This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 857470

NOMATEN
Centre of Excellence in Multifunctional Materials for Industrial and Medical Applications

Book of Abstracts

CoE NOMATEN WINTER SCHOOL 2023

27 – 30th November 2023

National Centre for Nuclear Research
Otwock, Poland

cea

NATIONAL CENTRE FOR NUCLEAR RESEARCH ŚWIERK

VTT

Spis treści

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Foreword

On behalf of the NOMATEN Center of Excellence directorate, we are pleased to welcome you to the 3rd NOMATEN Winter School held on November 28th -30th, 2023, at the National Centre for Nuclear Research in Otwock, Poland.

The third international CoE NOMATEN School will be devoted to understanding the functional properties of materials for industrial applications and novel radiopharmaceuticals for medical applications. CoE NOMATEN School is an internal collaboration event organized annually by different NOMATEN consortium partners (NCBJ, CEA, VTT). The first edition of the school was organized by CEA in Paris, France (2021), while the second event was organized by VTT in Espoo, Finland (2022). It enables team members to exchange knowledge and ideas on new developments and industrial solutions within the NOMATEN project. It is a platform for young scientists to meet with colleagues from other countries and an opportunity to build and strengthen ties between all three nuclear-oriented research institutions. The program of the Winter School 2023 includes topics related to the synthesis of new materials, modeling of materials deformation and radiation damage build-up, as well as material characterization and advanced solutions in radiopharmaceuticals and medical therapies. A rich program of the NOMATEN Winter School includes participation in plenary presentations and thematic sessions realized by experienced researchers, as well as sessions for young scientists and poster sessions. On the last day of the event, presentations of large scientific infrastructures built over past years at NCBJ (Polfel, Neutron diffractometer facility in MARIA Reactor dedicated to structural analysis of materials) and visits to newly established NCBJ Laboratories, including the Materials Research Laboratory, the XRay Lab, and the SEM & TEM Microscopy Laboratories has been planned. In parallel to NOMATEN Winter School, participants will also learn about theoretical and practical methods of intellectual property protection and patenting new scientific solutions as part of the intellectual property rights and protection training, which experts from CEA and VTT will conduct.

The NOMATEN 2023 Winter School is an ideal event for young scientists and PhD students of CoE NOMATEN who want to master basic and advanced materials preparation and characterization methods used in materials engineering. Participants will also learn how to prepare new radiopharmaceuticals and verify the interaction processes of this type of drug with living cells and tissues. The speeches will be delivered by experienced CoE NOMATEN scientists and guests from other Polish scientific institutions (e.g., Warsaw University of Technology, Medical University of Warsaw) who are experts in materials engineering, solid-state physics, and pharmacy. The expected number of participants registered for the 3rd NOMATEN Winter School is 75 people.

"The Book of Abstracts" comprises 29 extended abstracts that have been carefully selected on the basis of a peer review process, potential collaboration areas between NOMATEN participants, and their scientific interests. The authors present both the theoretical and experimental approaches to radiation damage studies, materials manufacture and characterization, and the development of advanced solutions in radiopharmaceuticals and medical therapies. The authors of this year's conference have carried out theoretical discussions, empirical studies, data analyses, and case studies and demonstrated solutions for new medical applications.

On behalf of the conference hosts, we would like to express our gratitude to the members of the NOMATEN Center of Excellence, the host of the event, the National Center for Nuclear Research, the Keynote Speakers, and all the Authors for their effort and willingness, to take part in 3rd edition of the NOMATEN Center of Excellence Winter School. We acknowledge support from the European Union Horizon 2020 research and innovation program under grant agreement no. 857470 and from the European Regional Development Fund via the Foundation for Polish Science International Research Agenda PLUS program grant No. MAB PLUS/2018/8.

We hope that this yearly event will foster the exchange of new ideas and promote new contacts between researchers from CEA, VTT, and NCBJ. We wish you an inspirational and fruitful conference and hope that you will enjoy everything the conference and the beautiful city of Warsaw have to offer.

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NOMATEN Winter School 2023 Topics:

- Synthesis of new materials
- Modeling of materials deformation and radiation damage build-up
- Materials characterization
- Advanced solutions in radiopharmaceuticals and medical therapies

Organizing Commitee:

- **Łukasz Kurpaska** – Functional Properties Group Leader, CoE NOMATEN, NCBJ, Poland
- **Marek Pruszyński** – Radiopharmaceuticals Group Leader, CoE NOMATEN, NCBJ, Poland
- **Paweł Sobkowicz** – Director for Scientific Operations, CoE NOMATEN, NCBJ, Poland
- **Mikko Alava** – Director of CoE NOMATEN Complexity in Functional Materials Group Leader, NCBJ, Poland
- **Jacek Jagielski** – CoE NOMATEN TEAMING Project Coordinator, NCBJ, Poland
- **Chirstopher Gallé** – CoE NOMATEN TEAMING Project Participant, CEA France
- **Frédéric Dollé** – CoE NOMATEN TEAMING Project Participant, CEA France
- **Maria Oksa** – CoE NOMATEN TEAMING Project Participant, VTT Finland
- **Jarosław Jasiński** – CoE NOMATEN Communication Group, NCBJ Poland
- **Monika Madigan** – CoE NOMATEN Communication Group, NCBJ Poland
- **Natalia Cacko** – CoE NOMATEN Communication Group, NCBJ Poland
- **Agnieszka Ślązak-Gwizdała** – CoE NOMATEN Communication Group, NCBJ Poland
- **Barbara Paprocka** CoE NOMATEN Communication Group, NCBJ Poland

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AGENDA OF THE EVENT

DAY 1 – TUESDAY 28.11.2023

7:05 – 7:10 Pick up from the Hotel (Novotel Entrance)

8:00 – 8:30 Arrival to NCBJ, Security Check and Entrance Procedures

(**Remember to bring your passports / ID cards with you!**)

8:30 – 9:00 Registration in the PNT Building, Welcome Coffee

SESSION 1. CENTRE OF EXCELLENCE NOMATEN INTRODUCTION
Chairpersons: M. Pruszyński & Ł. Kurpaska

9:00 – 9:05 Welcome – opening of the school (Director Krzysztof Kurek or Marcin Kardas)

9:05 – 9:10 NOMATEN – the EU Teaming Project – framework of the project and general information, Jacek Jagielski

9:10 – 9:15 The CoE NOMATEN – Presentation of the Centre of Excellence. Objectives and Scientific content of the School, Mikko Alava

9:15 – 9:20 Brief introduction to NCBJ, status of the CoE NOMATEN, Paweł Sobkowicz

9:20 – 9:25 Brief introduction to CEA, Partner of the CoE NOMATEN, Christophe Gallé and Frédéric Dollé

9:25 – 9:30 Brief introduction to VTT, Partner of the CoE NOMATEN, Maria Oksa

9:30–10:15 Invited talk no. 1 CEA – Alain Chartier – *Radiation damages in materials mimicked by Frenkel pairs accumulation*

10:15–11:00 Invited talk no. 2 VTT – Wade Karlsen – *High resolution digital image correlation for advancing the crystal plasticity modelling of nuclear reactor materials*

11:00 – 11:20 COFFEE BREAK

11:20 – 11:30 RG CoE NOMATEN: Complexity in Functional Materials, Mikko Alava

11:30 – 11:40 RG CoE NOMATEN: Materials Characterization, Iwona Jóźwik

11:40 – 11:50 RG CoE NOMATEN: Materials Structure, Informatics and Function, Stefanos Papanikolaou

11:50 – 12:00 RG CoE NOMATEN: Novel Radiopharmaceuticals for Medical Purposes, Marek Pruszyński

12:00 – 12:10 RG CoE NOMATEN: Functional Properties, Łukasz Kurpaska

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12:10 – 12:20 MSCA Project & Corrosion Lab Build up, Katarzyna Leśniak – Ziółkowska

12:20 – 12:30 General Comments and Q&A

12:30 – 13:30 Lunch Break and Discussions

Small rooms at PNT building will be available for internal discussions

SESSION 2. MATERIALS SCIENCE (NUCLEAR)
Chairpersons: Ł. Kurpaska & Ch. Gallé

13:30 – 13:50 Scientist from CEA – Elisa Leoni – *Gas Generation by Radiolysis: from R&D to Safety Assessment*

13:50 – 14:10 Scientist from VTT – Siddharth Suman – *Stress Corrosion Cracking Behaviour of Thermally Aged Alloy 182*

14:10 – 14:30 Scientist from NOMATEN – Sri T. Nori – *Impact of high temperature irradiation on mechanical and structural properties of HEA-ODS alloys*

14:30 – 14:50 Scientist from NOMATEN – Agata Sotniczuk – *NOMATEN toolbox for detecting corrosion phenomena*

14:50 – 15:10 Scientist from CEA – Oscar Sonzogni – *Determination and production of concentrated complex alloys (CCA) CFC/CC resistand to the specific conditions of molten salt nuclear reactors (MSR)*

15:10 – 15:30 Scientist from NOMATEN – Przemysław Kot – *Neutron diffraction study of phase stresses in Al/SiCp composite during tensile test*

15:30 – 16:00 COFFEE BREAK

16:00 – 16:20 Scientist from NOMATEN – Tymofii Khvan – *Understanding radtiation damage resistance of RAFM steels by experiments and simulations*

16:20 – 16:40 Scientist from NOMATEN – Damian Kalita – *Impact of He and Ni-ion irradiation on the performance of bcc-type HEA WtaTiV case study*

16:40 – 17:00 Scientist from other IPPT – Tomasz Mościcki – *Theoretical and experimental studies of superhard W-Ti-B coatings deposited using the HiPIMS method*

17:00 – 17:20 Scientist from NOMATEN – Magdalena Gawęda – *Amorphous silicon oxycarbide-based protective coatings for nuclear applications*

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SESSION 3 PhD MT180 (ORAL) SESSION

Chairpersons: F. Dollé and Ł. Kurpaska

The list of contributors is accessible at the end of the document (page 82).

18:20 – 18:25 Departure from the NCBJ directly to the Restaurant

19:15 Welcome Dinner – STREFA Restaurant, Próżna St. 9, 00-107 Warsaw

DAY 2 – WEDNESDAY 29.11.2023

7:05 – 7:10 Pick up from the Hotel (Novotel Entrance)

8:00 – 8:30 Arrival to NCBJ, Security Check and Entrance Procedures / Welcome Coffee

(**Remember to bring your passports / ID cards with you!**)

SESSION 4. MATERIALS SCIENCE (NON-NUCLEAR)
Chairpersons: M. Alava & M. Oksa

8:30 – 8:50 Scientist from CEA – Eloi de Villoutreys de Bringac – *Phase equilibria and solubility limits in the (Ce, Nd)-Fe-B system for new substituted permanent magnets*

8:50 – 9:10 Senior scientist from VTT – Mikko Vepsäläinen – *Electrochemical synthesis of metal-organic frameworks (MOFs)*

9:10 – 9:30 Scientists from NOMATEN – Javier Dominguez & Amil Aligayev – *2D Materials Catalysis: A Multiscale Quantum Chemistry Approach for Hydrogen Production from CH_4,CO_2 Purification, and Gas Splitting Applications*

9:30 – 9:50 Scientist from NOMATEN – Dario Massa – *Alloy informatics through Ab-initio Charge Density Profiles*

9:50 – 10:10 Scientist from WUT – Jan Wróbel – *DFT based modelling of high entropy alloys*

10:10 – 10:40 COFFEE BREAK

10:40 – 11:00 Scientist from NOMATEN – Kamran Karimi – *Multi-scale modelling of mechanical deformation in chemically complex alloys: a material informatics approach*

11:00 – 11:20 Scientist from NOMATEN – Maciej Ryś – *Modelling of size effects in spherical indentation of a single crystal*

11:20 – 11:40 Scientist from NOMATEN – Karol Frydrych – *Modelling spherical and Berkovich nanoindentation using the crystal plasticity finite element method*

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11:40 – 12:00 Scientist from NOMATEN – Amin Esfandiarpour – *Design of Multicomponent Alloys Based on Lattice Distortion, Short-Range Order, and Core Dislocations*

12:00 – 13:00 Lunch Break and Discussions

Small rooms at PNT building will be available for internal discussions

SESSION 5. RADIOPHARMACEUTICALS SCIENCES
Chairpersons: M. Pruszyński & F. Dollé

13:00 – 13:30 Bożena Sikora – Institute of Physics, Polish Academy of Sciences – *Multifunctional opto-magnetic nanoparticles with upconverting properties – designing, synthesis and applications in cancer diagnostic*

13:30 – 14:00 Joanna Giebułtowicz – Faculty of Pharmacy, Warsaw Medical University – *Application of metabolomics in pharmacy*

14:00 – 14:20 Izabela Cieszykowska – POLATOM / NCBJ – *CERAD project and 30 MeV cyclotron for medical isotope production in Poland*

14:20 – 14:40 Karolina Zajdel – NOMATEN / NCBJ – *Radiolabeling of up-converting nanoparticles for theranostic applications*

14:40 – 15:00 Marcin Zieliński – NOMATEN / NCBJ – *Differences in the biological response of MCF-7 breast cancer cells and heathy MCF-12A breast cells in conventional and ultra-high dose rate radiation therapy*

15:00 – 15:30 COFFEE BREAK

15:30 – 15:50 Scientist from CEA/Joliot – CAILLE Fabien – *Late-stage carbon-11 radiolabeling directly from carbon dioxide: from chemistry to drug PET imaging*

15:50 – 16:10 Scientist from CEA/JOLIOT – HUVELLE Steve – *Development of radiochemical tools for PET imaging of HIV infection*

16:10 – 16:30 Scientist from CEA/JOLIOT – HECK Marie-Pierre – *New multivalent scaffolds for anions and radioanions binding*

SESSION 6 PhD POSTER SESSION
Chairpersons: Ch. Gallé & Ł. Kurpaska

Posters accessible at the end of the document (page 112).

18:00 – 18:05 Departure from the NCBJ to Warsaw

19:00 – Free Time

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DAY 3 – THURSDAY 30.11.2023

7:05 – 7:10 Pick from the Hotel (Novotel Entrance)

8:00 – 8:30 Arrival to NCBJ, Security Check and Entrance Procedures / Welcome Coffee

(**Remember to bring your passports / ID cards with you!**)

VISITS TO NCBJ LABORATORIES
Organized by: R. Mikołajczak, P. Nowakowski, I. Jóźwik and Ł. Kurpaska

8:30 – 9:15 POLFEL Project Status & Neutron Irradiations in MARIA Reactor

9:15 – 9:30 Organization of the groups – Coffee Time

9:30 – 12:00 Visits, detailed information will follow

Group #1: NOMATENs SEM/TEM and XRD Laboratory (1 hour)

Group #2: Materials Research Laboratory (1 hour)

12:00 – 13:00 LUNCH

13:15 END OF THE SCHOOL

CLOSING REMARKS JACEK & MIKKO + ŁUKASZ & MAREK

13:30 Transportation to the Chopin Airport (Planned arrival to the Airport ca. 14:20)

13:30 NOMATEN IPR WORKSHOP – PATENT LANDSCAPE ANALYSIS
Chairpersons: M. Oksa, E. Jutila, M. Simons, P. Sobkowicz and Ł. Kurpaska

AGENDA
Online connection via GoTo Meeting Platform:
https://meet.goto.com/NCBJmeetings/patent-landscape-analysis-for-high-entropy-alloys

13:30 – 13:35 Introduction by P. Sobkowicz and M. Simons

13:35 – 14:25 Presentation of Patent Landscape by E. Julita

14:25 – 14:40 Discussion

14:40 – 15:00 Break

15:00 – 15:40 Group Work with by E. Jutila, M. Oksa, M. Simons and J. Järvenpää

15:40 – 15:50 Conclusions

End of the Workshop
Transportation to the Chopin Airport (Planned arrival to the Airport ca. 17.00)

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CoE NOMATEN Winter School 2023 Presenters

Biographies and Abstracts

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SESSION 1. CoE NOMATEN INTRODUCTION

Jacek Jagielski

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National Centre for Nuclear Research
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Professor Jacek Jagielski studied at the Faculty of Technical Physics and Applied Mathematics at the Warsaw University of Technology.In 1991, he received a Ph.D. title at the Institute for Nuclear Problems. In 1997 he obtained the title of doctor habilitatus (D.Sc.) in physical sciences, and in 2007 the title of professor granted by the President of Republic of Poland.

His research activities are connected to modification of materials using ion beams, material analysis, development of damage accumulation model (MSDA) and Monte Carlo simulations for quantitative analysis of defects in materials. He worked mainly on the use of ion beams for modification and analysis of materials: mechanical properties of metals, modification of polymers and ceramics, accumulation of defects in materials. In his work he combined theoretical topics with engineering, e.g. construction of three implanters or the construction of elements of the W7X stellarator.

Professor Jagielski has worked in many centers abroad, mainly in France, USA, Germany, Slovenia, Austria, South Africa and Japan. He published over 280 papers cited about 5000 times. His Hirsch index is 32 (Scopus) or 36 (Scholar). Co-author of eleven patents and patent applications. Directed four doctoral dissertations, one of them carried out in a co-tutelle system with CEA/Univ. Aix Marseille), and coordinated three European projects being involved in six more. He lead various research grants including multinational cooperations such as NATO Science for Peace, Coordinated Research Project by IAEA, Batelle in EMSL/PNNL Richland, WA USA and numerous bilateral projects. In 2018, NOMATEN project coordinated by prof. Jagielski was approved as Teaming for Excellence action.

Professor Jagielski currently holds the position of the director of the Materials Physics Department at the National Center for Nuclear Research in Świerk. He is an elected member of the Boehmische Physical Society (Los Alamos, USA) and an elected member of International Scientific Committees of Ion Beam Analysis and Ion Implantation and Other Applications of Ions and Electrons. He served as a referee in numerous scientific journals. Professor Jagielski is also an expert of French EMIR network of accelerators and an expert of HCERES, French organization responsible for the evaluation of scientific institutions.

Awarded with the Meritorious Medal for Mazovia, he is also an Officer of the French Order of Academic Palms.

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Mikko Alava

Director of Centre of Excellence NOMATEN
Complexity in Functional Materials Group Leader
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Professor Mikko Alava is a world-class expert in the physical properties of materials and their dependence on structure, including transport properties. He has worked extensively on materials science data analytics and applications of modern machine learning approaches. Mikko Alava holds a PhD in nuclear engineering (Helsinki University of Technology) in fusion plasma physics, from 1993. He is since 2009 a full professor of physics at Aalto University, Finland. Mikko Alava has worked after a research direction change from fusion to materials on statistical physics applications to the physics of materials and on challenging computational problems in understanding fracture, friction, plasticity and other complex properties, typical of functional materials and their dependence on structure – defects, surfaces and so on.

Lately, for 2012-17 he has been in Finland a vice-director of a national Center of Excellence in Computational Nanoscience (COMP) and he has extensive international science manage experience eg. from the European CECAM organization and others. The scientific achievements of the Director of the NOMATEN include over 250 scientific papers including 40 in first rate journals such as Science Advances, Nature Communications, PNAS, and Physical Review Letters. Professor Alava has supervised more than 20 PhD students and more than 20 post-docs, many of which occupy academic positions around world.

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Paweł Sobkowicz

Director for Scientific Operations of Centre of Excellence NOMATEN
National Centre for Nuclear Research
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Paweł Sobkowicz holds a PhD in theoretical physics. Between 1982 and 1993 he worked at the Institute of Physics, Polish Academy of Sciences. Since 1993 he has left the academic world and has been a member of management teams of several high-tech companies, both international and Polish. In 2012 he has joined the National Centre for Nuclear Research, with the task of managing the technology transfer processes and management of commercialization efforts, becoming in 2017, the Deputy Director for Innovation and Commercialization of the institute.

The experience gathered during the 20 years of commercial career covers many aspects, including human resources management, financial planning, sales management and general understanding of the decision processes in commercial environments. It is especially important in the context of efficient cooperation between the research communities and industry – the differences in language which is used by both communities is one of the most important factors slowing down or inhibiting successful commercialization. This experience complements the understanding of methods typical for research processes, with their inherent risks and uncertainties, as well as practical aspects of doing science.

In addition, he has returned to active research, using tools of statistical physics to describe complex social phenomena. In recognition of this work he has obtained the habilitation (D. Sc.) degree in 2016. Author of over 60 papers, cited over 500 times. Since 2018 Dr Sobkowicz is the Scientific Operations Director of the NOMATEN Centre of Excellence and the leader of the Industry Liaison Group

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Christophe Gallé

Centre of Excellence NOMATEN TEAMING Project Participant
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Christophe GALLÉ obtained in 1991 a PhD in Ingineering Geology at the Paris National School of Mines. In 1992, he joined the CEA Energy Division (DES) to work as a researcher for the nuclear waste management issue in strong relationship with French national companies dealing with nuclear energy (EDF, ANDRA, FRAMATOME). After a an year stay in Japan (1995) working at JAEA in a the framework of a CEA/JAEA agreement, he has been leading (from 2002) a research laboratory dedicated to research on the use of cementitious and clayed materials for nuclear deep disposal.

