites of the Heusler parent phase, and Sn occupy the Ga sites (Figure 1-a).

Thermomagnetic analysis (TMA) shows that the magnetic phase transition between the low temperature ferromagnetic phase and the high temperature paramagnetic phase occurs at around 520K. In order to reduce the Curie temperature closer to ambient conditions more suitable for magnetocaloric applications, we attempted to reduce the magnetic interactions by adding a non-magnetic element such as Cu. A set of four samples has been prepared in the (NiCoFeMnCu)₃Sn, with a Cu content varying from 6 to 18 at.

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Titre/Title:

Surface and cavity exciton-polaritons in J-aggregate films

Auteurs : **Marcelo Barreiro**^{1,2}, **Diogo Cunha**^{2,3}, **Mikhail Vasilevskiy**^{2,3}, **Andrei Postnikov**¹

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Résumé/Abstract :

Surface polaritons are hybrid excitations formed by strong coupling between electromagnetic waves and collective material responses, allowing light to be confined at the sub-wavelength scale with intense local field enhancements. Surface exciton polaritons (SEPs) appear in materials with strong excitonic responses [1] and are present in both inorganic - hosting Wannier-Mott excitons, which only exist at low temperatures - and organic semiconductors - which support Frenkel excitons, stable at room temperature [2], which makes them more suitable for practical use. Exciton-polaritons can also be confined in optical cavities like Fabry-Perot (FP) resonators, enabling control over their dispersion. Among organic materials, J-aggregates of organic dye molecules are especially promising due to their strong and narrow excitonic features [3]. However, modelling their optical behaviour is challenging due to molecular disorder, anisotropy, and interface roughness. This study examines surface and cavity exciton-polaritons in J-aggregate films using two modelling approaches: a 3D isotropic model and a 2D uniaxial model, both accounting for disorder. It explores how anisotropy and roughness influence SEP dispersion and reflectance. When placed in FP cavities, J-aggregates show complex dispersion features [4], including a guided wave and a nearly dispersion-less mode linked to the exciton energy - observed in photoluminescence but not reflectivity - whose nature remains unresolved.

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Titre/Title:

**Corrélations des gaz de Bose unidimensionnels piégés à température finie
One-body correlations and momentum distributions of trapped one-dimensional Bose gases at finite temperature**

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Résumé/Abstract :

We introduce a general approximate method for calculating the one-body correlations and the momentum distributions of one-dimensional Bose gases at finite interaction strengths and temperatures trapped in smooth confining potentials. Our method combines asymptotic techniques for the long-distance behavior of the gas (similar to Luttinger liquid theory) with known short-distance expansions. We derive analytical results for the limiting cases of strong and weak interactions, and provide a general procedure for calculating one-body correlations at any interaction strength. A step-by-step explanation of the numerical method used to compute Green's functions (needed as input to our theory) is included. We benchmark our method against exact numerical calculations and compare its predictions to recent experimental results.

Titre/Title:

Influence of laser speed on microstructure of copper enriched steels processed by additive manufacturing

Auteurs : Alan Vaissières¹, *Eduardo Reverte Palomino*¹, *Sébastien Allain*¹, *Julien Zollinger*¹

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Résumé/Abstract :

The increase in copper content in steels is inevitable as recycling becomes more widespread. The very low solubility of this element in the ferrous phases and its tendency to segregate cause difficulties during processing. On the other hand, additive manufacturing makes it possible to reach strongly nonequilibrium conditions, which could be advantageous for the elaboration of copper-rich steels. In this study, we investigate the influence of laser velocity on the microstructure formation of carbon steel with high copper contents (> 5 wt %). Copper trapping is studied for velocities between 200 and 1500 mm/min, which are in the stable processing range. The microstructures are characterised by SEM, to quantify microsegregations. The results are compared and discussed with available analytical models for solute trapping.

L'augmentation du taux de cuivre dans les aciers est inévitable avec l'intensification du recyclage. La très faible solubilité de cet élément dans les phases du fer et sa tendance à ségréger peut poser des problèmes durant l'élaboration. D'autre part, la fabrication additive permet d'atteindre des conditions hors-équilibre, ce qui pourrait être un avantage pour l'élaboration d'aciers enrichis en cuivre. Dans cette étude, nous nous intéressons à l'influence de la vitesse du laser sur la formation des microstructures d'acier au carbone avec des hautes teneurs de cuivre (>5 % massique). Le piégeage du cuivre est étudié pour des vitesses entre 200 et 1500 mm/min, qui sont dans la gamme du procédé utilisé. Les microstructures sont caractérisées pour quantifier les micro-ségrégations. Les résultats sont comparés et discutés avec les modèles analytiques de piégeage de soluté disponibles.