He became project leader in 2011 for several basic research programs dedicated to the behaviour of metallic alloys and polymers under irradiation and thermal solicitation in the context of Gen2&3 reactors lifespan extension and the development of new materials for gen IV sodium fast reactors (ASTRID). He has been the project leader of the CEA/DES Centre of Excellence for Nuclear Materials, MINOS, for 10 years. He obtained the HDR (Habilitation à Diriger des Recherches) from the University of Toulouse III in 2011. He published and/or was associated to around 20 articles in peer review journals. During these last few years, he has been involved in two main EU projects, TEAM-Cables (2017-2022, #755183), ENTENTE (2020-2024, #900018) and NOMATEN (2019-2026, #763604), in which he coordinates WP6 dealing of the capacity building programme of the NOMATEN CoE. In joined mid-2022, the head of Department of Materials, Physics and Chemistry of ISAS Institute (Institute of Applied Sciences and Simulation for low-carbon energy) at CEA Saclay, as Innovation and partnership assistant.

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Frédéric Dollé

Centre of Excellence NOMATEN TEAMING Project Participant
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Frédéric Dollé completed his PhD (organic chemistry) in 1991 from Strasbourg University (France). He then moved to Research Triangle Park, North Carolina, USA, to work for a pharmaceutical company (Rhône-Poulenc-Rorer, today SANOFI) for two years, before joining in 1993 the CEA and the Service Hospitalier Frédéric Joliot (Orsay, France). In 2000, he completed his HDR degree (habilitation à diriger des recherches, Paris-South University), and from 2000 to mid-2014, he was at Orsay in charge of the Chemistry / Radiochemistry section, a unit which supported all PET molecular imaging programs within the institute, before coordinating for another year, the newly created "Molecular Probes" team (as part of IMIV - Imagerie Moléculaire In Vivo - UMR1023), now also dealing with metabolism-related activities.

For over 20 years, his research interests have focused on the development of radiotracers for *in vivo* molecular imaging using PET, as well as the development and application of novel methods for the synthesis of 11C/18F-labelled probes (225 scientific publications, 12 book chapters, 7 patents – 1 licensed). In 2015, he joined the governing board level of his institute (at this time, Institut d'imagerie biomédicale (I2BM)) as scientific assistant to the director, also in charge of the relations with the newly created Paris-Saclay University. In February 2017, I2BM and IBITEC-S - another CEA institute - merged into a novel structure - Institut des sciences du vivant Frédéric Joliot - in which he is also today in charge of the doctoral (PhD) program and the CEA expertise hub / career development program. Appointed Director of Research at CEA (2021), he is still involved in EU projects, notably the CSA action (teaming) NOMATEN (2019-2026, #763604), in which he coordinates WP6 actions when Radiopharmaceutical Sciences are concerned.

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Maria Oksa

Centre of Excellence NOMATEN TEAMING Project Participant
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Dr Maria Oksa is Senior Scientist and Project Manager at VTT, with PhD degree from Aalto University on Materials Science. Dr Oksa has an extensive experience on research and development on advanced structural and coating materials for extreme conditions and high temperature applications, including material design, corrosion and mechanical testing, failure analysis, material characterization and lifetime management. She has acted as Team Leader, coordinated development of research services, contributed to several project preparations and scientific papers and she is the contact point on energy research to VTT's strategic collaboration partners.

She has also worked closely with the European Energy Research Alliance EERA, worked in the Secretariat and lately supported work with the SET Plan facilitation. Her research interests are on green transition and materials development to support the transition. Dr Oksa has strong experience on EU and national projects as coordinator, project manager and Work Package leader. Currently she is the coordinator of PREDIS project (https://predis-h2020.eu/). She is the project manager at VTT for the NOMATEN Teaming project and belongs to the project's Steering Committee and General Assembly.

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Łukasz Kurpaska

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Dr Łukasz Kurpaska studied at the Faculty of Material Science and Ceramics AGH University of Science and Technology in Cracow. In 2012, he received a Ph.D. title at the University of Technology of Compiegne, France. In 2019, he obtained the title of doctor habilitus (D.Sc.) in material engineering and a professors position at NCBJ. He is a Head of the Materials Research Laboratory (MRL) and a Research Group Leader at the NOMATEN Center of Excellence in the National Center for Nuclear Research (NCBJ). In his works, he mainly dealt with the structural and mechanical properties of ion-modified materials and the effect of high-temperature corrosion. He co-authored over 70 journal papers cited over 900 times (H – 18). He has been a director and manager of several projects funded by Polish agencies (FNP, NCBiR, MEN), IAEA, and EC. He received prestigious scholarships from the Ministry of Science and Higher Education in 2017, the French Embassy in Poland in 2014 and 2016, and the Fulbright Commission.

He works actively in the EERA JPNM (European Energy Research Alliance Joint Programme on Nuclear Materials) platform. He was a coordinator from the Polish site of three H2020 projects (M4F – Multiscale modeling for fusion and fission materials, GEMMA – Generation IV Materials Maturity and SafeG - Safety of GFR through innovative materials, technologies and processes) and one project funded in the frame of Horizon EUROPE calls; INNUMAT – Innovative Structural Materials for Fission and Fusion. He has been involved in preparing the NOMATEN project, approved by the European Commission. This project aims to create a new Centre of Excellence in Poland with strategic partners: CEA France and VTT Finland. He is involved in a project related to HTR technology, financed by the Ministry of Education. The project aims to rebuild MRL capabilities in testing materials for next-generation nuclear reactors. He is working with a number of Polish accreditation and certificate institutions, such as the Polish Center for Accreditation, Technical Inspection Authority, and Office of Nuclear Regulation. In 2021, he was elected a member of the scientific council of NCBJ. MRL is the only laboratory in Poland equipped with a set of 12 Hot Cells able to handle radioactive materials.

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Marek Pruszyński

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Dr. Marek Pruszyński studied chemistry (MSc specialization in analytical chemistry) at the Faculty of Biology and Chemistry at the University of Białystok in Poland. Since 2003, he works at the Institute of Nuclear Chemistry and Technology in Warsaw, where in 2008 he obtained PhD degree (specialization radiochemistry), and in 2019 doctor habilitus (DSc) and became Head of the Laboratory of Radiopharmaceuticals and Cellular Research. Since May 2021, he is an Associate Professor at the National Centre for Nuclear Research (NCBJ) in Świerk-Otwock and a Research Group Leader of the Novel Radiopharmaceuticals for Medical Application group at the NOMATEN Centre of Excellence at the NCBJ.

His research interest focuses on design and synthesis of theranostic molecular radiopharmaceuticals for targeted personalized medicine via: i) exploring new production routes of commercial and also potentially applicable new radionuclides in research reactor (Maria) and soon installed at NCBJ (CERAD centre) IBA Cyclone XP 30 cyclotron; ii) target's material preparation and its irradiation in reactor or cyclotron, radiochemical separation of interested radionuclide and target material recovery; iii) labeling of biomolecules (monoclonal antibodies and their fragments, peptides etc) with radionuclides via chelators or prosthetic groups; iv) development of multimodal nanomaterials for diagnostic and therapeutic applications in medicine; v) preclinical in vitro and in vivo evaluation of developed compounds and materials.

He co-authored over 30 full length journal papers (with IF) cited over 1100 times (H – 18). He has been also Principal Investigator of several projects funded by Polish agencies (NCN, NCBiR, NAWA), bilateral with Belgium and Czech Republic, as well as IAEA and EU COST. He received prestigious scholarships and awards from the Fulbright Commission, IAEA, Grzegorz Białkowski Award and Alavi-Mandell Award from the Society of Nuclear Medicine and Molecular Imaging for the article published in Journal of Nuclear Medicine (2014). He visited and worked for few months in several scientific institutions, including Institute of Nuclear Physics in Cracow and Institute of Organic Chemistry in Warsaw both Polish Academy of Sciences, JRC Karlsruhe, Joint Institute for Nuclear Research in Dubna, Institute of Nuclear Physics in Řež of the Academy of Sciences of the Czech Republic, Institute of Nuclear Chemistry at the Johannes Gutenberg University in Mainz, In Vivo Cellular and Molecular Imaging Laboratory at the Vrije Universiteit Brussel, Preclinical Molecular Imaging Laboratory at the Institute of Cancer Research in London. He was working for 3 years (2010-2013) as a post-doc at Prof. Michael Zalutsky's Group at Duke University Medical Center in Durham, North Carolina, USA. He is a member of the Polish Nucleonic Society, Polish Chemical Society and European Society of Molecular Imaging. He has supervised 5 MSc and BSc students, 4 PhD students and 2 post-docs.

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Iwona Jóźwik

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Dr. Iwona Jóźwik completed her studies in physics, earning a master's degree with distinction from the University of Maria Curie-Skłodowska in Lublin, Poland in 2001. In 2006, she successfully defended her Ph.D. in physics at the Faculty of Applied Physics and Mathematics of the Gdańsk University of Technology in Gdańsk, Poland. From 2001 to 2008, she worked at the Institute of Physics, Lublin University of Technology in Lublin, Poland. Since 2008, she has been employed at the Lukasiewicz Research Network – Institute of Microelectronics and Photonics in Warsaw, Poland (formerly known as the Institute of Electronic Materials Technology). In 2012, she received a stipend from the Ministry of Science and Higher Education in Poland in recognition of her outstanding work as a young scientist under the age of 35. In 2017, she joined the National Center for Nuclear Research in Świerk-Otwock, Poland.

She specializes in scanning electron microscopy (SEM) and sample preparation using focused ion beam (FIB) techniques. Her research interests encompass the application of low-energy scanning electron microscopy to directly visualize damage in ion-irradiated materials. She has an extensive publication record, with more than 90 scientific papers, an h-index of 17, and 926 citations according to Scopus. Starting in 2008, she has been a regular representative of Ł-IMIF (formerly ITME), and since 2017, she has represented also NCBJ at conferences, technical meetings, and in negotiations with industrial partners. She has been involved in collaborative projects with various research centers, including the Centre de Spectrometrie Nucleaire et de Spectrometrie de Masse in Orsay, France; the Laboratoire de Physico-Chimie des Matériaux Luminescents at the Université de Lyon 1, France; the Environmental Molecular Sciences Laboratory at Pacific Northwest National Laboratory in Richland, WA, USA; the Centre for High-Resolution Transmission Electron Microscopy at Nelson Mandela University in Port Elizabeth, South Africa; and the Helmholtz-Zentrum Dresden-Rossendorf e.V. (HZDR) in Germany. She has coordinated several scientific projects funded by the National Science Centre and has also been involved in numerous national and international research projects as the Primary Investigator. She led a Work Package in the international project NOMATEN during Phase 1 of the Teaming For Excellence EU project from 2019 to 2021. She continued her involvement in NOMATEN MAB+ as the Principal Investigator, responsible for characterization using scanning electron microscopy and related techniques, and in NOMATEN Teaming. Currently, she holds the position of Leader of the Materials Characterization Research Group at NOMATEN CoE, NCBJ, Poland.

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Stefanos Papanikolaou acts as a Habilitated Professor and Research Group Leader of the Materials Structure, Informatics and Function (MASIF) Group, in the NOMATEN Center of Excellence for Multifunctional Materials in the National Center for Nuclear Research in Poland. His BSc is in Physics from the National University of Athens. His MS and PhD degrees are in Physics from the University of Illinois, Urbana-Champaign. He performed his postdoctoral work in the Department of Physics at Cornell University, and then he held positions at Yale University, Johns Hopkins University and West Virginia University. Papanikolaou won the internationally competitive 5-year VIDI excellence grant by the Netherlands research council in 2013 and a research excellence award in 2018. His research interest is in materials informatics and machine learning. Prof. Papanikolaou has received his habilitation in Poland since 2022.

He actively works on fusion-related materials science, simulations and machine learning. Papanikolaou has been at the forefront of the international research community in the field of materials science and micromechanics of advanced alloys and specifically, crystal plasticity, especially in the context of stochastic aspects and non-linear dynamical phenomena. Having a strong background in theoretical condensed matter physics, statistical mechanics and strongly correlated electron phenomena, he represents an ideal upcoming world leader of the ever emerging Materials Informatics field in materials science. An example of such leadership has been the organization of the 1st Materials Informatics conference in Warsaw, Poland, in 2022, at the NCBJ premises, first of its kind in Poland. He has also published numerous manuscripts in machine learning aspects of crystal plasticity. Papanikolaou leads the MAterials Structure, Informatics and Function (MASIF) group at the NOMATEN CoE, and leads the materials informatics research at NCBJ and in Poland. He has 80+ peer-reviewed publications, including more than 20 in machine learning aspects, with 2000+ total citations, and publications in high impact journals such as Nature, Nature Physics, Materials&Design, npj Comput. Materials, Scripta Materialia etc.. The MASIF group has 5 doctoral students, 3 postdoctoral associates and 2 machine learning experts. Papanikolaou received his Bachelors from Athens, Greece, and then his Physics Masters and Doctoral degrees at the University of Illinois in USA, and then developed a materials science and engineering career in USA, with the focus on statistical and stochastic aspects in mechanical deformation of advanced alloys. The MASIF group has been funded by multiple funding agencies, including NSF (Materials) (2017-2020), DOE (Basic Energy Sciences, 2016-2019) and AFOSR (2015-2017) in USA, as well as NWO in Netherlands (Vidi grant, 2013-2018).

He received the 2018 WVU award for excellence in tenure-track research. Papanikolaou is currently writing a book on Materials Informatics Methods and Applications, towards future graduate students in Materials Science and Engineering programs. Finally, professional service and recognition has been evidenced through chairing and organizing the first materials informatics conference in Poland last summer (2022), has organized more than 20 symposia in major conferences, has been involved in the leadership of major regional (ASEE-NCS) and national (MRS) societies, and being on the editorial board of three peer-reviewed journals (Mat.Theory, J. Mechanics, Frontiers in Physics). He is currently one of four selected Associate Editors of Materials Theory at Springer/Nature, and one of six Associate Editors of Frontiers in Physics -- Condensed Matter Physics at Frontiers.

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Invited Speakers

Alain Chartier

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Dr Alain Chartier studied at the University of Paris XI in Orsay, and received his PhD title in 1999. He obtained his accreditation to supervise research (HDR) in 2010. He is currently Research Director in material sciences at CEA-Saclay. His researches deal with atomic scale modeling and simulations in three domains: radiation damages in materials, and recently corrosion and geopolymers. He published more than 80 papers cited over 1800 times (h-index 28).

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Radiation damages in materials mimicked by Frenkel pairs accumulation

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Molecular dynamics simulation of radiation damages in materials frequently refer to studies in which displacement cascades, threshold displacement energies and sometimes, thermal spikes are performed. Each of these techniques are meant to address the primary damage – i.e. single events – produced by electronic loss and/or ballistic interactions. Recent attempts have tried to explore the effect of the irradiation dose by accumulating these single events. However, this demarche is limited to low doses since very cpu demanding. One may circumvent single events and access higher doses – in some specific cases – by shortcutting part of the story. Instead of repeating 'single event' one after the other to get the effect of dose, the final state can be used as a starting point.

Here, we show that as long as single events end up with point defects or very small clusters, it is convenient to accumulate point defects to reach doses up to 10 dpa or more [1]. Such a simulation procedure offers great potential for understanding complex mechanisms at work when materials are in severe irradiation environments. For example, one can (i) identify the specific defect responsible for amorphization in titanate pyrochlores [1], (ii) shed light on the wrinkling responsible for the anisotropic swelling in graphite [2], (iii) exhibit Frank loops as part of the monitoring mechanism for UO_2 lattice swelling [3], (iv) while voids/vacancies are responsible for volume swelling in MgO [4], (v) evidence that C15 clusters are seeds for both ½ <111> and <100> loops in iron [5], (vi) support the finding that A15 clusters too are seeds of loops in fcc metals [6] and (vii) that oriented loops under irradiation and stress are related to preferential nucleation rather than differential growth [7].

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Dr. Wade Karlsen is a Principal Scientist at VTT Technical Research Centre of Finland. where he also serves as the Technology Manager for the new VTT Centre for Nuclear Safety hot laboratory facilities. He was granted a Ph.D. in Materials Science and Engineering from the Oregon Graduate Institute of Science and Technology, U.S.A. (now Portland State University) in 1997.

He then took a post-doctoral research scientist position in the Laboratory of Engineering Materials of Helsinki University of Technology (now Aalto) in Finland. In 2004 he joined VTT's nuclear materials research group, focused on nuclear power plant materials degradation due to environmental effects, thermal aging and neutron irradiation. His primary specialty is in analytical transmission electron microscopy, particularly of radiation defects and radiation-induced segregation. In his role as Technology Manager he is familiar with the utilization of mechanical testing, autoclave exposure and bellows-driven special mechanical testing devices for study of materials performance, particularly of neutron-irradiated materials in the hot cell environment.

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High resolution digital image correlation for advancing the crystal plasticity modelling of nuclear reactor materials

Dr KARLSEN, Wade; VTT Technical Research Centre of Finland, Ltd.
Dr LINDROOS, Matti; VTT Technical Research Centre of Finland, Ltd.
Dr SOARES, Guilherme; VTT Technical Research Centreof Finland, Ltd.

The plastic behavior of irradiated materials used in nuclear reactors can be modelled by describing it via constitutive equations capturing the important contributing factors. To reflect the microstructural context, the flow stress must be decomposed into its fundamental components associated with the microstructure features peculiar to the particular steel, such as carbides, the dislocation network, deformation confinement inside grains, and strain localization in cleared channels. To study strain localization in particular, at VTT we are developing high resolution digital image correlation techniques for employment with in situ tensile testing in the SEM chamber, to capture the manifestation of the local deformation behavior on a sub-grain scale. The captured images are quantified, and the results are then employed to improve, parameterize and verify the crystal plasticity modelling approach VTT is employing for grain scale calculations as part of the overall multiscale modelling approach.

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SESSION 2
MATERIALS SCIENCE (NUCLEAR)

Elisa Leoni

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After a Master Degree in Chemistry, Elisa LEONI obtained her joint PhD Thesis in Material Sciences from the University of Milan (IT) and the University of Marseille (FR). Her research post-doctoral work at the French Alternative Energies and Atomic Energy Commission – CEA, was focused on *"The effect of Radiolysis on the corrosion of stainless steel"*.

She, then, joined Orano (formerly AREVA) as R&D Project Manager where she worked on R&D Programs in support to the safety demonstration of Intermediate Level Long lived (IL-LL) waste: design, specifications of waste packages and licensing process. Her technical expertise was mainly focused on radiolysis and corrosion issues related to the radioactive waste management. After ten years as Technical Expert, she moved to the department in charge of the definition of the waste management strategy of Orano's legacy IL–LL Waste to be disposed of in the deep geological disposal (Cigéo). In this framework she was involved in different international working groups such the IAEA's Technical Working Group on Radioactive Waste Management and Technologies –WATEC.

She, then, joined the Institute for Radiation Protection and Nuclear Safety (IRSN) (the French Technical support Organization to the Regulator) both as technical expert and coordinator of the WP – ROUTES of the EURAD H2020 Project (Homepage | Eurad (ejp-eurad.eu)) – European Joint Program on radioactive waste management. In 2022 she moved back to CEA where she is now the Head of the Laboratory of Radiolysis of Organic Matter (LRMO) whose research activity is mainly focused on the effect of the irradiation on polymeric materials.

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Gas Generation by Radiolysis: from R&D to Safety Assessment

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Radiolysis is ubiquitous throughout all aspects of a nuclear fuel cycle. Radiolysis may promote the chemical transformation of molecules and materials with the formation of potentially degradation products and corresponding changes in physical and chemical properties. One of the major safety concern related to radiolysis is gas production. Gas production shall be assessed at each step of the nuclear cycle: from reactor operations to radioactive waste management.

In the first part of this talk, an overview of fundamental phenomena related to radiolysis of aqueous solutions and organic matter and the safety concerns related to the associated gas production will be presented.

Then the presentation will be focused on the R&D conducted at CEA in support to safety assessment, especially in the field on nuclear waste management. The safety assessments rely both on experiments specifically designed to obtain radiolytic yields as function of the particle nature (α, β/γ), dose and dose rate, temperature and atmosphere (oxidizing or not) (see Fig. 1) . The main results of the R&D conducted in the last decade will be presented together with the ad hoc simulation tools developed to calculate gas production [2-3].

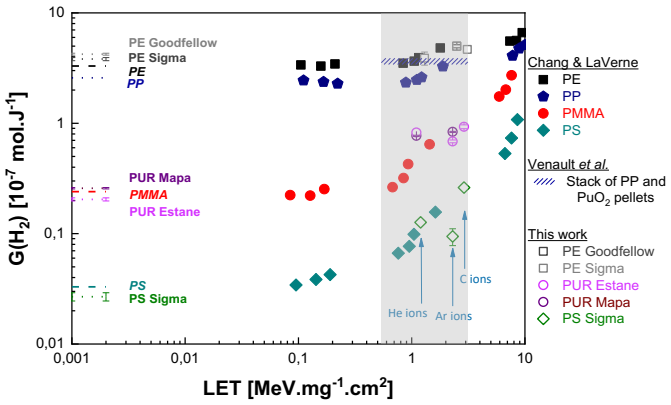

Figure 1 Hydrogen radiolytic yields as function of LET (Linear Energy Transfer) for different types of polymers irradiated under inert atmosphere. Figure reproduced from [1] (copyright 5427670663720)

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Dr. Siddharth Suman obtained Ph.D. in Mechanical engineering from Indian Institute of Technology, India. He is presently working as a research scientist at Centre for Nuclear Safety, VTT Technical Research Centre of Finland, Finland. He was also Marie Skłodowska-Curie Actions Fellow in the Department of Nuclear Energy and Safety, Paul Scherrer Institute, Switzerland. His research was focused on 'Experimental evaluation of synergistic effects of irradiation, hydrogen, and high temperature on the fracture behaviour and stress corrosion cracking of nuclear Reactor Pressure Vessels steels'.

As an independent researcher, he explores multifaceted aspects of sustainable energy especially, but not exclusively, solar-thermal conversion, hybrid nuclear-renewable integrated energy systems, artificial intelligence in energy systems, pink hydrogen, multi-scale modelling of hydride embrittlement. In collaboration with different scientists across the globe, primarily India, research is focused on Additive manufacturing of Biomaterial, Multi-scale modelling of hydrogen embrittlement, Laser machining of anisotropic material like Glass fiber reinforced polymer, Optical solar reflector, Application of artificial intelligence for engineering applications, Heat transfer in Non-Newtonian Fluids. Dr. Suman has published well acknowledged articles in international journals and has featured in the 'World's Top 2 % Scientists' list released by Stanford university since 2021.

He has also been conferred Young Scientist award twice by the Venus International Foundation, and the Society of Aeronautical Engineers. He has been invited to deliver guest lectures by various educational institutions to popularize sustainable energy. He has also completed one year training program in scientific journalism and write for various media houses to communicate science and develop scientific temperament among masses.

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Stress Corrosion Cracking Behaviour of Thermally Aged Alloy 182

SUMAN, Siddharth; VTT Technical Research Centre of Finland

To understand the effects of long-term thermal ageing on stress corrosion cracking (SCC) of alloy 182 in nuclear power plants, thermal ageing of as-welded alloy 182 was performed at 400 °C for 800 h, 2400 h, and 5500 h. Stress corrosion cracking initiation as well as crack growth tests were conducted in hydrogenated hightemperature water. SCC initiation was not affected by thermal ageing, but the number of tests were too low to make statistically sound conclusions. The SCC crack growth rates were moderately lower in thermally-aged samples. However, the differences in growth rates were diminishing with more aggressive testing conditions (higher temperature and KI). There is thus no evidence for adverse effects of thermal aging on SCC in Alloy 182 in long-term operation.

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Dr. Sri Tapaswi Nori received his Ph.D. in 2021 from Purdue University, USA. He worked on the three-dimensional characterization of high-temperature ultra-fine precipitate strengthened steel following neutron irradiation. He later joined the NOMATEN Centre of Excellence, National Centre for Nuclear Research (NCBJ), as an Assistant Professor, where he is currently working. His research is focused mainly on the assessment of microstructure and mechanical properties of structural materials such as the concentrated solid solution alloys for nuclear applications.

He is experienced in material characterization via techniques such as scanning and transmission electron microscopy and synchrotron X-ray-based diffraction and spectroscopy. He won several research grants such as the ESTEEM3 project, Nuclear Science User Facilities Rapid Turn-Around Experiment, and Center for Integrated Nanotechnologies user proposal.

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Impact of high-temperature irradiation on mechanical and structural properties of oxide dispersion strengthened-concentrated solid solution alloys

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In the past few years, oxide dispersion strengthened (ODS)-concentrated solid solution alloys (CSAs) emerged as potential structural materials for Gen. IV nuclear reactors. The alloys can possess the best radiation resistance even at high temperatures (>400°C) as demonstrated in the limited studies [1, 2]. However, there is a lack of comprehensive understanding of the effects of high-temperature irradiation on the structural and mechanical properties of ODS-CSAs. Hence, this work aims to examine high-temperature irradiation effects such as defect evolution, chemical segregation, and hardening in some of the NiCo-based ODS-CSAs. In the current work, ODS-NiCoFe, ODS-NiCoFeCr, and ODS-NiCoCr were studied following Ni^{2+} irradiation at 580°C and 700°C via various transmission electron microscopy techniques and nanoindentation.

Defects induced by irradiation could lead to adverse effects such as irradiation swelling and hardening. The interfaces between the matrix and nano oxide particles and the grain boundaries act as defect sinks. Thus, these can be the regions of significant chemical redistribution during irradiation. Chemical segregation indicating Cr and Fe depletion and Ni and Co enrichment is expected near the grain boundaries specifically in Cr containing ODS-CSAs following irradiation. All such key findings which will culminate in evaluating the high-temperature radiation resistance of some of the ODS-CSAs will be presented.

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Agata Sotniczuk received Master (2015) and Ph.D. (2022) title at the Faculty of Materials Science and Engineering at Warsaw University of Technology in Poland. From 2020, she is working at the Warsaw University of Technology and till now she has been Consultant in five Bachelor and four Master thesis. In 2022 she joined NOMATEN CoE as a Support Specialist in Corrosion. In NOMATEN CoE she was responsible for setting-up Corrosion and Electrochemical LAB which now offers both standard and local corrosion analysis using Scanning Electrochemical Microscopy (SECM). Her work encompasses investigating the effect of microstructural features, phase structure and chemical composition on physicochemical surface properties of titanium and its biomedical alloys.

She is focusing on the influence of proteins, products of immunological systems, and bacteria metabolism on the corrosion resistance of biomedical alloys. In order to investigate this phenomena she is exploiting electrochemical techniques, mainly electrochemical impedance spectroscopy (EIS) together with spectrometric methods such as ICP-AES and ICP-MS. Her corrosion studies are supplemented by post-immersion surface analysis by spectroscopic techniques such as XPS, AES and microscopic methods such as AFM or FIB-TEM analysis. She is Co-Author of 20 publications from JCR list, mostly in the Corrosion and Materials Science oriented journals, that were cited over 200 times (H-9).

She has been PI of two projects financed by the NCN in Poland and two fellowship projects financed by NAWA in Poland and European Organization KMM-VIN. In 2022 she received award for the best Ph.D. thesis from the Polish Corrosion Society which is a member of European Federation of Corrosion (EFC). She gained her experience during international research stays in the Institute of Biomaterials, University of Erlangen–Nuremberg (Germany); Clemson University-Medical University of South Carolina (USA) and Chimie ParisTech (France). Now, she is focusing on designing new orthopedic alloys with desired strength-ductility trade off.

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NOMATEN toolbox for detecting corrosion phenomena

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Corrosion processes of metal-based materials are commonly investigated by standard electrochemical methods such as Cyclic Polarization (CV) or Electrochemical Impedance Spectroscopy (EIS) as well as by spectrometry techniques such as Inductively Coupled Plasma Mass Spectrometry (ICP-MS). Coupling this techniques allow us to obtain information related to the oxidation and dissolution phenomena that contribute to the overall corrosion process. Currently in NOMATEN CoE, special emphasize is put on analysing corrosion behaviour of metals and their alloys devoted to nuclear and medical applications for which corrosion resistance is triggered by the presence of nanometric air-formed oxide layer on their surface.

Nanometric oxide film tend to evolve during the time of exposure to the environmental conditions, which is reflected by changes in the values of corrosion parameters designated from the results of electrochemical tests as well as by changes in the amount of released metal ions. In order to provide an insight into the kinetics of corrosion/oxidation and to indentify mechanisms of materials' degradation, corrosion tests are supported by post-immersion surface characterization by the "top-view" and "cross-section" analysis with SEM and FIB combined with TEM respectively. The aim of this lecture is to introduce this path of corrosion investigations based on the latest research performed within NOMATEN MAB project, and experiments planned to be completed within the projects that were recently granted by the members of Corrosion and Electrochemical group: (i) Magnificor (MSC Actions – Horizon 2020) and (ii) Sonatina 7 (National Science Centre in Poland). Moreover, in this lecture the concept of research approaches, currently developing in NOMATEN CoE, will be introducted. Precisely, research methodologies such electrochemical *in situ* Raman spectroscopy, and corrosion measurements in micro- and submicron scale using Scanning Electrochemical Microscopy (SECM), will be described during the lecture.

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Oscar Sonzogni studied at Bordeaux INP engineering school ENSCBP and obtained a Master's degree in Materials Science in 2022. He did his Master Degree Apprenticeship at ArianeGroup on the assessment of large Laser – Powder Bed Fusion (Additive Manufacturing) machines for aerospace parts manufacturing. He is currently preparing a PhD at CEA on the "Determination and elaboration of BCC/FCC Complex Concentrated Alloys resistant to Molten Salt Reactor operating conditions". The thesis work is carried out at CEA DRMP, Service de Recherche en Matériaux et procédés Avancés in partnership with Université Paris Est, ICMPE. This research has received funding from the Euratom Research and Training Program, Horizon EUROPE, INNUMAT project – Innovative Structural Materials for Fission and Fusion.

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Development of NiMoCrAl alloys resistant to molten chloride salts corrosion

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Molten Salt Reactors (MSR) are a type of nuclear reactor working with molten salts as heat gatherer with nuclear combustible usually dissolved in the salts. This design could lead to improved efficiency and safety compared to high-pressure water reactors.[1] One of the biggest challenges to their widespread use is finding structural materials that can withstand both the corrosion in chloride salts, and neutron irradiation at 600/700°C. Literature shows that Ni-Mo-Cr alloys seem to be good candidates to resist to molten chloride corrosion [2]. In addition, it has been shown that chromia (Cr_2O_3) or alumina (Al_2O_3) protective layers can enhance corrosion resistance [3]. Our goal in this study is to investigate the influence of substitution of Cr by Al in a NiMoCr system on its molten chloride corrosion. For that, the selection criteria are the following: be single or two-phased with contents close to equimolarity, good corrosion resistance and acceptable hardness (<500HV). In a first stage, interesting compositions are identified using CALPHAD method. In the second stage, investigations focus on the fabrication of $NiMoCr_{a-x}Al_x$ alloys by arc melting and their characterization using electronic microscopy, hardness measurements and X-ray diffraction. In a third stage, corrosion resistance is assessed on sample selection after immersion in $NaCl\text{-}MgCl_2$ salts for one week. First results show that substitution of Cr by Al from 15%at causes the precipitation of other phases (i.e. Ni_3Al and σ phases) and induces a significant increase in hardness.

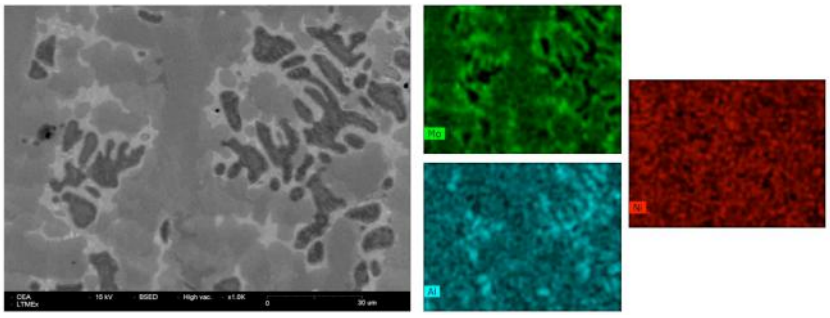

Figure 1. Electronic Microscopy of $Ni_{70}Mo_{10}Al_{20}$ alloy. Left: Back Scattered Electronic Microscopy, others: EDS analysis

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Dr inż. Przemysław Kot studied at Faculty of Physics and Applied Computer Science AGH University of Science and Technology in Cracow. In 2022, he received a Ph.D. title. He is a member of Material Characterisation group at the NOMATEN Centre of Excellence in the National Centre for Nuclear Research. He is a director of project founded by Polish agency NCN. He conducted several experiments on neutron diffractometers: HK9 at UJF CAS, FSD and EPSILON in JINR, where he helped facilitate the operation of the diffractometer. In his works, he mainly dealt with the in-situ neutron/X-ray diffraction stress and texture measurements and development of theoretical models for the study of elastic-plastic deformations in polycrystalline and multiphase materials. He is coordinator of stress/texture diffractometer implementation at the Maria research reactor.

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Neutron diffraction study of magnesium AZ31 plastic deformation mechanisms and phase stresses in Al/SiC$_p$ composite during thermal cycling and mechanical loading

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In the present work the mechanical behaviour of the Al/SiCp composite and AZ31 magnesium were studied using neutron diffraction. To do this, the time of flight (TOF) neutron diffraction was applied. The advantage of diffraction methods is that the mechanical behaviour of different peaks and phases of polycrystalline material, therefore different lattice strains and stresses can be independently studied during sample loading by measuring in several different directions of scattering vector.
The experimentally obtained phase stresses evolution in both constituents of the Al/SiCp composite during thermal processing and elastic-plastic deformation were explained with a proposed Developed Thermo-Mechanical Self-Consistent model (DTMSC). The advantage of the DTMSC model is a prediction of the thermal inter-phase stresses, and subsequently simulation of their relaxation during the elastic-plastic deformation. [1]

Measurements of the highly textured AZ31 magnesium alloy during the compression and tension test were made for a load applied in different directions relative to the sample. Simultaneous measurement of many hkl reflections (TOF method) and measurement in 9 different directions allowed to determine stress tensors for selected groups of crystallites (including twins). These data and the developed method of crystallite groups allowed for the first time to determine the critical shear stresses for various slip and twinning systems directly from diffraction measurements (in previous works, the interpretation of the results required model assumptions regarding crystallite interactions). These results were used as model parameters, making the model less ambiguous. A very good agreement between model and experimental results was obtained. [2]

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Dr. Tymofii Khvan studied at the Faculty of Physics of V.N. Karazin Kharkiv National University in Ukraine. His mature research career started during his Bachelor's studies in 2016, after a short scientific visit to the Belgian Nuclear Research Center SCK-CEN, where he started joint work under the EUROfusion project. Three more like visits, four publications in international journals, a comprehensive study on plasma-facing fusion materials, and two travel grants from the FuseNet educational network are the features of his late University years. After that, during 2018-2023, he received a Ph.D. in Engineering Sciences at the University of Liege, Belgium. His research mainly focuses on the microstructural and mechanical properties of structural materials for nuclear applications, which Tymofii characterizes using experimental and computational methods. During Ph.D. studies, Tymofii participated in the H2020 project (M4F –Multiscale modeling for fusion and fission materials, technologies, and processes), worked at the JRC-Petten under the Open Access program, collaborated with Bruker Nano GmbH, OCAS NV, Plansee SE, etc.

In the summer 2023, he successfully passed the selection for the POLONEZ BIS 3 – a prestigious EU research grant under the Marie Skłodowska-Curie Action to perform his proposed research at the National Center for Nuclear Research (NCBJ). Now, he is an Assistant Professor at the NOMATEN Center of Excellence at the NCBJ. His project is dedicated to the extension of the applicability of the experimentally computational tool he developed during his Ph.D., which is capable of predicting the plastic properties of neutron-irradiated ferritic/martensitic steels while dealing only with virtually safe, fast, and cheap experiments on the ion-irradiated material. This approach is believed to accelerate the delivery of research data in nuclear material sciences.

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 857470

Mechanical and structural properties of RAFM steels - Impact of radiation damage

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Reduced activation ferritic/martensitic (RAFM) steels are the main candidates for the construction of structural components in future nuclear reactors [1]. RAFM-based materials require a careful approach for their selection and characterization, as they must ensure the safe and stable employment of a nuclear device over its full lifetime. Constantly enduring neutron irradiation, high temperatures, and mechanical stresses, the structural materials tend to degrade their mechanical properties [2]. As neutron irradiation for research purposes is a long, expensive, and complicated process, the nuclear materials scientific community is increasingly looking towards an attractive solution of ion irradiation. However, this type of irradiation implies limitations in terms of non-uniform and shallow damage accumulation. Therefore, non-conventional testing procedures are applied to deduce the maximum information about the impact of the ion damage on the mechanical properties.

We propose to establish a computationally experimental protocol built around high-temperature nanoindentation experiments, electron microscopy techniques, and the finite element method to characterize the plastic properties of metallic materials after ion irradiation, serving as a surrogate for neutron damage. The nanoindentation process in reference and ion-irradiated Eurofer97 steel is modeled using numerical simulations, which are validated through experimental data. The radiation-modified constitutive laws are then deduced and used as inputs for macroscale simulations, representing neutron-irradiated materials. Electron microscopy, together with focused ion beaming, is used to observe microstructural features associated with radiation damage or the nanoindentation deformation process. This approach may eventually serve as a tool to predict the effect of irradiation damage by avoiding neutron irradiation and will accelerate the delivery of new research data on materials for nuclear applications.

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Damian Kalita graduated Materials Engineering at the Faculty of Material Science and Ceramics AGH University of Science and Technology in Cracow. In 2021, he received a PhD title in the field of Materials Science at the Institute of Metallurgy and Materials Science, Polish Academy of Sciences. His PhD thesis was focused on the development of the fabrication technology of the body centered cubic (BCC) Ti-Nb-based alloys exhibiting the superelastic effect with the application of powder metallurgy and additive manufacturing methods.

Currently, he is employed as postdoc in the Materials Characterization Research Group at the NOMATEN Centre of Excellence in the National Centre for Nuclear Research (NCBJ). In his work he is concentrated on the development of the new irradiation-resistant refractory high entropy alloys (HEA) for the nuclear fusion applications. He is also the expert in the field of scanning electron microscopy (SEM) and transmission electron microscopy (TEM) at NOMATEN. He co-authored 26 scientific papers cited over 500 times (h-index 10). His scientific interests include among others refractory alloys, high entropy alloys, phase transformations and advanced electron microscopy.

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Impact of He and Ni-ion irradiation on the performance of BCC-type HEA – WTaCrV case study

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The rapidly increasing global demand for energy consumption requires the development of new advanced nuclear reactor technologies characterized by higher safety, better efficiency, and lower long-term environmental effects. The upcoming fusion systems could meet these needs, but their efficiency will greatly rely on the performance of the structural materials. The key components of fusion reactors will be exposed to extreme conditions, including high operating temperatures, and radiation-induced damage resulting from the interaction with high-energy neutrons and He-irradiation. The materials currently used in operating fission reactors have not been designed to withstand such conditions.

In the presented work, the novel body-centered cubic (BCC) WTaCrV refractory high entropy alloy (HEA) was synthesized using the magnetron sputtering method. To simulate the conditions present in a fusion reactor, the material was subjected to He-ion irradiation, followed by heavy ion irradiation using Ni-ions. Structural characterization of the material was systematically performed using scanning and transmission electron microscopy, while changes in its mechanical properties were studied using nanoindentation.

We observed that He-irradiation resulted in the formation of a high density of nanometric He-bubbles within the microstructure of the alloy. Surprisingly, the fine structure of the He-bubbles remained stable under the heavy ion irradiation up to 2 dpa. Despite the relatively high damage caused by the He and Ni irradiation processes, only slight irradiation hardening was observed, indicating a high irradiation resistance of the developed alloy.

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Dr Tomasz Moscicki studied at the Faculty of Power and Aeronautical Engineering Warsaw University of Technology in Warsaw. In 2007, he received a Ph.D. title at the Institute of Fundamental Technological Research PAS, Warsaw, Poland. In 2017, he obtained the title of doctor habilitus (D.Sc.) in mechanical engineering. From February 2019 he is a member of the Scientific Council of IPPT PAN. From January 2020 he is head of Division of Technological Laser Applications in Department of Experimental Mechanics. Also in 2020 he obtained a professors position at IPPT PAN. In his works, he mainly deals with the structural and mechanical properties of superhard materials such as transition metal borides. Actually, during his work he studies the influence of deposition parameters on properties of thin films deposited by Pulsed Laser Deposition (PLD), Magnetron Sputtering (MS) and also hybrid method PLD+MS.

He is also expert in laser technologies such as laser welding, laser ablation, nanoparticle synthetizing and he studies a plasma induced during those processes. His interests include not only experimental research but also theoretical modeling of the mechanical and thermal properties of deposited films, which is the topic of his current research project. He co-authored over 40 journal papers cited over 730 times (H – 15). He has been a manager of four projects funded by Polish agencies (NCN, NCBiR). He received 4 individual and team awards for academic achievements from the Director of Institute of Fundamental Technological Research PAS (between 2016-2022). He was a reviewer above 70 scientific articles and was an expert in National Science Center of Poland (above 50 projects applications) in mechanical and material engineering.