Titre/Title:

Modélisation non linéaire d'un récupérateur d'énergie électromagnétique pour la marche humaine et résolution analytique.

Nonlinear modeling for a human walking electromagnetic energy harvester and analytical resolution

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Résumé/Abstract :

Avec la prolifération des objets connectés et des dispositifs électroniques embarqués, la récupération d'énergie lors de la marche humaine devient un sujet de recherche de plus en plus étudié. Nous présentons un modèle électromécanique de récupérateur d'énergie électromagnétique, constitué d'une bille aimantée se déplaçant à l'intérieur d'un tube conducteur équipé d'une bobine de récupération. Le modèle fournit une représentation mathématique du mouvement dynamique de la bille engendré par les mouvements du pied pendant la marche, et décrit comment ces mouvements permettent de générer de l'énergie via le champ magnétique induit dans la bobine. Le modèle proposé se concentre sur la phase de balancement du pied au cours de laquelle le déplacement de l'aimant dans le tube produit un courant électrique dans la bobine de récupération. Cela permet ainsi la conversion de l'énergie mécanique en énergie électrique. L'équation différentielle décrivant le mouvement de la bille, obtenue via les équations de Lagrange, est une équation forcée de Mathieu-Van der Pol généralisée comprenant un terme d'amortissement non-linéaire. Afin de résoudre cette équation multiphysique dans le cas faiblement non-linéaire, la méthode des échelles multiples (MSM) est utilisée. Les résultats obtenus sont comparés à ceux issus du solveur numérique ODE45 de Matlab®. Il est observé que la méthode MSM fournit de très bonnes approximations des solutions temporelles ainsi que de la puissance. En perspective, l'optimisation du récupérateur à partir des expressions obtenues.

Titre/Title:

Caractérisation et analyse numérique de fils d'acier inoxydable austénitique 304L soumis à une déformation par traction et par laminage à froid

Characterisation and numerical analysis of 304L austenitic stainless steel wires under tensile and cold rolling deformation

Auteurs : Aymeric Wassermann^{1,2}, *Gautier List*¹, *Eric Fleury*¹, *Olivier Jacquelin*²

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Résumé/Abstract :

The phenomenon of strain-induced martensite in 304L stainless steel is well known to increase the mechanical strength of the rolled samples. The martensite being harder than the austenite, this transformation is also responsible for a pronounced damage by wear of the rolls and dies. The present study focuses on the rolling of wire, particularly for complex shapes like flat wires with rounded edges, intending to get a deeper understanding of martensite formation during the rolling of 304L under industrial conditions. In addition to tensile tests performed until rupture over a temperature range of 20 C to 200C and strain rates ranging from 10^{-5} to 10^{-1} s^{-1} , interrupted tensile tests were particularly undertaken to investigate the variation of the volume fraction of martensite with the plastic strain. In parallel rolling experiments on a laboratory rolling mill were conducted with thickness reduction ratios of 20%, 40%, and 60%. Microstructural analyses using Electron BackScatter Diffraction (EBSD) revealed an inhomogeneous distribution of martensite, with a particularly larger value of the volume fraction of martensite in the centre of the rolled samples in comparison to their surfaces. Numerical simulations provided insights into the temperature distribution through the thickness of the rolled samples, explaining the lower martensite volume fraction at the surface and highlighting the significant impact of triaxiality on martensite formation.

Titre/Title:

Développement d'un bioprocédé pour stimuler mécaniquement les cellules via lévitation acoustique

Development of a bioprocess to mechanically stimulate cells by acoustic levitation

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Résumé/Abstract :

La stimulation mécanique des cellules est un élément clé dans la production de sécrétomes. Parmi les bioprocédés existants, la lévitation acoustique s'impose comme une méthode sans contact, aux conditions limites bien définies, et permettant ainsi d'appliquer des sollicitations mécaniques contrôlées aux cellules. Jusqu'à présent, ce procédé a uniquement été utilisé pour organiser des cellules dans un milieu fluide en vue de former des sphéroïdes ou du tissu. Dans notre cas, il s'agit du développement d'un bioprocédé permettant de léviter des gouttes d'hydrogel,ensemencées des cellules et d'appliquer des compressions cycliques à des fréquences réglables. Des gels à base d'alginate (1 à 12 %) ainsi que des hydrogels issus gelée de Wharton ou de collagène de queue de rat sont ainsi lévités. Puis par ombroscopie, le volume et la forme de la goutte sont analysés au cours du temps. Les premiers résultats montrent des pertes de volume par évaporation (environ 15 min), influencées par la température, l'humidité et la viscosité, affectant également la stabilité de la goutte. Ces données permettent d'alimenter un modèle numérique sur les compressions cycliques de la goutte. De futures expériences intégreront des cellules souches afin de mieux comprendre l'impact des sollicitations mécaniques sur leurs réponses.