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Theoretical and experimental studies of superhard W-Ti-B coatings deposited using the HiPIMS method

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High-power impulse magnetron sputtering (HiPIMS) is thin film deposition from standard magnetrons using pulsed plasma discharges, where a large fraction of the material used in the deposition process arrives at the workpiece as ions instead of commonly used neutrals. HIPIMS utilizes extremely high power densities of the order of kW/cm^2 in short pulses of tens of microseconds at low duty cycle (on/off time ratio) of < 10%. Distinguishing features of HIPIMS are a high degree of ionisation of the sputtered material and a high rate of molecular gas dissociation. The benefit of having an ionized deposition flux is that it can be guided and manipulated by electric and magnetic fields. This allows for increased control of the microstructure and properties of the coatings.

In this work as an example the superhard (H>40 GPa) and "flexible" (W,Ti)B_2 coatings are presented. The "flexible" means that ceramic films are characterized by increased ductility and high crack resistance. The deposited coatings are dense, partially crystalline and possess void free microstructure. Such interesting properties can be obtained by two different ways: addition of alloying element to WB_2 hexagonal structure and choosing of optimal condition of deposition such us substrate temperature, additional polarization of substrate (bias voltage) and selection of HiPIMS parameters like power, pulse duration and frequency.

The explanation of special features of presented coatings is not ease and need studies in different scales, starting from atomic scale. In this work potentially superhard $W_{1-x}Ti_xB_2$ polymorphs hP6-$P6_3$/mmc-WB_2 and hP3-P6/mmm, were thoroughly analysed with titanium doping in the range of x=0-25%, within the framework of the first-principles density functional theory, from both a structural and a mechanical point of view. The obtained results were subsequently compared with the properties of material deposited by the magnetron sputtering method (fig. 1).

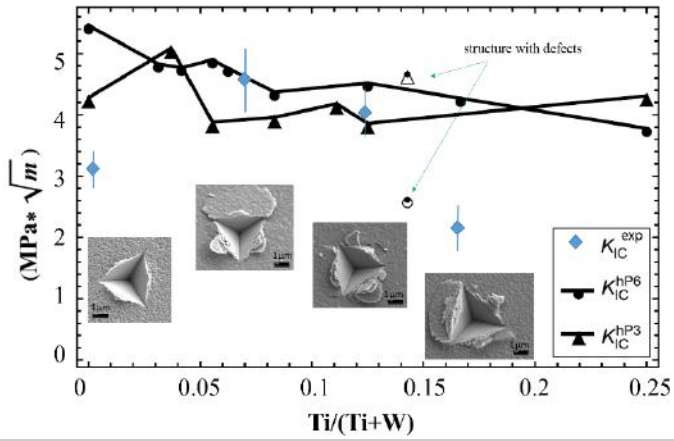

Figure 1. Theoretical and experimental fracture toughness of W-Ti-B coatings

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Magdalena Gawęda, PhD Eng., graduated from AGH University of Krakow, Poland. In 2020, at the Faculty of Materials Science and Ceramics, she successfully defended her doctoral thesis titled "Bioactivity of black glasses based on ladder-like silsesquioxanes" earning a Doctor of Natural Sciences degree in the field of Chemical Sciences. Prior to this achievement, she had acquired a Master's degree in Materials Science (2015) and an Engineer title in Chemical Technology (2014), all from the same university. Between 2014 and 2016, she participated in the Advanced Spectroscopy in Chemistry Erasmus Mundus Joint Master Degree program, which led to her receiving a double diploma from Université Lille-I, France, and Jagiellonian University in Krakow, Poland. Her master's thesis, titled “Optimisation of measurement methodology of fixed cells using imaging techniques, vibrational spectroscopy, microscopy (AFM, SNOM) and chemometric analysis” was result of this program. She is a recipient of the Minister of Science and Higher Education scholarship for the outstanding achievements for a 2014/2015 academic year.

Dr. Gawęda professional pursuits encompass two primary areas. Firstly, she is engaged in the design, preparation, and process optimization of polymer-derived ceramics (PDCs), with a specific focus on protective coatings for steel intended for use in hostile environments. Her second area of expertise revolves around structural examination of materials, with a specialization in vibrational spectroscopy. Her valuable contributions to the field of materials science and chemical analytics are substantiated by 19 scientific articles (*h*-index: 10) published in esteemed journals, including Applied Surface Science, Spectrochimica Acta - Part A, and Ceramics International. She actively participates in international conferences where she presents her research findings.

Since 2021, she has been employed at the National Centre for Nuclear Research, and starting in 2022, she has become an integral part of the Materials Characterization Group at NOMATEN CoE. In this role, she leverages her expertise in structural examination. She conducts extensive ex-situ and in-situ Raman spectroscopy studies on materials used in nuclear reactors to assess their performance under the hostile working conditions of high temperature and radiation. Dr. Gawęda actively contributed to the establishment of a new LA-ICP-MS/LIBS laboratory. Notably, in 2023, she was awarded the Sonatina 7 grant titled "Amorphous silicon oxycarbide-based protective coatings on steel for cladding materials in nuclear reactors" by the National Science Centre.

This project has received funding from the European Union’s Horizon 2020 research and innovation programme under grant agreement No 857470

Amorphous silicon oxycarbide-based protective coatings for nuclear applications

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Silicon oxycarbide (SiOC) is a class of two-phase materials composed of an amorphous silica-based matrix with oxygen ions partially substituted by carbon, along with a dispersed graphite-like disordered free carbon phase. SiOC is of particular interest due to its favourable mechanical parameters[1], excellent adhesion to the metallic substrates[2], as well as its chemical and thermal stability[3]. The functional properties of SiOC can be further customised by adjusting the quantity of free carbon phase[4] and ionic substitutions[5,6]. This presentation discusses the utilization of other advantageous qualities of SiOC, namely its radiation tolerance and resistance to helium bubble formation[7].

The presentation reveals the groundwork and preliminary research for the Sonatina grant, which focuses on the development of protective amorphous silicon oxycarbide-based coatings for construction components used in nuclear reactors. They objective is to enhance radiation tolerance and high-temperature stability of steel components. These materials will be prepared following the concept of polymer-derived ceramics by pyrolysis of self-synthesized ladder-like silsesquioxanes with designed carbon and iron (as the modifying cation) content, which will be deposited onto AISI 316L austenitic stainless steel. The work plan includes comprehensive structural, microstructural, and mechanical studies conducted both before and after irradiation with light and heavy ions, as well as *in-situ* investigation at elevated temperatures. The anticipated results will provide significant scientific value and have a direct application in the use of SiOC/steel composites in nuclear reactors, bridging the gap between fundamental research and industrial implementation.

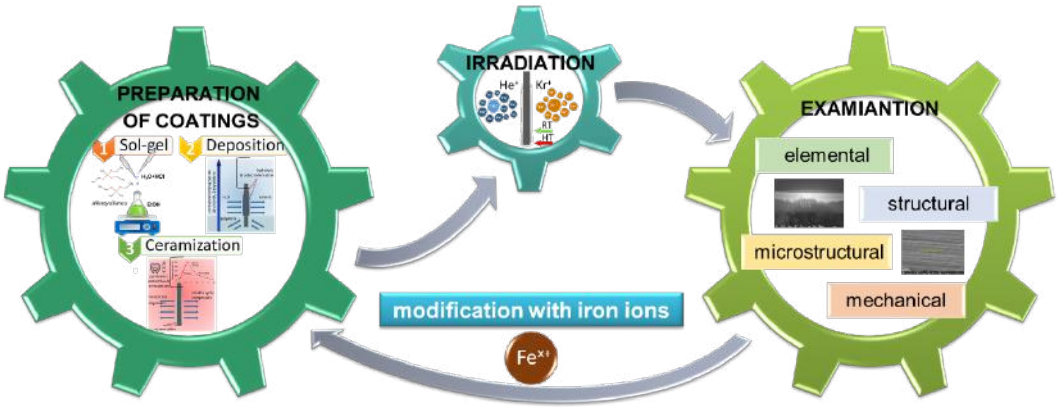

Figure 2. Schematic description of characterization methodology for amorphous SiOC-based coatings.

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SESSION 4 Materials Science Non-Nuclear

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PhD student Eloi de Villoutreys studied Material Science at Chimie ParisTech – PSL engineering school in Paris. He is currently preparing its PhD entitled “Optimization of the manufacturing processes of Nd-Fe-B permanent magnets by an alloy design method” at CEA Paris-Saclay. In 2023, he participated to the E-MRS Spring Meeting and won an award for its poster in the Symposium: Advanced Sustainable Materials for Energy Applications.

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Phase equilibria and solubility limits in the (Ce, Nd)-Fe-B system for new substituted permanent magnets

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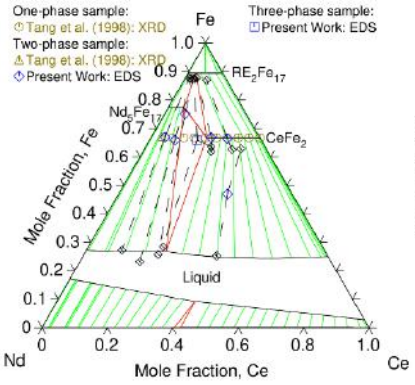
Worldwide pressure on the supply of Nd-based (Nd-Fe-B) permanent magnets due to the energy transition is pushing manufacturers to develop new magnets with reduced Nd content, replaced by other less critical Rare Earths (RE) like Ce and La [1]. Their elaboration requires a fine control of the microstructure composed of $(Nd,RE)_2Fe_{14}B$ main grains and others phases present at the grain boundaries (GBP). The overall objective of this study is to improve manufacturing conditions, which control the distribution of the microstructure of the future magnet. New Ce-substituted magnets involves developing a numerical approach for the thermodynamic of these systems. This work focuses on the effect of the addition of Ce to the Nd-Fe-B base system. This implies a deep understanding of the thermodynamic of GBP that effectively form and not form. Presence of GBP like the Nd-rich one are needed to maintain coercivity while other like FeB are deleterious. The presence of $REFe_2$ can be beneficial but only distributed in adjacent grains [2]. An experimental study has been carried out on the (Ce, Nd)-Fe-B system in order to improve our understanding of its thermodynamic, and results has been complied in a database according to the CALPHAD method. In addition, ab-initio and quasi-harmonic calculations were conducted to complete experimental thermodynamic results. Application simulations were performed to replicate and predict the effects of heat treatment on phase compositions.



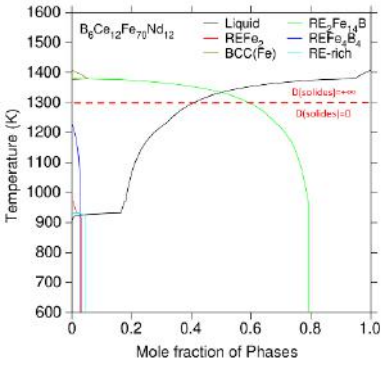


Figure 1. (Left) Phase diagram of the Ce-Fe-Nd at 1023 K Figure 2. (Right) Solidification of a $B_6Ce_{12}Fe_{70}Nd_{12}$ sample without diffusion in solids below 1300 K

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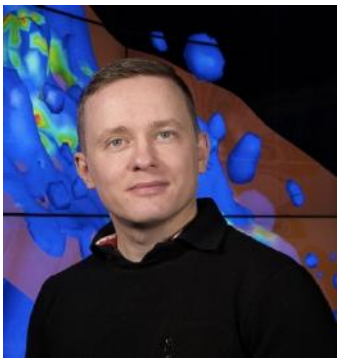

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Dr Mikko Vepsäläinen holds a Doctor of Science (D.Sc.) degree in Environmental Technology, which he obtained from Lappeenranta University of Technology in October 2012. Prior to this, he earned a Master of Science (M.Sc.) in Applied Chemistry from the University of Jyväskylä in December 2005. Dr. Vepsäläinen currently serves as a Research Team Leader at VTT in Espoo, Finland, a position he has held since 2021. In this position, he leads a diverse research team comprising 18 scientists and technical people and a large R&D portfolio. Prior to his current role, Dr. Vepsäläinen had a position in Australia at CSIRO from 2012 to 2021, where he served as a Postdoctoral Fellow, Research Scientist and Senior Research Scientist. Before this, he worked as a Senior Scientist at the Technical Research Centre of Finland VTT and R&D Manager at a private company, Savcor Forest Oy.

His research is centred on electrochemistry, corrosion, and nanomaterials. He has published 25 peer-reviewed journal papers, 2 book chapters and several conference proceedings and public reports. He has an h-index of 17 with over 3200 citations and he is the inventor of 8 international patent families in water quality monitoring and treatment and electrochemical systems. During his tenure at the Australian governmental research organization CSIRO, he led the development of the Vesi™ (formerly known as Sensei™) in-situ water quality monitoring system. He also ventured into the electrochemical synthesis of metal-organic frameworks (MOFs) and their application in water treatment and water quality monitoring. He has industrial and academic research experience on corrosion, fouling, and scaling in water systems. The work at VTT Technical Research Centre of Finland and Savcor Forest Oy has centred on understanding and mitigating these complex phenomena. His findings have contributed to the safe operation of industrial water systems and informed strategies for the secure long-term storage of nuclear waste.

In recognition of his contributions to the scientific community, Dr. Vepsäläinen has received accolades, including the CSIRO Julius Career Award in 2018 and the CSIRO AcceleratiON award in 2015, both in Australia. Additionally, he was honoured as the CSIRO Mineral Resources Young Scientist of the Year in 2015. Beyond his research, he contributes to international organizations, such as the SIAPWS Executive Committee.

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Electrochemical synthesis of metal-organic frameworks (MOFs)

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Electrochemical synthesis provides an innovative approach to the formation of metal-organic frameworks (MOFs). This method can offer advantages, such as enhanced reaction rates, selective crystallite growth, and lower energy consumption compared to conventional synthesis methods. During the process, metal ions from electrodes undergo redox reactions and coordinate with organic linkers, leading to the formation of MOF structures on electrode surfaces. By manipulating parameters like current density, electrolyte concentration, and polarity, researchers can optimize MOF yield and quality. This electrochemical strategy not only offers an efficient route for MOF synthesis but also paves the way for integrating MOFs into electronic devices and sensors.

Challenges in scaling up MOFs synthesis have hindered their widespread commercialization. In our recent work, we have demonstrated the combined electrosynthesis and flow-synthesis of HKUST-1 metal-organic frameworks [1]. In another research work, we demonstrated that cycling of electrode potential during electrosynthesis enables continuous MOFs production by preventing passivation of the electrode surface [2]. The electrosynthesis methods described in the papers reduce the postprocessing requirements simplifying the large-scale synthesis and reducing the costs by up to 88%.

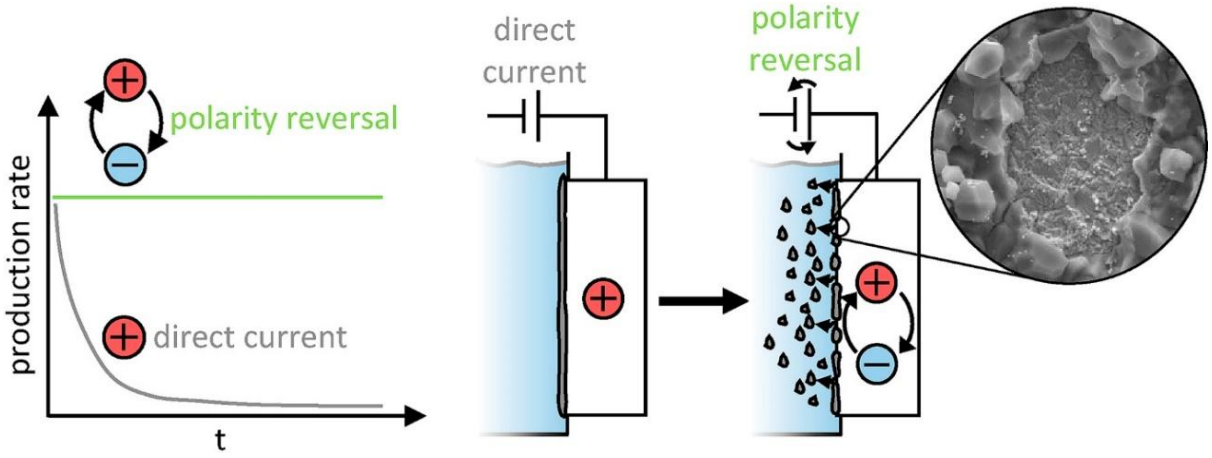

Figure. *Passivation of the electrodes during MOFs electrosynthesis can be prevented by a low-frequency polarity switch.*

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Dr. F. Javier Dominguez achieved his PhD in Computational and Applied Physics with Summa Cum Laude honors at the National University of Mexico (UNAM). During his doctoral and postdoctoral studies, he joined The Institute for Advanced Computational Science at Stony Brook University, where he focused on modeling plasma-material interactions in tokamak plasmas, collaborating with the Princeton Plasma Physics Laboratory in the USA. Before joining NOMATEN, he was the recipient of the A. von Humboldt Research Fellowship and a Siemens Foundation scholarship at the Max Planck Institute for Plasma Physics in Germany. During this period, he created the innovative FAVAD software workflow using machine learning methods to characterize and visualize defects in damaged materials. Notably, FAVAD won the IAEA challenge, showcasing its excellence. In 2023, he attained the title of doctor habilitus (D.Sc.) in physics and an institute professor position at NCBJ. His academic contributions include over 40 journal papers with a cumulative citation count exceeding 300 and an H-index of 11. He's been invited to speak at institutions like Aalto University, Karlsruhe Institute of Technology, University of Helsinki, VTT, IPPT, and DIFFER lab. Within NOMATEN CoE, his primary research focus on developing multi-scale numerical models seeking to understand how single crystal materials and high-entropy metal alloys respond under extreme conditions, such as high temperatures and irradiation doses. The overarching goal is to engineer and design materials suitable for applications in fusion, fission, and various industrial sectors.

Dr. Dominguez actively participates in platforms like the EERA JPNM, INNUMAT project, Humboldt Foundation, and EuMINe COST ACTIONS. His collaborative efforts bridge the theoretical and experimental domains, spanning research institutes across the USA and Europe. Additionally, Dr. Dominguez serves as a mentor and is a dedicated member of the Polonium Foundation. He's also an active participant in the Societas Humboltanian Polonorium, holds IOP trusted reviewer certification, and serves on the editorial board of Frontiers Condensed Matter. Notably, he has also developed quantum chemistry software designed for investigating the catalytic properties of 2D materials in NCBJ. This software finds diverse applications, from hydrogen production and water splitting to gas separation, electron conductivity, and sensor development with already collaborations with international and polish research institutions, scientific publications, and presentations in international conferences dedicated to chemistry of materials.

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Amil Aligayev, a current Ph.D. student, is affiliated with the Materials Structure, Informatics, and Function (MASIF) research group in the NOMATEN Center of Excellence for Multifunctional Materials under supervision of Prof. Stefanos Papanikolaou at the National Center for Nuclear Research (NCBJ) in Poland. In 2021, Mr. Aligayev attained his Master of Science degree from the Department of Condensed Matter Physics at the University of Electronic Science and Technology of China (UESTC) in the P.R. China. His academic journey commenced with a BSc degree obtained with high honors from the Faculty of Physics at Baku Engineering University, spanning from 2014 to 2019. His research topic is predominantly centered on the domain of experimental and computational modelling studied of hydrogen production, catalysis, and the development of electronic nanodevices. His work is intently focused on elucidating optimal structural configurations for electrolysis and photoelectrochemical applications. Employing a methodology in materials science, he integrates theoretical expertise, multi-scale simulation techniques, and experimental methodologies, with a particular emphasis on the synthesis of nanoparticles and 2D materials for the purpose of designing high-performance catalytic systems. Endowed with a robust foundation in theoretical condensed matter physics and chemistry, he exemplifies a promising scholar in the burgeoning field of Materials Informatics within the broader context of materials science.

His scholarly contributions encompass several published works in Physica Status Solidi (b), Phys. Chem. Chem. Phys., J. Environmental Chemical Engineering and Diamond & Related Materials, etc., with a specific emphasis on subjects related to gas adsorption and hydrogen production. This work led Mr. Aligayev to obtain the ENEN+ award to attend ANIMMA 2023 summer schools in Advancement in Nuclear Instrumentation Measurement Methods and their Application, CECAM workshops focused in ab initio calculations, and e-MRS sessions where his work was selected to be published in the proceeding of the materials chemistry of materials. In addition, he is actively engaged in the synthesis of low-dimensional nanoparticles and quantum dots for applications in the realm of photoelectrochemistry. He collaborates with a cadre of Chinese researchers at the Science Island Branch of the Hefei Institute of Physical Science-Chinese Academy of Sciences (CAS), the University of Science and Technology of China (USTC) and La Rochelle Université in France. His research endeavors make substantive contributions to the ongoing global quest for knowledge in materials science and augur well for prospective innovations in the field of sustainable energy technologies.

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2D Materials Catalysis: A Multiscale Quantum Chemistry Approach for Hydrogen production from CH_4, CO_2 Purification, and Gas Splitting Applications

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Two-dimensional carbon-based materials, such as graphene, graphenylene, g-C3N4, and graphyne, have shown promise for various applications, including electronics, optics, energy storage, and gas separation. Their unique electronic and optical characteristics make them particularly appealing for hydrogen production. In this study, we use computational chemistry models to investigate how methane and carbon dioxide adsorb onto single-layer sheets, focusing on their effects on optical absorption and electrical conductivity at room temperature. To closely mimic experimental conditions, we utilize the self-consistent charge tight-binding density functional theory (SCC-DFTB) [1-5] and validate our findings with ab initio calculations using VASP [2-3]. Through classical molecular dynamics (MD) simulations, we observe hydrogen molecules forming from CH4 and CO+O species from CO2[2,3]. Additionally, we explore how molecular adsorption affects optical absorption. We find that methane and methylene (CH2) significantly influence the optical properties of porous carbon sheets, making them favourable for gas diffusion [2-4]. Our MD simulations suggest the potential of porous carbon sheets for gas separation, especially for CH4, while CO2 has a limited impact on the optical properties of these 2D materials [2]. For electron transport analysis, we employ the open-boundary non-equilibrium Green's function method. Studying the conductivity of carbon sheets under voltage bias up to 300 mV provides valuable insights into their electrical properties under optical absorption conditions [2,3]. Our computational modeling results contribute to a better understanding of the potential applications of these materials in hydrogen production and advanced electronics [1,5].

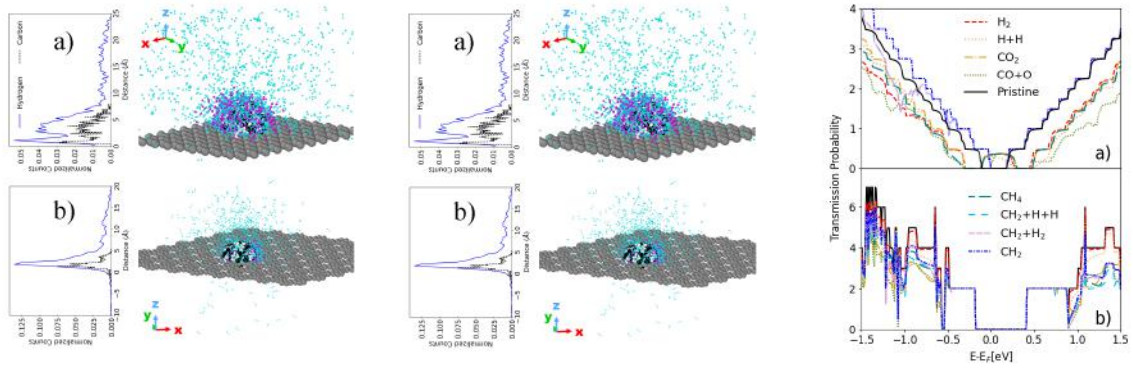

Figure: Left panel, visualization of the hydrogen production by graphene and graphenylene. Total transmission probabilities summed over all channels in the nanoribbon graphene direction in a) and through the pores of graphenelyne in b). -

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Mr. Dario Massa obtained his B.Sc. degree in Physics at the University of Rome La Sapienza, and his M.Sc. degree in Physics at the University of Padova, in Italy, where he also worked as a research fellow in the theoretical modelling of van der Waals interactions. Currently, he is a Ph.D. student in the Materials Informatics group of Prof. Stefanos Papanikolaou at NOMATEN Center of Excellence in the National Center for Nuclear Research (NCBJ), where he develops novel ways of combining Machine Learning and quantum simulations techniques to speed up the research on alloys and defects, in collaboration with renewed national and international institutions. He is also an AI intern at IDEAS-NCBR in Warsaw, in the intelligent algorithms group of Prof. Piotr Sankowski, where he is involved in multiple projects bridging advanced Machine Learning techniques and Materials Science.

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Alloy Informatics through Ab Initio Charge Density Profiles: Case Study of Hydrogen Effects in Face-Centered Cubic Crystals

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Materials design has traditionally evolved through trial-error approaches, mainly due to the non-local relationship between microstructures and properties such as strength and toughness. We propose 'alloy informatics' as a machine learning based prototype predictive approach for alloys and compounds, using electron charge density profiles derived from first-principle calculations. We demonstrate this framework in the case of hydrogen interstitials in face-centered cubic crystals, showing that their differential electron charge density profiles capture crystal properties and defect-crystal interaction properties. Radial Distribution Functions (RDFs) of defect-induced differential charge density perturbations highlight the resulting screening effect, and, together with hydrogen Bader charges, strongly correlate to a large set of atomic properties of the metal species forming the bulk crystal. We observe the spontaneous emergence of classes of charge responses while coarse-graining over crystal compositions. Nudge-Elastic-Band calculations show that RDFs and charge features also connect to hydrogen migration energy barriers between interstitial sites. Unsupervised machine-learning on RDFs supports classification, unveiling compositional and configurational non-localities in the similarities of the perturbed densities. Electron charge density perturbations may be considered as bias-free descriptors for a large variety of defects.

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Dr Jan Wróbel is an Assistant Professor at the Faculty of Materials Science and Engineering (FMSE), Warsaw University of Technology (WUT). His research focuses on the *ab initio* modelling of materials properties based on the density functional theory (DFT). He was using this method both for his Master's thesis at the Faculty of Physics WUT and Ph.D. thesis at FMSE-WUT. After a defence of his Ph.D. thesis in 2012, Dr Jan Wróbel moved for a post-doc to the world-renowned Materials Modelling group head by Prof. Sergei Dudarev at Culham Centre for Fusion Energy in the United Kingdom, where he was involved during 2.5 years in the Accelerated Metallurgy project. In this project, he was responsible together with Prof. Duc Nguyen-Manh for the DFT modelling of phase stability of multicomponent alloys for fusion applications.

After his come back to Poland, Dr Jan Wróbel was the project leader of the HOMING project titled "*Ab-initio modelling of phase stability and properties of high-entropy alloys*" financed by the Foundation for Polish Science. Now, he is the principal investigator of the SONATA project titled "*Microstructure evolution of Ta-Ti-V-W high-entropy alloys: from ab initio modelling to additive manufacturing technology*" supported by the National Science Foundation in Poland. He is also the project manager at WUT of the European INNUMAT project titled "*Innovative Structural Materials for Fission and Fusion*" funded by European Commission-Euratom. Since the year 2017, he has been also the task leader within the IREMEV (Irradiation Effects Modelling and Experimental Validation) package in the EUROfusion project.

Dr Jan Wróbel is an author of 48 papers in international journals with peer reviewers that have more than 1300 citations. The Hirsch index of Dr Jan Wróbel is 18. He won the Scholarship for Young Scientists funded by the Foundation for Polish Science. Dr Jan Wróbel was a visiting scientist and a member of the "Materials for Fusion and Fission" group at the Materials Department of University of Oxford head by Prof. Steve Roberts. He has completed also an internship in the group of Prof. Georg Kresse at the University of Vienna, in which the VASP code (the most popular program for DFT calculations) was created and is being now developed. He received the title of doctor habilitus in materials engineering in 2023.

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DFT-based modelling of high-entropy alloys

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Due to the enormous number of combinations of components and their concentrations, the experimental investigation of all combinations of high entropy alloys (HEAs) is impossible. Therefore, the theoretical understanding of the influence of components and their concentrations on the phase stability and basic properties of HEAs is very important. The ab initio method using density functional theory (DFT) is preferred for modelling HEAs due to its ability to predict material properties without requiring experimental data. However, its drawback is its time-consuming nature, limiting the number of atoms it can handle. Combining DFT with higher-scale methods is often necessary to address this limitation.

I will review the chosen DFT-based methods. Primarily, I will focus on the combination of DFT, the cluster expansion method and Monte Carlo (MC) simulations, which can be applied to investigate the phase stability of alloys as a function of temperature and alloy composition and to generate the representative structures for further DFT calculations. On the example of non-magnetic bcc Cr-Ta-Ti-V-W and magnetic fcc Fe-Cr-Mn-Ni alloys, I will present how the short-range ordering and order-disorder transition temperature depend on the concentration of elements and how this can be used to design novel alloys with improved homogeneity of atoms.

Next, I will present the methodology of the development of thermodynamic databases using DFT-based MC simulations in order to study the regions of stability of fcc and bcc phases in Fe-Cr-Mn-Ni alloys as well as the fractions of each phase in the region of their coexistence. Finally, I will present the methodology of developing interatomic potentials for molecular dynamics simulations by using the combination of DFT and machine learning methods, which enables us to predict their elastic and point defect properties and melting temperatures.

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Kamran Karimi joined the Nomaten Center of Excellence as an adjunct professor in April 2021. Prior to joining Nomaten, he held postdoctoral positions in France and Canada working on research projects related to amorphous plasticity, fracture, and statistical seismology. Kamran received his PhD from Carnegie Mellon University, his master's degree from Sharif University of Technology with a specialization in structural mechanics, and a bachelor's degree in Civil engineering from the University of Tehran, Iran. Kamran's current research is focused on applications of materials informatics in understanding microstructure-property correlations in complex multicomponent alloys and metallic glasses with a special emphasis on material modeling, coupled multi-physics and multi-scale problems under extreme loading conditions.

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Multiscale Modeling of Mechanical Deformation in Chemically Complex Alloys

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In my presentation, I will give an overview of three primary areas that have been my focal research interests at NOMATEN CoE: ***i***) crystal and amorphous plasticity, ***ii***) transport properties of high-entropy alloys (HEAs), and ***iii***) micro-structural informatics. In ***i***), my research has employed statistical physics to unravel the microscopic basis of plasticity based on the collective dynamics of shear transformation zones in amorphous solids as well as dislocations mechanics in crystalline metals. Within the context of HEAs, my focus has been on the role of chemical complexities (i.e. local disorder/ordering) investigating their impact on alloy strengths. In ***ii***), I have explored the sluggish diffusion of defects in HEAs and its impact on thermo-mechanical properties. In the area of micro-structural informatics in ***iii***), I have utilized the power of machine learning (ML) and graph neural networks GNNs to infer (hardness) properties solely based on the (surface) microstructural information. Building upon these achievements, we are currently expanding the scope of the above studies by ***i***) employing ML to identify relevant microstructural metrics for predicting bulk plastic properties in bulk metallic glasses as well as HEAs within the microstructure-property paradigm, ***ii***) utilizing machine-learned interatomic potentials for accelerated material discovery, and ***iii***) extending the GNN's capabilities to infer microstructural signatures and defects based on micro/nano mechanical response (as input data) in different metallic systems and distinct alloy compositions.

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Dr. Maciej Ryś graduated from the Faculty of Metals Engineering & Industrial Computer Science at AGH University of Science and Technology, as well as the Faculty of Mechanical Engineering at Cracow University of Technology. In 2019, he earned his Ph.D. with distinction from Cracow University of Technology. During his doctoral studies, he completed an internship at the Institute of Fundamental Technological Research of the Polish Academy of Sciences, where he later joined as a Research Assistant.

He served as the principal investigator in the PRELUDIUM 9 NCN project and also contributed as a co-contractor to seven other NCN projects. In recognition of his scientific achievements, he was honored with the Michał Życzkowski Scientific Award by the Committee on Mechanics of the Polish Academy of Sciences in 2021. In 2023, Dr. Ryś joined the Complexity in Functional Materials group, led by Professor Mikko Alava, at the NOMATEN Centre of Excellence (CoE) at the National Centre for Nuclear Research (NCBJ). His recent research has predominantly focused on theoretical and finite element modeling of size effects in metallic single crystals, as well as the modeling of moving interfaces in shape memory alloys (SMA) under cyclic loading.

Dr. Ryś research interests encompass local and non-local constitutive modeling of materials, addressing coupled problems such as thermomechanics, mechanically induced phase transitions, plasticity, and damage, and applying advanced finite element methods (FEM) to model materials' behavior.

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Modelling of size effects in spherical indentation of a single crystal

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The need to include an intrinsic length scale in elastoplastic material modeling at small dimensional scales has become apparent in recent years. Various concepts, such as geometrically necessary dislocations (GND) and associated pile-up effects, dislocation source limitations, surface effects, and several other mechanisms, have been proposed as relevant factors across different scales and scenarios. It is widely accepted that, particularly at the micron scale, size effects in plasticity are associated with geometrically necessary dislocations (GNDs), which are mathematically related to the incompatibility of plastic (or equivalently elastic) deformation.

In order to predict scale effects on hardness in the spherical indentation, a gradient crystal plasticity model is developed by merging the small-strain Cosserat crystal plasticity [1] framework with the concept of a natural length scale arising from minimal gradient enhancement in crystal plasticity [2]. This approach incorporates the incompatibility tensor in two distinct manners, resulting in the presence of two different length scales.

The first length scale is linked to the formation of GNDs, which contributes to isotropic strain hardening. This part of the model involves a length scale that evolves during plastic deformation and is explicitly determined in terms of standard parameters [1]. The second length scale is associated with lattice curvature and rotation effects introduced into the model through the Cosserat framework [4]. The relevance of curvature effects and the associated length scale in modeling the size effect in indentation of single crystals is indicated.

The model's validity is established through 3D finite-element simulations of spherical indentation on a single crystal of copper. It is shown that the Cosserat framework is a convenient and computationally efficient tool, involving only three additional global unknowns in 3D simulations [3, 4]. The numerical simulations successfully predict indentation size effects and exhibit good agreement with experimental observations.

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Dr Karol Frydrych graduated from the Faculty of Civil Engineering at Warsaw University of Technology in Warsaw in 2013. He won the KMM-VIN Research Fellowship Grant that enabled him to conduct research at the Friedrich Alexander Universität in Erlangen Nürnberg (FAU, Germany) in 2017. Also in 2017, he received a PhD title (with a distinction) at the Institute of Fundamental Technological Research of Polish Academy of Sciences (IPPT PAN, Warsaw). After defending his PhD thesis, he did a postdoctoral internship at the Laboratoire d'Étude des Microstructures et de Mécanique des Matériaux (LEM3, Metz, France) in 2017-2018. Since 2020 he is a tenured assistant professor at the Institute of Fundamental Technological Research of Polish Academy of Sciences. In 2021 he joined the NOMATEN Centre of Excellence (CoE) at the National Centre for Nuclear Research (NCBJ) to work in the Materials Structure, Informatics and Function (MASIF) group led by prof. Stefanos Papanikolaou.

Since 2023 he also serves as an industry liaison specialist at NOMATEN CoE. In his works, he dealt with various aspects of crystal plasticity, including modelling of mechanical response and microstructure evolution of single crystals and polycrystalline metallic materials subjected to large plastic deformation and nanoindentation. To this aim, he also implemented several models himself, such as the Three-Scale Crystal Plasticity (3SCP) model and the Sequential Elasto-ViscoPlastic Self-Consistent (SEVPSC) model. The research interests spanned such materials as aluminium, copper, steel, magnesium, titanium, zinc and high entropy alloys. Currently he joins these interests with state-of-the-art machine learning techniques thus contributing to the materials informatics field. He is single author of 4 research papers, a co-author of 13 research papers (and a first author of 10 of them). The papers were cited over 200 times (HI – 9). His PhD thesis was awarded the 3rd place in the Polish stage of the ECCOMAS contest in 2017. He also obtained the prof. Życzkowski Polish Academy of Sciences Mechanics Committee award in 2019.

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Modelling spherical and Berkovich nanoindentation using the crystal plasticity finite element method

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Instrumented nanoindentation is a popular technique to study mechanical properties of nuclear materials. Unfortunately, correct interpretation of the results obatined is by no means trivial. There are issues like orientation of the indented grain, size effect and indenter tip shape imperfections. Accounting for the effect of irradiation by indenting ion-implanted material adds another level of complication.

The crystal plasticity finite element method seems to be the optimal tool to simulate nanoindentation. On the one hand, it accounts for the crystalline nature of metallic materials. On the other hand, it is a continuum method and it enables to simulate the test in the same length and time scales as in the real experiment. In the presentation, we show a method to establish model parameters based on indentation test [1]. We also show how the model can be modified in order to account for unconventional plastic behaviour of high entropy alloys [2]. Then, we show how the imperfections of Berkovich indenter's tip can be accounted for, cf. Fig. 1. Finally, some results concerning applications of machine learning in the analysis of indented surfaces are presented.

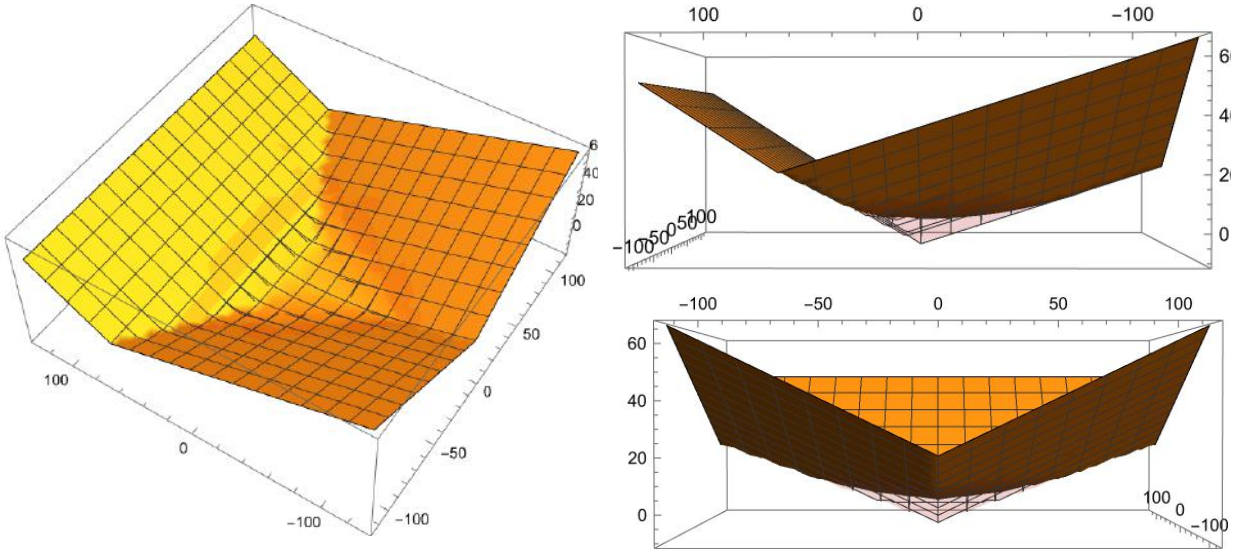

Fig. 1. Plot of the analytical function accounting for the Berkovich tip imperfection.

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Dr. Amin Esfandiarpour is an Assistant Professor and a member of the Complexity in Functional Materials Group at NOMATEN COE, led by Professor Mikko Alava. He earned his Ph.D. in Physics from Payame Noor University (Center of Graduate Study) in Tehran, Iran, in 2015.

In 2017, he secured funding for his first postdoctoral research from the Iran National Science Foundation (INSF) and conducted his research at the University of Isfahan, Iran. In 2019, he started his second postdoctoral position in the Kai Nordlund's group at the University of Helsinki. In August 2020, he joined the NOMATEN Center of Excellence at the National Center for Nuclear Research (NCBJ).

Dr. Esfandiarpour's research primarily focuses on gaining a fundamental understanding of material behavior at the atomic scale under deformation and irradiation. He employs various methods, including density functional theory, molecular dynamics, object dynamics Monte Carlo, and hybrid molecular dynamic/Monte Carlo simulations. His work revolves around complex metallic alloys, such as high and medium entropy alloys, and high entropy metallic glass. Specifically, he investigates the creation and evolution of dislocations in crystalline materials induced by irradiation or deformation and their interactions with other microstructures, such as nano-precipitates and grain boundaries in high and medium entropy alloys. This research is essential for designing novel materials for harsh environments through atomistic simulations and collaboration with experimental groups.

He has co-authored 18 peer-reviewed journal papers, cited over 190 times, and maintains an H-index of 9. Dr. Esfandiarpour actively shares his knowledge at major conferences, thanks to two international postdoctoral experiences collaborating with experts like Professor Mikko Alava, Professor Kai Nordlund, and Professor B.J. Lee. He serves as a Review Editor for Frontiers in Materials/Computational Materials Science and has reviewed more than 30 manuscripts for Elsevier journals since 2020. He has also co-supervised Master's and Ph.D. theses.

In addition to his research pursuits, Dr. Esfandiarpour has invested in personal development through workshops, such as "Intercultural Collaboration and Communication for Team Leaders" in Warsaw on May 26th, 2023, to enhance his leadership and collaboration skills. He is currently organizing a symposium on high entropy alloys as part of the "Multiscale Materials Modeling (MMM11)" conference, scheduled to be held in Prague next year.

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Design of Multicomponent Alloys Based on Lattice Distortion, Short-Range Order, and Core Dislocations

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Designing alloys that are both ductile and strong for structural materials is a challenging task. Given the inherent ductility of face-centered cubic (FCC) multicomponent alloys, our focus has been on designing strong multicomponent alloys with an FCC structure. This design approach is based on solid solution strengthening and the enhancement of strength through chemical short-range order (CSRO).