Mechanical stimulation of cells is a key element of bioprocesses to activate their production of secretome. More particularly, acoustic levitation [1] is progressively becoming an interesting tool to apply controlled mechanical stimulations on stem cells, by being a contact-free method with well-defined boundary conditions. Until now, the process has been solely used to organize cells within a fluidic environment for spheroid or tissue formation [2]. In this work we develop a bioprocess to levitate single drop-shaped gel containing cells and apply cyclic compressions on them with adjustable frequencies. Alginate-based gels at different concentrations (1 to 12%) Preliminary results show volume changes due to evaporation [3] (around 15 min), influenced by temperature, humidity as well as viscosity, which affect the droplet's stability. These data will be used to feed an in silico model of the cyclic compressions on acoustically levitated droplets. Further experiments will investigate how material properties influence the levitating droplet before implementing stem cells in order to better understand mechanical stimuli on their responses.

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Titre/Title:

Analyse en corrélation 2D de spectres Raman à basses fréquences de molécules chirales : exemples de cristaux de phénylalanine

2D-correlation low-frequency polarized Raman spectroscopy of chiral molecules: example of phenylalanine crystals

Auteurs : Yechi Romiald Yavo¹, Grégoire Herzog¹, Manuel Dossot¹

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Résumé/Abstract :

Low-frequency Raman spectroscopy is a technique that studies vibrational modes below the traditional cut-off at 80-100 cm⁻¹ due to conventional optical filter. This technique can provide unique information on the solid state and structural characteristics, among other properties, owing to its sensitivity to intermolecular forces. In fact, low-frequency Raman spectroscopy has now enjoyed a surge in popularity with applications found in many research areas[1]. A particularly important application is the possibility to differentiate racemic crystals from enantiopure crystals [2], as will be shown in this communication. The low-frequency Raman spectra of racemic and enantiopure crystals exhibit significant spectral variation, which we attribute to different hydrogen-bond networks in the chiral crystal structures. Using the example of phenylalanine, we observed that when comparing racemic versus enantiopure crystals, the observed low-frequency vibrational modes and their relative scattering intensities are strongly dependent on the laser polarization state. To improve the spectral data interpretation, we used 2D correlation spectroscopy [3] of these low-frequency Raman spectra. The communication will demonstrate the interest of this kind of analysis to clearly differentiate the racemic from the pure enantiomeric form of crystalline powder of phenylalanine.

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Titre/Title:

**Élaboration in-situ d'alliages Ti-Nb par LPBF : étude d'optimisation paramétrique
In-situ fabrication of Ti-Nb alloys by LPBF: a parametric optimization study**

Auteurs : Delong Zhao¹, Wafa Elmaya¹, Pascal Laheurte¹

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Résumé/Abstract :

La fusion laser sur lit de poudre (L-PBF), procédé de fabrication additive, permet la réalisation de pièces complexes par fusion sélective de poudres métalliques couche par couche [1]. Malgré les avancées en élaboration in situ par L-PBF, l'optimisation de la densité et de l'homogénéité reste délicate [2]. Cette étude porte sur l'élaboration in situ d'alliages Ti-Nb à partir de poudres élémentaires. Un plan d'expérience de type Box-Behnken à trois facteurs est utilisé pour évaluer l'influence des paramètres d'impression (puissance laser, vitesse de balayage, espacement des hachures) exploitant une large plage de densité d'énergie (140-326 J/mm³) sur la qualité des pièces (densité et homogénéité chimique). La porosité (Φ) et la fraction de particules de Nb non fondues (I) ont été quantifiées en post-traitant des micrographies grâce au logiciel Ilastik et à des scripts Python. Une fenêtre optimale a pu être identifiée par la méthode des surfaces de réponses (P=165-170W, H=0,049-0,053mm, v=400mm/s). Le rôle et l'influence des paramètres ont été discutés. Une stratégie d'impression utilisant les paramètres optimaux identifiés avec une refusion par couche a permis d'aboutir à des pièces de densité élevée et une homogénéité intéressante.