In the initial phase, we explore depinning stress in several equimolar Cantor family alloys with an FCC crystal structure, such as CrCoNi, CrMnCoNi, CrFeCoNi, CrMnFeCoNi, and FeNi. Our findings reveal that CrCoNi exhibits the highest depinning stress, attributed to its significant lattice distortion and relatively high dislocation roughness.

Replacing Cr with V in the CrCoNi medium entropy alloy results in increased lattice distortion. According to the solid solution strengthening theory [1], this suggests that VCoNi may exhibit greater strength compared to CrCoNi. Thus, in the second step we investigate the strength and lattice distortion of four VCoNi concentrated solid solution alloys (CSSAs) including $V_{0.33}Co_{0.33}$ $Ni_{0.33}$, $V_{0.35}Co_{0.2}$ $Ni_{0.45}$, $V_{0.33}Co_{0.17}$ $Ni_{0.5}$, and $V_{0.17}Co_{0.33}$ $Ni_{0.5}$. We find that the alloy composition $V_{0.33}Co_{0.17}$ $Ni_{0.5}$ displays the largest depinning stress at both 5 and 300 K.

In addition, to investigate the impact of CSRO on the strength of these alloys, we introduced CSRO into
the microstructure using two distinct approaches. The first method involved employing hybrid Molecular-dynamics/Monte-Carlo simulations to identify the most stable distribution of atom types in each alloy at various temperatures. It became evident that these simulations successfully generated CSRO within the microstructure. Moreover, we determined the CSRO motif and concentration in an equimolar VCoNi alloy through experimental results [2]. Subsequently, we replicated this experiment through modeling, introducing CSRO into the microstructure as our second method. By employing both techniques, we analyzed the influence of CSRO on the magnitude of depinning stress. Our results clearly demonstrated that in both methods, CSRO had a significant impact on the strength of non-equimolar VCoNi alloys.

References:

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SESSION 5
RADIOPHARMACEUTICALS SCIENCE

Bożena Sikora-Dobrowolska

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Dr. Bożena Sikora-Dobrowolska has been working as an assistant professor at the Institute of Physics of the Polish Academy of Sciences for 9 years. So far, she has been mainly involved in scientific and research work as part of numerous projects, one of which she managed independently. It quickly turned out that she was the leader of the team that she had founded and successfully managed so far (resulting in several publications and two defended doctorates, as well as numerous master's and bachelor's theses). She can conduct research in the fields of chemistry, biology, and physicochemical characterization, and in 2022 she additionally completed training in the basics of data analytics.

Dr. Bożena Sikora-Dobrowolska studied at the Faculty of Chemistry, University of Warsaw in Warsaw. In 2014, she received a Ph.D. title at the Institute of Physics of the Polish Academy of Sciences, Warsaw. Additionally, in 2012, she ended postgraduate studies in evidence law, criminology, and related sciences at the Center for Forensic Sciences of the University of Warsaw. She is a Research Group Leader at the Laboratory of Physics, Institute of Physics of the Polish Academy of Sciences. In her works, she designs, prepares, researches, and apply in biology, the multifunctional nanoparticles. She co-authored 25 journal papers cited over 300 times (H – 11).

In 2015, she spent one month at the School of Automation, Huazhong University of Science and Technology in Wuhan (China) in cooperation with Prof. Wenzhong Liu. During her stay, she characterized magnetic nanoparticles. Then, in 2016, she spent two months in Brazil at the Instituto de Fisica, Nfflcleo de Fsica Aplicada Universidade de Brasilia. During her stay, she carried out the characterization of magnetic nanoparticles in an alternating magnetic field (magnetic hyperthermia). Then in the next 2 months, she spent two months in Brazil at Depto de Genética e Morfologia CNANO - Instituto de Ciências Biológicas, Universidade de Brasília. As part of the internship, she conducted photodynamic therapy experiments on animal models.

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Multifunctional opto-magnetic nanoparticles with upconverting properties - designing, synthesis and applications in cancer diagnostic.

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The process of upconversion of infrared (NIR) light to visible light (VIS) has numerous potential applications in biology and medicine. In particular, up-converting nanoparticles (UCNPs) can be local light sources in the imaging of pathological tissues and can locally generate reactive oxygen species (ROS), capable of destroying cancer tissues. ROS production occurs by energy transfer from UCNPs emitting visible light to the photosensitizer located on their surface. The photosensitizer can effectively produce ROS that is harmful to cells.

Additionally, Fe_3O_4-based nanoparticles with magnetic properties (SPIONs) can be used in magnetic resonance imaging (MRI) as contrast agents. Also under the influence of an alternating magnetic field, they can cause a local increase in temperature, thereby causing the death of pathological tissues (hyperthermia). Our research aims to produce multifunctional opto-magnetic nanoparticles based on upconverting β-$NaYF_4$ doped with rare earth ions connected with the magnetic Fe_3O_4. The β-$NaYF_4$ nanoparticles are encapsulated in SiO_2. The Fe_3O_4 nanoparticles or photosensitizers capable of generating ROS are covalently attached to the surface of β-$NaYF_4$@SiO_2 nanoparticles.

The research showed that under the influence of NIR light, the upconversion of β-$NaYF_4$ nanoparticles causes the stimulation of photosensitizers (Rose Bengal) and the generation of reactive oxygen species. The Fe_3O_4 magnetic nanoparticles used in hyperthermia cause an increase in temperature under the influence of an alternating magnetic field in an aqueous solution.

The use of these nanoparticles on 4T1 cancer cells resulted in a significant decrease in their survival under the influence of an alternating magnetic field or NIR compared to studies without the use of stimulating factors.

In conclusion, multifunctional upconverting nanoparticles show potential in applications in biology and medicine.

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Dr Joanna Giebułtowicz studied at the Faculty of Pharmacy, Medical University in Warsaw. In 2011, she received her Ph.D. degree, while in 2017, she obtained the title of Doctor Habilitus (D.Sc.) in pharmacy. She works at the Department of Drug Chemistry, Pharmaceutical and Biomedical Analysis at the Faculty of Pharmacy, Medical University in Warsaw. She had research scholarships at the Department of Pharmacy at UCLAN University in Preston (England), Physiolution GmbH (Germany), and Jihočeská univerzita v Českých Budějovicích (Czech Republic). She also completed a teaching internship at Iuliu Haţieganu University of Medicine and Pharmacy. She is a member of the Faculty Council and the Pharmaceutical Sciences Discipline Council. In her work, she has primarily focused on the development, validation, and application of various analytical methods for determining pharmaceuticals in clinical and environmental matrices, as well as the detection and structure elucidation of unknown metabolites, impurities, and degradation products of pharmaceuticals and ingredients of dietary supplements. She also applies liquid chromatography coupled with mass spectrometry in targeted and untargeted metabolomics, especially pharmaco-metabolomics. She is a member of Polish Pharmaceutical Society and Polish Society of Mass Spectrometry.

Dr Giebułtowicz has co-authored over 100 journal papers cited more than 1,000 times (H-index: 19 WoS). She is a multiple recipient of scientific awards from the Rector of the Medical University of Warsaw. Dr Giebułtowicz has served as a manager, coordinator, key researcher, or researcher in several projects funded by Polish agencies (NCN, MEiN) and the European Commission. She has supervised six Ph.D. theses and more than 35 MSc students. In 2021-2022, she was the Deputy Head of the organizing committee of the Interdisciplinary Conference of Drug Sciences, ACCORD 2022. Currently, she is the Head of the organizing committee for the Interdisciplinary Conference of Drug Sciences, ACCORD 2024.

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Application of metabolomics in pharmacy

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Metabolomics is a relatively new field within systems biology, alongside genomics and proteomics, and as such, it is still an emerging area of research with many unanswered questions. One of the key interests in pharmacometabolomics is predicting an individual's response to a drug or understanding the drug's behavior by analyzing small compounds (metabolites from various metabolic pathways) found in the patient's bodily fluids. Importantly, this predictive testing can be conducted using samples collected before the first administration of the drug.

Metabolites from different metabolic pathways, such as carbohydrate and sugar metabolism, lipid and fatty acid metabolism, nucleotide and nucleoside metabolism, protein and amino acid metabolism, and steroid metabolism, can be employed to differentiate between groups (responders vs. non-responders), predict severe side effects, or assess pharmacokinetic parameters. The advantage of this phenotypic approach is that metabolite levels reflect the influence of various factors affecting drug metabolism, including environmental factors, genetic variability, and enzyme activity.

During the presentation, I will provide an overview of the applications of metabolomics in the field of pharmacy

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Dr Izabela Cieszykowska works as an assistant professor at NCBJ Radioisotope Centre POLATOM. She graduated from the Faculty of Chemistry of Nicolaus Copernicus University (Toruń, Poland) in 2000. She received her PhD in chemistry from the Institute of Nuclear Chemistry and Technology (Warsaw, Poland) in 2007. In 2023, she completed postgraduate studies in Clinical Research Methodology at the Medical University of Warsaw. In the early years of her professional career, she conducted research on the manufacturing of sealed radioactive sources used in brachytherapy, such as 125I seeds and 106Ru and 125I ophthalmic applicators, as well as 57Co sources used in Mössbauer spectroscopy. In subsequent years, she focused her interests on producing radionuclides and radiopharmaceuticals used in nuclear medicine and related regulatory issues.

She was involved in numerous Polish and international research projects, e.g., aimed at producing 99Mo from LEU fission products, 99Mo and 99mTc in cyclotrons and linear accelerators, 44Sc in cyclotrons, and 47Sc nuclear reactors. She is the Head of the Laboratory of Radionuclides in the R&D Department. She deals with producing 177Lu and 90Y-based radiopharmaceutical investigational medicinal products used in treating neuroendocrine tumors as part of a non-commercial clinical trial founded by the Medical Research Agency in Poland. She is the internal auditor of the PN-EN ISO 9001 and GMP quality system in radiopharmaceuticals production and worked as an IAEA technical expert in GMP production of radiopharmaceuticals. She co-authors many scientific articles in international journals and one patent and is a reviewer of articles in scientific journals. She is also involved in educational activities. She is a member of the scientific council of NCBJ in the 2021-2025 term.

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CERAD project and 30 MeV cyclotron for medical isotope production in Poland

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CERAD project - Center of Design and Synthesis of Radiopharmaceuticals for Molecular Targeting is the new research facility being built at NCBJ/POLATOM. Its main component is a 30 MeV cyclotron (Cyclone 30XP, IBA) which will accelerate protons and alpha particles to 30 MeV and deuterons to 15 MeV. This powerful tool will be employed for the production of novel radioisotopes for medical use, which were not available in Poland up to today such as F-18, Sc-44/43, Cu-64, Cu-67, Ge-68, Zr-89, I-123, and At-211. Installation of a new high-current cyclotron at NCBJ, with equipment and infrastructure combined with an already existing scientific base, creates unique and pro-development research capabilities, offering new possibilities to design innovative radiopharmaceuticals. The CERAD project has found its place on the Polish Roadmap of Large Research Infrastructure. This project is co-financed under the Smart Growth Operational Programme 2014-2020, Priority IV: INCREASING THE RESEARCH POTENTIAL, Measure 4.2. Development of modern research infrastructure of the science sector.

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Dr. Karolina Zajdel studied at the Pomeranian Medical University (Szczecin, Poland) where she defended MSc thesis "The analysis of the effect of non-physiological concentrations of human growth hormone on the cell cycle of hematopoietic cells, with particular insight into cell proliferation" in 2013 at the Faculty of Medicine, Biotechnology and Laboratory Medicine. Next, she received PhD degree with distinction in the field of Medical Sciences and Health Sciences (defense 2022) at the Mossakowski Medical Research Centre Polish Academy of Sciences (Warsaw, Poland) in the Electron Microscopy Research Unit, title of thesis "Assessment of functionality and cytotoxicity of NaYF4:Yb3+-Er3+ luminescent nanoparticles for bio-medical applications".

Currently, she is a member of Novel Radiopharmaceuticals for Medical Purposes group at the NOMATEN Centre of Excellence in the National Centre for Nuclear Research (Otwock, Poland). Dr. Zajdel works on radiolabeling with metallic radionuclides of various up-converting nanoparticles (UCNPs) doped with rare-earth ions (e.g. Er3+-Yb3+, Ho3+-Yb3+ or Tm3+-Yb3+) to obtain multimodal diagnostic or theranostic nanotracers.

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Radiolabeling of up-converting nanoparticles for theranostic applications

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Various types of nanostructures are undergoing intensive development and their innovative applications are featured in biological and medical sciences. Currently, among the available nanostructures, the new generation of up-converting nanoparticles (UCNPs), doped with rare-earth ions, is of great interest due to their luminescent properties. The specific pairs (e.g. Er^{3+}-Yb^{3+}, Ho^{3+}-Yb^{3+} or Tm^{3+}-Yb^{3+}) can naturally emit radiation in the visible or UV range when exposed to near-infrared. Luminescence emission is based on a nonlinear optical process called energy up-conversion. This process enables the observation and tracking of UCNPs inside cells and tissues, making them effective and sensitive optical nanosensors. This phenomenon is also very beneficial, because it facilitates deep tissue imaging, reduces background signal, allows for multi-color emission, and ensures high photostability.

Current attempts are focused on exploring the integration of rare-earth ions and radioisotopes into a single nanoparticle. Incorporation of both luminescent lanthanide ions and radioisotopes, makes possible to design dual-modal imaging nanomaterials suitable for applications in diagnostics. The combination of two distinct imaging modalities, such as fluorescence imaging (photoluminescence) and either Positron Emission Tomography (PET) or Single-Photon Emission Computed Tomography (SPECT) enables acquisition of complementary information, better image visualization and interpretation. So far, the UCNPs have been efficiently labeled with radioisotopes, including diagnostic like ^{18}F, ^{64}Cu, ^{68}Ga and ^{124}I, as well as therapeutic like ^{90}Y, ^{125}I, ^{153}Sm and ^{177}Lu.

In our studies, narrowly size-distributed $NaYF_4$:Yb^{3+}/Er^{3+} UCNPs with a hexagonal crystal structure and strong green/red luminescence were synthesized. Creating a luminescent nanoparticle with radiodetection capability would offer an innovative nanotracer for biomedicine. We have chosen to combine unique properties of $NaYF_4$:Yb^{3+}/Er^{3+} UCNPs with ^{90}Y to create a theranostic agent as ^{90}Y is a β^--particle emitter used for treatment in nuclear medicine. To avoid potential yttrium leakage, we plan incorporation of radioactive ions into the core matrix surrounded by a shell. The core-shell strategy ($NaYF_4$:Yb^{3+}/Er^{3+}@$NaYF_4$) enables the combination of unique features of nanoparticles and their tailoring to bind with specific ligands such as drugs, peptides or antibodies. Therefore, the next phase of research will focus on further functionalization of UCNPs surface using various polymers followed by coupling to biomolecules. Such an approach of nanoparticle modification presents prospect to produce highly advanced theranostic nanomaterials capable of integrating targeted cancer therapy and diagnostics within a single nanoplatform.

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PhD Eng. Marcin Zieliński studied at the Interdepartmental Study of Biotechnology at the Warsaw University of Life Sciences (SGGW). Biotechnology is a multidisciplinary field as it integrates the coordinated use of different fields such as biochemistry, genetic engineering, molecular biology, microbiology and structural biology. In 2017, he received a PhD title at the same university.

In his previous scientific and research work at the Department of Bioengineering of the Institute of Biotechnology and Antibiotics (IBA) in Warsaw (2005-2020), he conducted development work in the field of genetic engineering, molecular biology, biochemistry and microbiology. He was mainly involved in developing technologies for obtaining, isolating and purifying human recombinant proteins - mainly with therapeutic applications, e.g. human insulin and its analogues, growth hormone, interferons (α, β, γ), monoclonal antibodies. Some of the technologies developed at the Institute were implemented into production by Bioton S.A. company, for which IBA was initially a R&D base.

Another important achievement was participation in the project "Research on a vaccine against the SARS-CoV-2 virus and support for research work on the search for an effective therapy." As part of this project, he participated in the development of a technology for obtaining the recombinant MPro protease of the SARS-CoV-2 virus in *Escherichia coli* bacteria. Currently, he works at the National Centre for Nuclear Research. He started working in Radiological Metrology and Biomedical Physics Division where he was involved in radiobiological research, cancer biology and research on the impact of ionizing radiation on cells. Then he joined the NOMATEN Centre of Excellence Novel Radiopharmaceuticals for Medical Applications Research Group for a position Assistant Professor / Research specialist in *in vitro* assays. He is responsible for conducting *in vitro* cell cultures (mainly cancer cell lines) and for preclinical evaluation of developed compounds - radiopharmaceuticals (e.g. specificity, affinity, immunoreactivity, internalization, toxicity, clonogenic test, comet test, double-stranded DNA damage - histone γ-H2AX foci test and other).

He is the author/co-author of 8 papers in journals such as Protein Expression and Purification, Virology Journal, Plasmid, Cellular & Molecular Biology Letters, Reports of Practical Oncology and Radiotherapy and 26 conference posters. He holds 5 national and international patents. He participated in over 25 courses/trainings, e.g. techniques for overproduction and purification of recombinant proteins, Western blotting, proteomics, protein electrophoresis, mammalian cell cultures, stem cells & transfection, bioluminescent reporter gene systems, training in the use of the device capillary electrophoresis ProteomLAB PA 800 Protein Characterization System and FACSAria Becton Dickinson flow cytometer. He is a member of the Polish Radiation Research Society and the Polish Society of Nuclear Medicine.

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Differences in the biological response of MCF-7 breast cancer cells and healthy MCF-12A breast cells in conventional and ultra-high dose rate radiotherapy

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Radiotherapy (RT) with other treatments, such as surgery and chemotherapy is used to treat over 50 % of cancer patients. It remains highly efficient at eliminate cancer cells and regardless of significant technological improvements related to tumor targeting by image-guidance, the dose required for tumor control is still limited by normal tissue toxicity. Ultra-high dose rate radiotherapy delivers RT in milliseconds and has been associated in preclinical studies with less side effects on healthy tissues, when compared to conventional dose rate RT (CONV) delivered in minutes, while the effect on tumors appeared similar. The exact biochemical mechanisms that cause the FLASH effect have not yet been fully elucidated. Generally, in response to ionizing radiation, indirect DNA damage occurs through radiolysis of water and the subsequent formation of reactive oxygen species (ROS) which damage DNA. To confirm differencesin the response to the postulated depletion of the intracellular oxygen pool and to assess its consequences, several more detailed *in vitro* studies are needed - for example, the examination of the corresponding levels of DNA damage and the subsequent response to DNA damage. In these preliminary studies, it was planned to use the Western blot method to examine (at the protein level) the response of selected cell lines to doses of ionizing radiation typical for conventional and ultra-high dose rate radiotherapy. MCF-7 and MCF-12A cells have been subjected to electron beam irradiation at two different doses: 0.083 Gy/s and 10 Gy/s. Cell lysates were used for proteomic analysis with the following sets of antibodies: 1) Oxidative stress defense Western blot cocktail, 2) Non-homologous end joining antibody panel, 3) DNA damage kinases panel and 4) Cell cycle and apoptosis Western blot cocktail. The use of these antibody panels allowed us to take a very broad look at the proteomic changes taking place in the examined cells depending on the method of radiotherapy.

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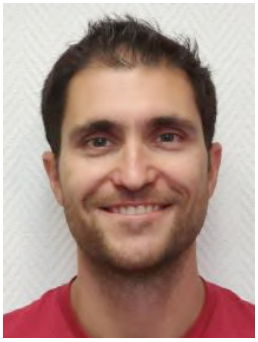

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Fabien CAILLÉ is a radiochemist at the Service Hospitalier Frédéric Joliot (SHFJ) of the French Atomic Energy Commission (CEA) in Saclay and member of the UMR "Laboratoire d'imagerie biomédicale multimodale Paris-Saclay (BIOMAPS)" research unit. Graduated from the engineer school of chemistry of Toulouse in 2008, Fabien Caillé completed a PhD in organic chemistry and physico-chemistry at the University of Orléans in 2011 under the supervision of the Pr. Franck Suzenet and Dr. Eva Jakab Tóth. His work was dedicated to the synthesis and characterization of bimodal contrast agents for MRI and optical imaging. In 2012, Fabien Caillé moved to New Haven CT (USA) to work under the supervision of Pr. Gilles Tamagnan at Molecular Neuroimaging LCC in collaboration with the University of Yale to the design and labeling of radiotracers for PET imaging of neurodegenerative disorders. In 2013, Fabien Caillé completed a second post-doctoral fellowship at the University of Rouen under the supervision of Pr. Géraldine Gouhier to synthesize cyclodextrin-based smart contrast agents for MRI. Since the end of 2013, Fabien Caillé hold a permanent position at the CEA-SHFJ in the research group of Dr. Bertrand Kuhnast focusing on the development of carbon-11 and fluorine-18 labeled radiotracers for PET imaging. He is also the head of the radiochemistry production platform for preclinical applications. Fabien Caillé is the co-author of 60 peer-reviewed scientific publications and 1 book chapter in the field of chemistry applied to medical imaging. He has been the coordinator of 8 financed scientific projects and is a leader of the SRS-TT international forum.