Laser Powder Bed Fusion (L-PBF), an additive manufacturing process, is an effective method for fabricating complex functional parts by using laser beam to melt selectively metal powders layer by layer [1]. Despite advances in-situ alloying by LPBF, optimizing density and homogeneity remains challenging [2]. This study investigates in-situ Ti-Nb alloying through using premixed elemental powders. A three-factor Box-Behnken experimental design was employed, examining the influence of scanning parameters (laser power, scanning speed and hatch spacing) through a large volumetric energy density of 140-326 J/mm³, on density and chemical homogeneity of manufactured samples. Porosity and unmelted-Nb particle rate (I) were quantified from optical micrographs and scanning electron microscopy images via Ilastik software segmentation and Python scripts. An optimal window of the scanning parameters was identified by a response surface methodology (P=165-170W; H=0.049-0.053mm; v=400mm/s) yielding to a low porosity (< 0.4 %) and low unmelted particles (<8 %). Quadratic response-surface models fitted well ($R^2=0.983$ for Φ ; $R^2=0.930$ for I), showing the role of each scanning parameters on the quality of manufactured parts. By first identifying optimized parameters via Design of Experiments and then combining with remelting strategy, this approach efficiently produces high-density and homogenous Ti-Nb parts.

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Titre/Title:

Apprentissage profond pour détecter les joints de grains dans les images MEB en électrons rétrodiffusés

A deep-learning approach for grain boundary detection in SEM backscattered electron images

Auteurs : Pengru Zhao¹, Lionel Germain¹, Frédéric Sur², Nathalie Gey¹, Xavier Le Goff³

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Résumé/Abstract :

Nombreuses propriétés des matériaux sont intimement liées à leur microstructure, ainsi la caractérisation microstructurale est essentielle pour comprendre et optimiser le comportement des matériaux. La taille et la morphologie des grains est traditionnellement mesurée par annotation manuelle (méthode chronophage) ou par des techniques de traitement d'images semi-automatiques qui peuvent être sensibles à des défauts de surfaces ou des inclusions microstructurales et ne peuvent aider si le contraste entre grains adjacents est faible. Les méthodes d'apprentissage profond ouvrent de nouvelles perspectives. Dans cette étude, notre objectif est de développer un réseau de neurones convolutifs pour détecter les joints de grains de micrographies MEB acquises en mode électrons rétrodiffusés. L'approche est appliquée à des images acquises sur des échantillons de dioxyde d'uranium. Nous avons utilisé un modèle UNet à supervision profonde pour améliorer les performances, ainsi que la fonction de perte cDice [1], conçue pour préserver la topologie des joints prédits. La métrique Betti matching error [2] a été choisie pour évaluer le nombre et la position des caractéristiques topologiques. Enfin, notre approche est comparée à la méthode SEraMic [3], fondée sur le traitement d'image, qui exploite plusieurs micrographies MEB acquises en mode électrons rétrodiffusés d'une même région acquise à différentes inclinaisons.

Numerous materials properties are closely related to microstructure, making microstructural characterization essential for understanding and optimizing materials behavior. Grain size and morphology are traditionally measured either by manual annotation (a time-consuming process) or by semi-automatic image-processing techniques that can be sensitive to surface defects or microstructural inclusions and become ineffective when the contrast between neighboring grains is low. Deep-learning methods offer new possibilities. In this study, we intend to develop a convolutional neural network that detects grain boundaries in scanning electron microscope (SEM) images acquired in backscattered-electron (BSE) mode. The approach is applied to images of uranium dioxide samples. We employ a deeply supervised UNet architecture to boost performance and use the cDice [1] loss function to preserve the topology of the predicted boundaries. The Betti matching error [2] is selected to evaluate the number and the position of topological features. Finally, our approach is compared with the SEraMic method [3], an image-processing technique that leverages multiple SEM-BSE images of the same region taken at different tilt angles.

Titre/Title:

Selective hydrogenation of butadiene by single metallic atoms anchored on graphene-based catalysts

Auteurs : *Safouan ZIAT*¹, *Theo BEQUET*¹, *Florian BRIX*¹, *Luc MOREAU*¹, *Bertran KIERREN*¹, *Emilie GAUDRY*¹

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Résumé/Abstract :

Petroleum cracking processes yield highly unsaturated hydrocarbons, which likely poison reactions widely used in the chemical industry. Effective removal of such unsaturated hydrocarbons is crucial, commonly achieved through catalytic hydrogenation. Traditional noble metals are efficient, but lack the desired selectivity. Single metallic atoms anchored on graphene-based catalysts have recently shown excellent performances for such reactions, but a deep understanding of the mechanisms involved has not yet been achieved. In this work, we focus on butadiene hydrogenation because of its practical relevance in industrial processes and the relative simplicity of its mechanism, which is expected to be smoother than that involving more complex molecules, potentially containing oxygen.

In this work, using Density Functional Theory, we have systematically computed adsorption energies of hydrogen, butadiene and butenes on 32 structural models of single atom catalysts consisting of isolated atoms anchored on N-doped graphene systems. Both the support and the active site are modified, by tuning the nitrogen content and the transition metal, and their impact are discussed in relation to the adsorption strength and adsorbate conformation, paving the way to a better understanding of the catalytic activity. Additionally, barriers for hydrogen dissociation have been determined for a reduced number of catalyst models.

These results aim to help the analysis of surface science experiments planned in the group, with scanning tunneling microscopy (STM) and spectroscopy (STS), using samples elaborated by Molecular Beam Epitaxy (MBE). This approach aims to advance our understanding via the comparison of computational results with experimental measurements.

Titre/Title:

Etude du potentiel d'une espèce Bacillus comme agent de cicatrisation des microfissures des bétons

Study of the potential of a Bacillus species as an agent for healing microcracks in concrete

Auteurs : Mathias Lejeune¹, Sébastien Roux¹, Jean-Michel Mechling¹

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Résumé/Abstract :

La pérennité des ouvrages en béton est fortement influencée par leur état de fissuration. La précipitation de carbonate de calcium bio-induite semble être une solution potentielle de réparation des microfissures des bétons. La bio-minéralisation de calcite à partir d'un inoculum d'endospores de Bacillus a été étudiée sur milieu gélosé dans les conditions de culture optimales et son augmentation au cours du temps a été analysé par ATG-ATD. Ce potentiel de bio-minéralisation a ensuite été confirmé sur un milieu gélosé modélisant l'alcalinité des bétons. Enfin la viabilité au cours du temps et la capacité de comblement de fissuration sur pâtes pures de 3 types de ciment a été démontrée.

Titre/Title:

Structure et dynamique des assemblages de nanodisques lipidiques mimétiques de l'apoA-1 en intégrant des données expérimentales et des simulations de dynamique moléculaire
Structural and dynamics of apoA-1 mimetic peptide lipid nanodisc assemblies by integrating experimental data with molecular dynamics simulations

Auteurs : Rohith Ravi¹, Mounir Tarek¹

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² Laboratoire de Physique et Chimie Théoriques-UMR 7019, CNRS, Université de Lorraine, 54500 Vandoeuvre-lès-Nancy, France.

Résumé/Abstract :

Apolipoprotein A-1 (ApoA-1) is the major protein component of high-density lipoproteins (HDL) and plays a critical role in reverse cholesterol transport (RCT) as well as disease progression. Its structure consists of a series of tandem amphipathic helical domains. Based on this structure and helix theory, amphipathic helical peptides were designed as potential therapeutic tools in biomedical applications¹. In particular, we focus on the 14A, 4F, 4FP4F peptides, which have demonstrated superior therapeutic efficacy in animal models of cardiovascular diseases (CVDs) the leading cause of death worldwide. In each year, more than 17.6 million deaths were attributed to CVDs globally. Despite the significance of peptide-lipid nanodisc assemblies in biomedical therapy, there is still a lack of detailed structural, dynamic, and biophysical characterization of these assemblies. To address this gap, we combined small-angle X-ray scattering (SAXS) and nuclear magnetic resonance (NMR)² spectroscopy with molecular dynamics (MD) simulations to validate our models³. Our study characterizes lipid-peptide and peptide-peptide interactions, which play a crucial role in stabilizing nanodiscs, an essential component in lipid metabolism pathways. Our findings will contribute to the future design and development of ApoA-1 mimetic peptide-lipid nanodisc assemblies for therapeutic applications. Keywords: All-atom Molecular Dynamics, Nanodiscs, HDL, Apolipoprotein-A1 mimetic peptides, SAXS, Solid-state NMR.

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Séminaire de l'école doctorale C2MP
Impression : 150 exemplaires
Reprographie centrale UL, Site Montet
rue du doyen Marcel Roubault
54500 Vandœuvre-lès-Nancy
Éditeurs : Comité d'organisation séminaire C2MP 2025
Couverture et affiches : Khaoula CHERKANI
Site du séminaire : ENIM 1 Route d'Ars-Laquenexy, 57070 Metz
le 26 juin 2025

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2 poster sessions

Plenary sessions

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CEA Paris

11h40 - 12h40

Pr Alain Blanchard :

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