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Late-stage carbon-11 radiolabeling directly from CO_2: from chemistry to drug PET imaging

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Carbon-11 ($t_{1/2}$ = 20.4 min) is a radioisotope of choice for positron emission tomography (PET) imaging. Applied to drug isotopic labeling, carbon-11 and PET imaging are powerful tools to support pharmaceutical development.

Carbon-11 is produced in a cyclotron as carbon dioxide $[^{11}C]CO_2$. To date, the majority of radiolabeling approaches is reduced to methylations with methyl iodide/triflate synthesized from $[^{11}C]CO_2$ through time-consuming processes with moderate yields, limiting the scope of radiotracers to methylated molecules. There is therefore a need to develop new carbon-11 labeling strategies directly from $[^{11}C]CO_2$ to broaden the scope of radiolabeled molecules of interest.

The CEA-SHFJ and the CEA-SCBM have developed several innovating labeling strategies to meet this need. A Staudinger/aza-Wittig sequence was developed to trap $[^{11}C]CO_2$ and form inter or intramolecular ureas and carbamates.[1–3] This strategy was applied to the radiosynthesis of [^{11}C]domperidone to study the brain penetration of this antiemetic drug with PET.[4] The development of a redox equilibrium between potassium formate and $[^{11}C]CO_2$ enabled the formation of the radical anion $[^{11}C]CO_2^{\cdot-}$ to afford carboxylic acids *via* the Giese addition on alkenes.[5] This was exemplified to explore the biodistribution of [^{11}C]oxaprozin in healthy mice with PET. Finally, a photo-induced reduction of $[^{11}C]CO_2$ with [Re] and [Ru] complexes afforded radiolabeled [^{11}C]CO, which is used in carbonylation reactions to form radiolabeled amides.[6]

These innovating radiolabeling approaches were automated to demonstrate their applicability to the production of radiotracers for PET imaging. However, carbon-11 radiochemistry has still a bright future ahead as many molecular scaffolds remain difficult to radiolabel.

[1]Del Vecchio *ACIE* **2018**, 9892; [2]Babin *Chem. Commun.* **2021**, 6680; [3]Del Vecchio *Chem. Commun.* **2020**, 11677; [4]Breuil *Pharmaceutics* **2022**, 1658; [5]Malandain *JACS* **2023**, 16760; [6]Monticelli *Nat. Commun.* **2023**, 4451.

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Steve Huvelle was born in 1989 in France. He graduated from Paris Diderot University in 2014. He received his Ph.D. from PSL University prepared in Curie Institute. During this time, his research focused on self-immolative spacers and their applications in chemical biology. After post-doctoral studies in the University of Tours working on antibody-drug conjugates, he moved to ENSCP Chimie ParisTech in 2020 as a post-doctoral associate in organometallic catalysis. His current research fields include metal-catalyzed [2+2+2] cycloaddition reactions. He is currently post-doctoral fellow in the Development of Radiopharmaceuticals and Imaging Agents team and carrying out syntheses of new radiotracers for PET imaging of infectious diseases.

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 857470

Development of radiochemical tools for PET imaging of HIV infection

Steve Huvelle[1,2], Antoine Pinon[1], Christine Coulon[1], Catherine Chapon[2], Thibaut Naninck[2], Roger Legrand, Bertrand Kuhnast[1], Fabien Caillé[1]

[1] Université Paris-Saclay, Inserm, CNRS, CEA, Laboratoire d'Imagerie Biomédicale Multimodale Paris-Saclay (BioMaps), 91401 Orsay
[2] Université Paris-Saclay, Inserm, CEA, Center for Immunology of Viral, Auto-immune, Hematological and Bacterial diseases (IMVA-HB/IDMIT), Fontenay-aux-Roses, France.

Increasing evidences are making remission an achievable goal for new anti-HIV therapies. Safer and more potent antiretroviral drug (ARD) combinations can significantly improve control of viremia and open the way for new strategies aiming at minimizing the viral reservoir. Early control of these reservoirs together with the limitation of pharmacological sanctuaries where the exposure to ARD is suboptimal are among the key scientific challenges to address. New in vivo imaging technologies may be of considerable help to tackle with anti-HIV therapy challenges.

Positron emission tomography (PET) is the state-of-the-art molecular imaging technique to quantitatively assess kinetics of drugs diffusion and physiological changes at the whole-body scale in real time. The aim of this work is to radiolabel both antiretrovirals and a HIV-recognizing antibody in order to determine the drug biodistribution and the viral particles locations in vivo. Dolutegravir is a integrase strand transfer inhibitor ARD which can be isotopically radiolabelled with fluorine-18, a radioisotope of choice for PET imaging. We have recently described the radiosynthesis of [^{18}F]Dolutegravir in a three-step process in 5% radiochemical yield (RCY). Aiming at clinical applications for this radiotracer, we have developed a novel two-step radiosynthesis of [^{18}F]Dolutegravir from a trimethyltin precursor based on a copper-mediated radiofluorination. Optimization of the reaction conditions afforded [^{18}F]Dolutegravir in 20% RCY. This strategy was automated on a kit-based, pharmaceutically compliant, AllInOne® synthesizer and a full quality control according to the European Pharmacopeia guidelines was realized to demonstrate that ready-to-inject [^{18}F]Dolutegravir was suitable for human injection. We believe that this study will grow our knowledge about HIV persistence and will give us new therapeutic options to treat-and not only contain- this disease.

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 857470

Marie-Pierre Heck

CEA Centre de Saclay
DRF/JOLIOT/DMTS/SCBM
Université Paris-Saclay
91191 Gif sur Yvette cedex, France

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Dr. Marie-Pierre Heck studied organic chemistry at the University Louis Pasteur of Strasbourg (France). In 1994, she obtained a Ph.D. degree at the University of Strasbourg on the synthesis of glycosylated amidines of therapeutic interest under the supervision of Dr. Charles Mioskowski. Then, she completed a 2 years post-doctoral training with Prof. Chi-Huey Wong at the Scripps Research Institute (La Jolla, California) where she developed glycosidase inhibitors and Sialyl Lewis X Mimetics.

Since 1996, she has been working at the Commissariat à L'Energie Atomique (CEA, Alternative Energies and Atomic Energy Commission of France) where she is leading the chemistry group "Development of new methodologies in organic synthesis and synthesis of bioactive molecules". In 2008, she received the Habilitation à Diriger des Recherches in chemistry from the University of Paris IX, called now University Paris-Saclay. Her main fields of interest are organic chemistry in relation and applications to biological problems, sugar chemistry, macrocyclic chemistry, supramolecular assemblies, cage-molecules for gas encapsulation and macrocycles for anions chelation for labeling, imaging and therapy applications. She has coordinated the ANR GHOST project (2009-2012, "Water-soluble cucurbiturils for gases sensing," 3 partners), she was work package leader in the European FP7 METACODE Project (2011-2015, "Code-engineered of new- microbial cell factories", involving 8 partners from 5 European countries) and she was work package leader in the ANR M3ODALITY project (2017-2022, "Innovative dual PET/NIRF tools for molecular imaging", 4 partners). Since 2021, she is research director and CEA expert senior for chemistry. Marie-Pierre Heck has supervised 11 PhD students, 7 post-docs and > 20 Master students.

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 857470

New multivalent scaffolds for anions and radioanions binding

Marie-Pierre HECK,[1] Elise Cartier,[1] Julie Patissou[1]*

[1] SCBM, CEA-Saclay, Université Paris-Saclay, France
marie-pierre.heck@cea.fr

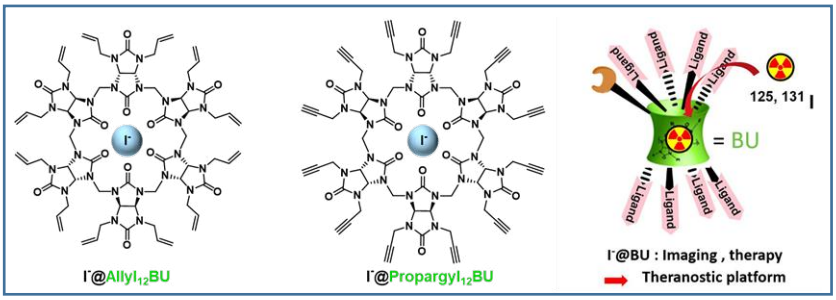
Anions are ubiquitous in nature and play important roles in biological mechanisms, clinical diagnosis, industries and environment. There recognition and monitoring are of primordial importance. Numerous progress have been achieved in supramolecular chemistry, but when considering anions of large sizes, various geometries, and being sensitive to pH, the design of efficient anion receptors operating in water is very challenging.

Among them, Iodides owning a large atomic radius with low charge density, are the most difficult halides to complex. Scaffolds allowing the binding of radioactive isotopes $^{131}I^-$, $^{123}I^-$, $^{124}I^-$ and $^{125}I^-$ are expected to find radiopharmaceutical applications.

Bambusurils, BU[6], are cyclic oligomers that can strongly encapsulate anions inside their cavity thanks to twelve C-H--X$^-$ bounds.[1] These neutral cavitands with a jigger-like conformation are prepared from a cheap and easy synthesis, and can be functionalized with various groups to be soluble either in organic or in aqueous media. It was shown that BU exhibit highly specific recognition for iodides in organic media making them the most efficient sequestering agents currently known.

In our laboratory, two families of bambusurils, allylBU[6][2] and propargyBU[6],[3] have been developed and post-functionalized by various chemical groups to increase their water solubility, and their affinity constants for iodides.[3,4] Furthermore, we have also shown that BU can be used as multivalent plateforms to link ligands such as oligosaccharides. Thus, multivalent glycosylBU platform bearing 8 to 24 iminosugars derivatives has demonstrated great efficiency for glycosidase inhibition.[5]

Disposing of such radiopharmaceuticals based on anion-chelation for a late stage labeling and able to target biological receptors should be a major breakthrough in nuclear medicine.



[1] a) Svec, J.; Necas, M.; Sindelar, V. *Angew. Chem., Int. Ed.* **2010**, *49*, 2378; b) Lizal, T.; Sindelar, V. *Isr. J. Chem.* **2018**, *58*, 326; [2] Rivollier, J.; Thuery, P.; Heck, M.-P. *Org. Lett.* **2013**, *15*, 480.
[3] Lafosse, M.; Cartier, E.; Solmont, K.; Rivollier, J.; Azazna, D.; Thuéry, P.; Boulard, Y.; Gontier, A.; Charbonnier, J.-B.; Kuhnast, B.; Heck, M.-P. *Org. Lett.*, **2020**, 22, 3099.
[4] D. Azazna, M. Lafosse, J. Rivollier, J. Wang, I. Ben Cheikh, M. Meyer, P. Thuéry, J.-P. Dognon, G. Hubert, M.-P. Heck, *Chem. Eur. J.*, **2018**, 24, 10793.
[5] Lafosse M., Liang Y., Schneider J. P., Cartier E., Bodlenner A., Compain P., Heck, M.-P. *Molecules* **2022**, *27*, 4772.

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 857470

During the 3rd Edition of the NOMATEN Winter School all preset PhD students presented their thesis subject in 180s (according to the rules of the MT180 competition). List of the PhD students together with the affiliation and research topic is given in the table below. Introductory slide and one-slide presentation prepared by each student are presented below the table.

Name of the PhD student	Affiliation	Thesis subject
DIF Brahim	VTT	*ITER-grade tungsten research: insights from crystal plasticity modeling and small punch test*
GAULI Bibesh	VTT	*Green aromatics production from lignocellulosic biomass via catalytic aromatization*
GNICHI Dina	CEA	*Understanding the corrosion mechanisms of zirconium alloys under an electric field*
HAUWELLE Alexandre	CEA	*Synthesis and carbon-11 isotopic labeling of Serodolin, a biased ligand of 5-HT7 receptors*
LI Yunli	NCBJ	*Design and preparation of Co-free high-entropy alloys with single FCC structure*
MAMMADLI Bakhtiyar	NCBJ	*Detecting material properties with digital image correlation and principal component analysis*
NAGHDI Amirhossein	NCBJ	*Machine learning interatomic potentials for mesoscale crystal defect modeling*
OLEJARZ Artur	NCBJ	*Low ball-to-powder-ratio sintered CoCrFeNi high entropy alloys: Cr-rich structure evolution and enhanced mechanical properties*
PATISSOU Julie	CEA	*Synthesis and evaluation of new supramolecular receptors for molecular imaging and therapy*
PONCHELLE Mathilde	CEA	*Theranostic micellar nanocarriers for imaging, targeted radiosensitization and internal radioisotope therapy*
SHOKAIR Ihab	NCBJ	*Copper-mediated nucleophilic approach for the radioiodination of various prosthetic groups*
SUCHORAB Kinga	NCBJ	*Understanding oxidation of zirconium and its alloys in air and water vapour operating conditions - high temperature Raman studies*
WYSZKOWSKA Edyta	NCBJ	*Impact of radiation damage on the structural and mechanical properties of fcc Ni_xFe_{1-x} single crystal alloys*

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 857470

NOMATEN Winter school
November 27-30, 2023
NCBJ, Otwock-Świerk, Poland

NOMATEN
Centre of Excellence in Multifunctional Materials for Industrial and Medical Applications

MT180 – PhD oral session

Teasing presentations for poster session

NATIONAL CENTRE FOR NUCLEAR RESEARCH ŚWIERK

cea

VTT

Chair : Frédéric Dollé (CEA) | Łukasz Kurpaska (NCBJ)

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 857470

DIF Brahim
GAULI Bibesh
GNICHI Dina
HAUWELLE Alexandre
LI Yunli
MAMMADLI Bakhtiyar
NAGHDI Amirhossein
OLEJARZ Artur
PATISSOU Julie
PONCHELLE Mathilde
SHOKAIR Ihab
SUCHORAB Kinga
WYSZKOWSKA Edyta

In collaboration with

via ADI UPSaclay co-tutelle (2022)

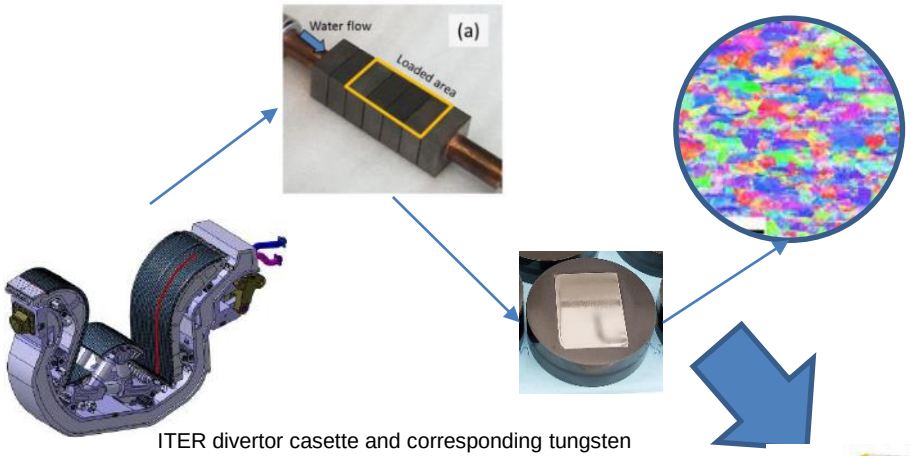
In collaboration with

Brahim Dif

ITER-grade tungsten research:
insights from crystal plasticity modeling and small punch test

VTT, Nuclear Energy group, Reactor Analysis

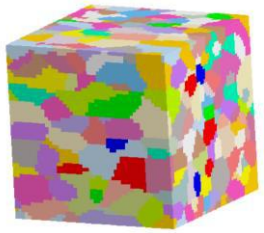
ITER-grade W research



ITER divertor casette and corresponding tungsten monoblocks

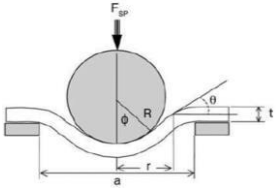
- SEM-EBSD maps of ITER-tungsten
- Polycrystalline morphology with Elongated grains

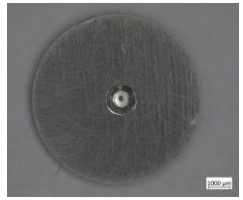
- Crystal plasticity modelling
- Initial Parametrization based on tensile data



Representative volume element

Tension along rolling direction





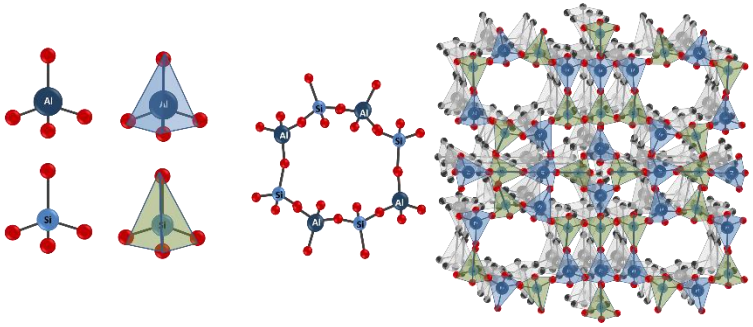
- Investigating W mechanical behaviour: Small punch testing (EN10371 standard 2021)
- Developing a rig to perform SP tests in hydrogen environment

Bibesh Gauli

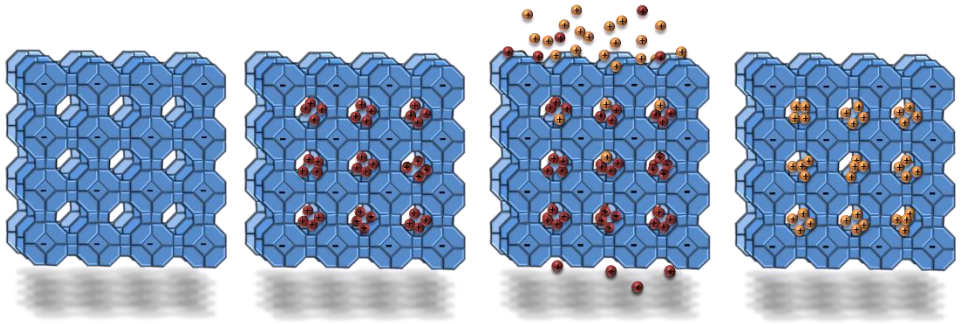
Green aromatics production from lignocellulosic biomass via catalytic aromatization

VTT, Chemical and polymer synthesis group

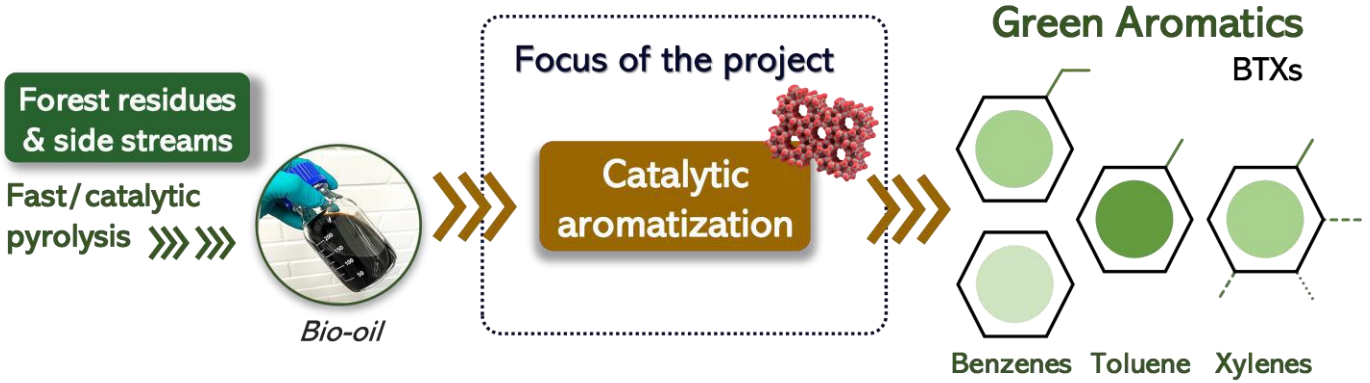
Funded by: BUSINESS FINLAND



The building blocks of 3D zeolite structures. Red is oxygen.



Zeolite cage structure (left), with mobile ions shown (second from left)



Process flow scheme to produce *BTX from biomass.

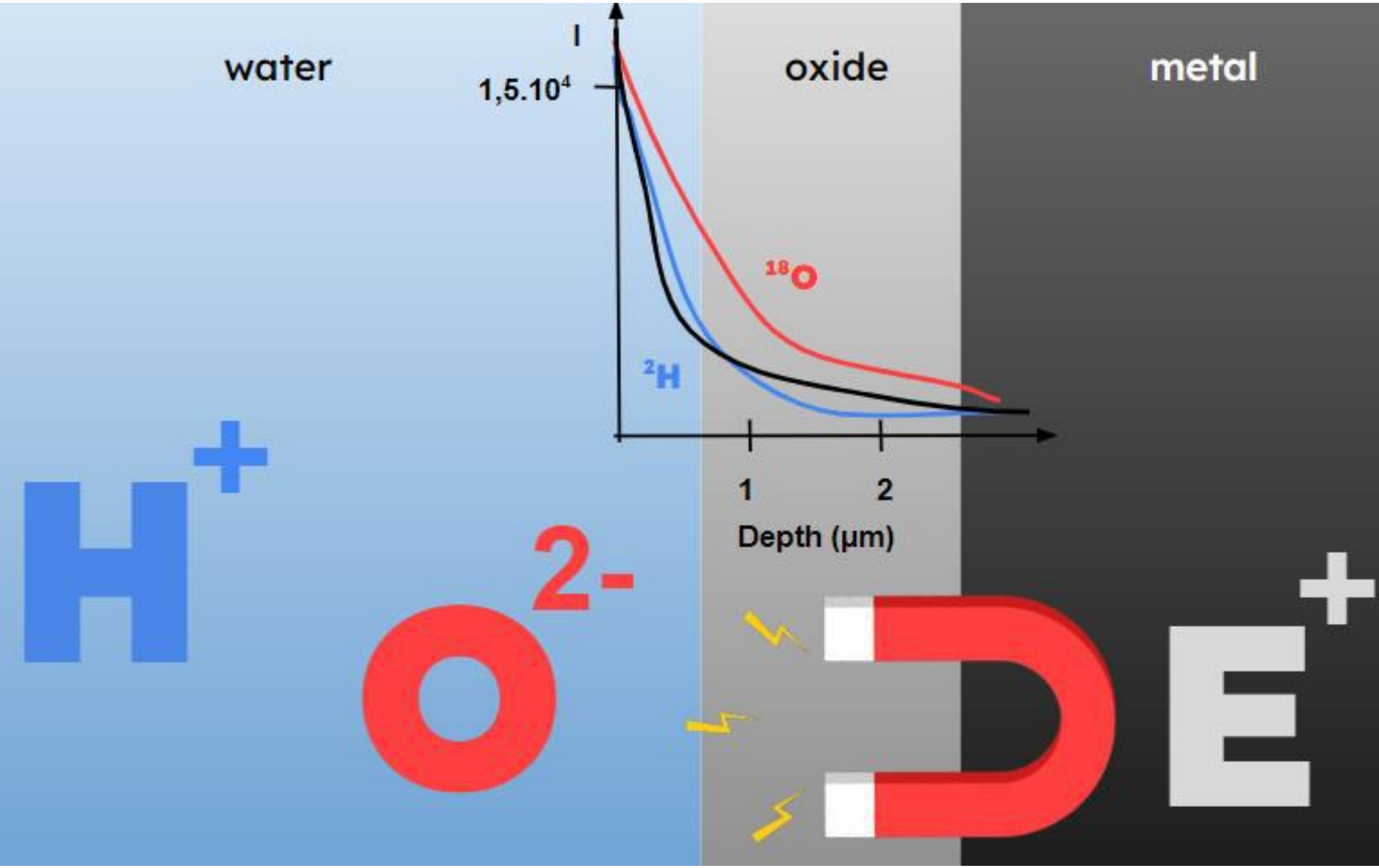
*BTX: Benzene, toluene, and xylene

Dina Gnichi

Understanding the corrosion mechanisms of zirconium alloys under an electric field

CEA / DES / DRMP / SEMI / LM2E

In collaboration with :


water
oxide
metal
I
1,5.10⁴
¹⁸O
²H
1
2
Depth (µm)
H+
O2-
E+

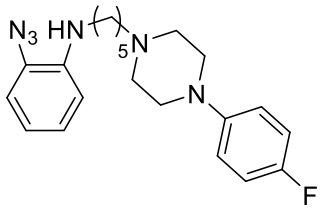
Alexandre Hauwelle

Synthesis and carbon-11 isotopic labeling of Serodolin, a biased ligand of 5-HT7 receptors

CEA / DRF / JOLIOT / SHFJ / BioMaps

Aim: PET imaging using isotopically labeled [^{11}C]Serodolin to better understand the distribution of this drug.

Precursor

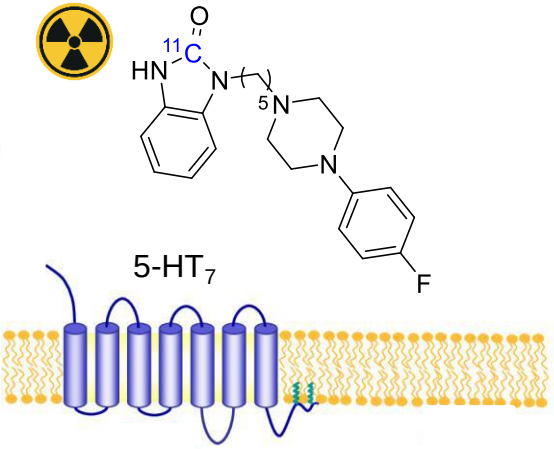


4 Steps Synthesis

Mel$_{plus}$ Research

Automated radiolabeling with [^{11}C]CO_2

Serodolin



In vivo PET imaging

RC Yield = 25%

Radiolabeling via Staudinger/Aza-Wittig with specific activity of **60 GBq/µmol**

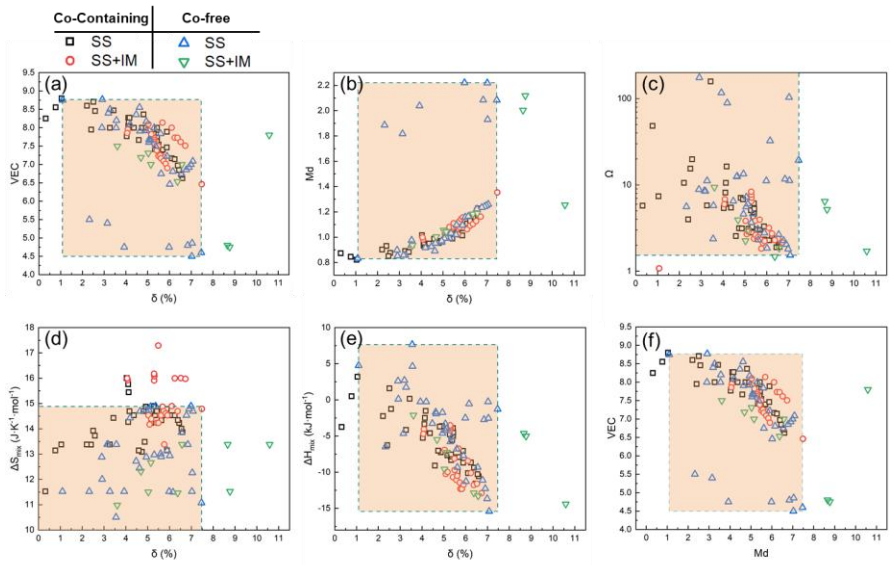
Yulin Li

Design and preparation of Co-free high-entropy alloys with single FCC structure

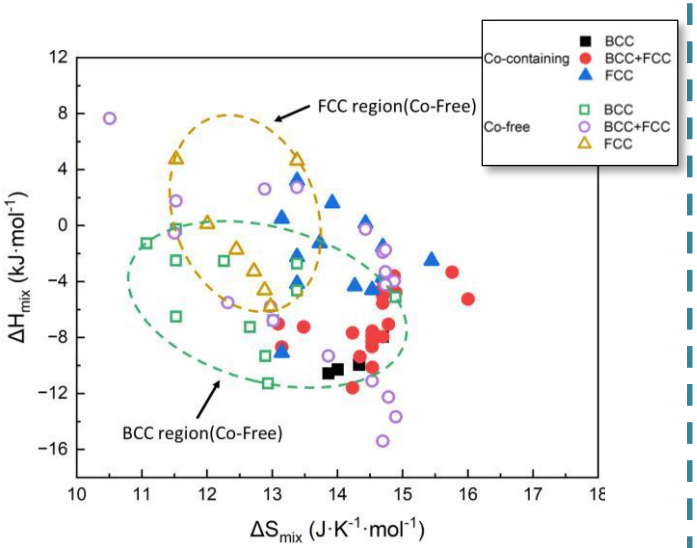
NOMATEN CoE, NCBJ, Functional Properties of Materials group

NATIONAL CENTRE FOR NUCLEAR RESEARCH ŚWIERK

Effect of physical parameters on phase stability in HEAs



Solid solution phases distribution in ΔH_{mix} - ΔS_{mix}



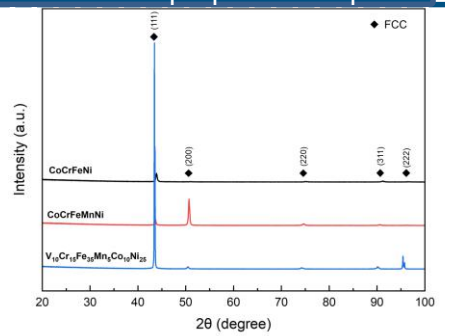
Solid solution formation rule in Co-free HEAs:

- **VEC:** < 8.77
- **Md:** < 2.22
- **ΔS_{mix}:** 10.51 ~ 14.90
- **ΔH_{mix}:** -15.40 ~ 7.66
- **Ω:** > 1.54
- **δ:** < 7.46

FCC phase formation rule in Co-free HEAs:

- **ΔS_{mix}:** 12.01 ~ 13.38
- **ΔH_{mix}:** -6.64 ~ 4.64

Structures of prepared samples



Parameters and structures of prepared samples

Materials	VEC	Md	ΔS_{mix}	ΔH_{mix}	Ω	δ	Structure
CoCrFeNi	8.25	0.874	11.53	-3.75	5.75	0.32	FCC
CoCrFeMnNi	8.00	0.890	13.38	-4.16	5.79	3.27	FCC
$V_{10}Cr_{15}Mn_5Fe_{35}Co_{10}Ni_{25}$	7.95	0.931	13.38	-6.26	3.98	2.41	FCC

Preparation: Arc melting, Characterization: X-ray diffraction

Bakhtiyar Mammadli

Detecting material properties with digital image correlation
and principal component analysis

NOMATEN CoE, NCBJ, Material Structure, Informatics and Function (MASIF) group

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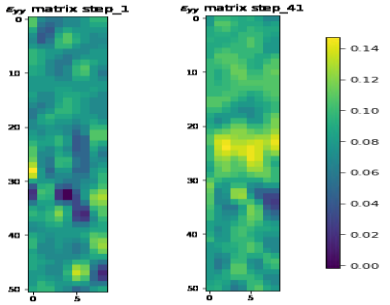
Detection of Yielding

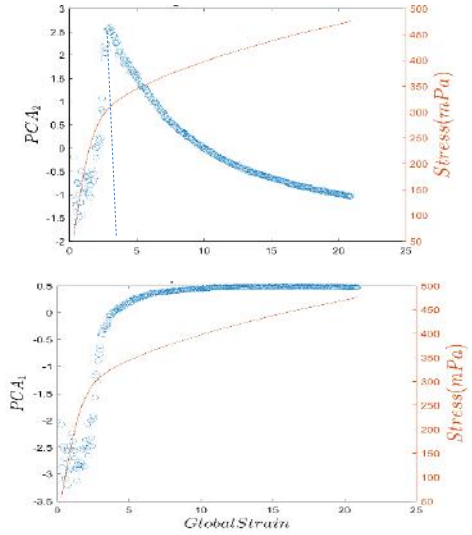
DIC test of $FeMnNiCo)_{100-x}Mo_x$,$x=5$

In collaboration with Dr. Krzysztof Muszka's team at AGH University of Science and Technology in Krakow, Poland

Before Yielding

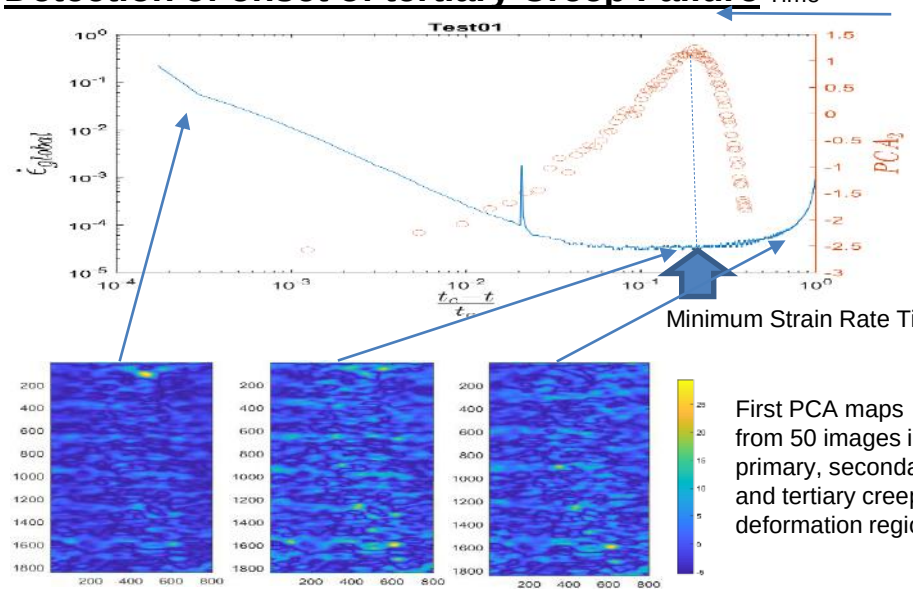
After Yielding





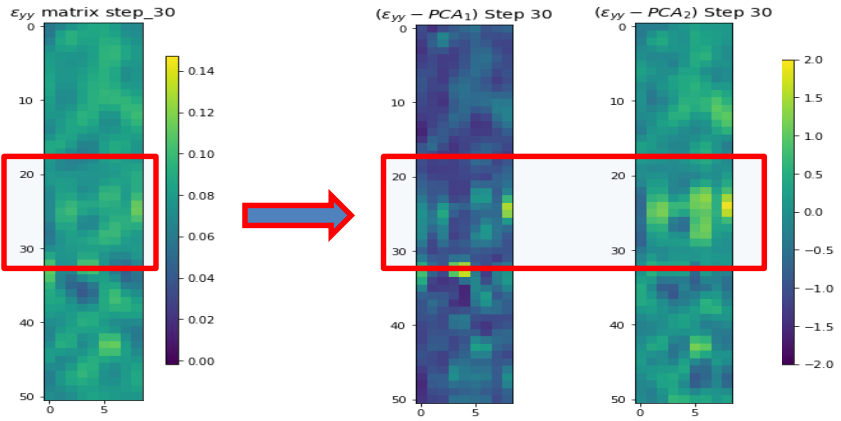
Detection of onset of tertiary Creep Failure

Time

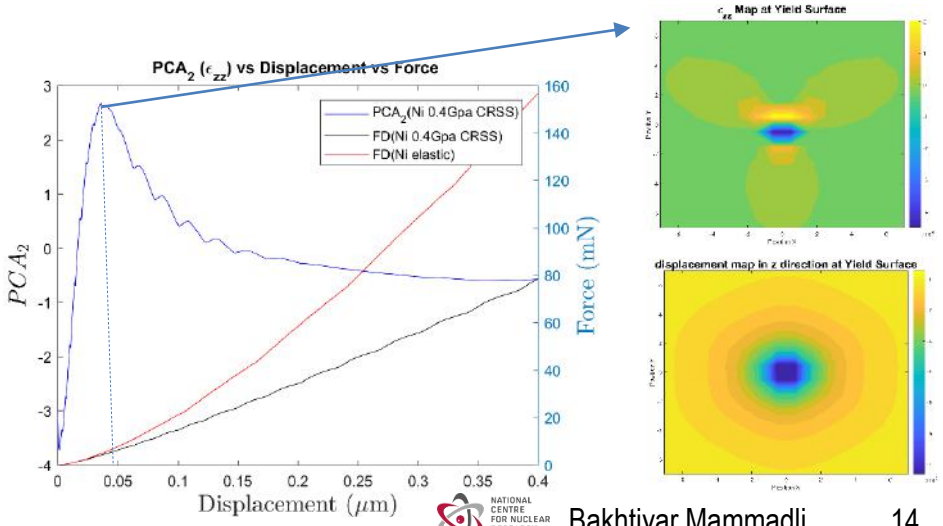


First PCA maps from 50 images in primary, secondary and tertiary creep deformation regions

Detection of Necking Instabilities



Detection of Indentation (CP-FEM) Yield Surface



Amirhossein Naghdi Dorabati

Machine learning interatomic potentials for mesoscale crystal defect modeling

NOMATEN CoE, NCBJ, Material Structure, Informatics and Function (MASIF) group

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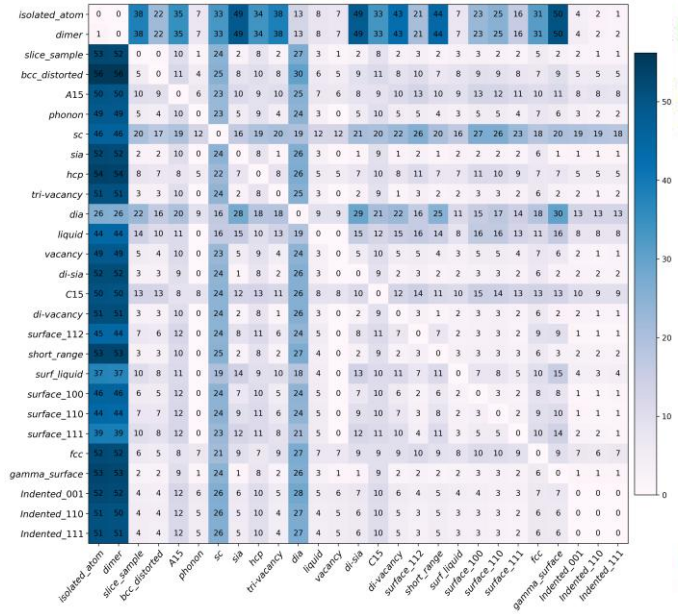
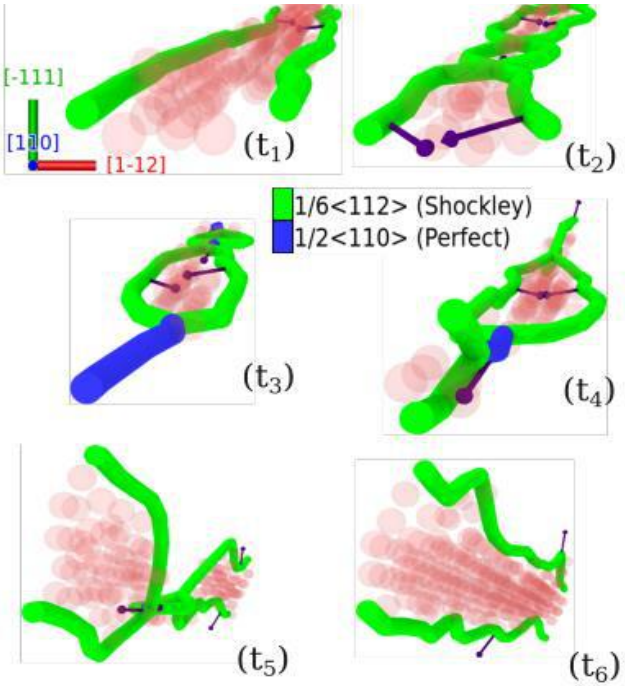
Project 1

Developed a novel method for MLFF developement



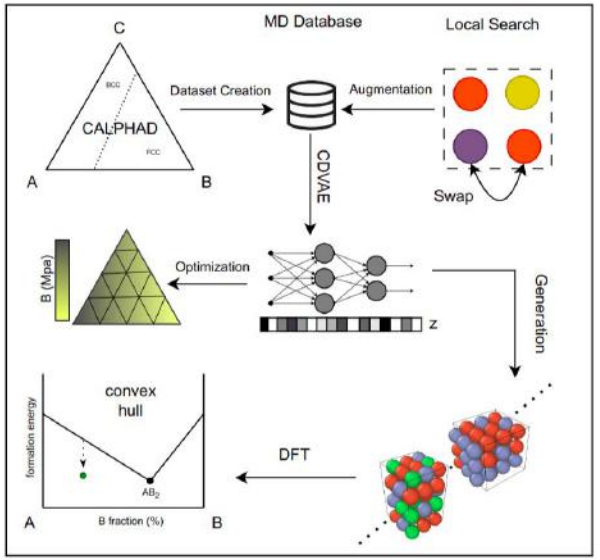
Project 2

Modeling of complex extended defects via MLFFs



Project 3

Composition search with deep generative models



Artur Olejarz

Low ball-to-powder-ratio sintered CoCrFeNi high entropy alloys: Cr-rich structure evolution and enhanced mechanical properties

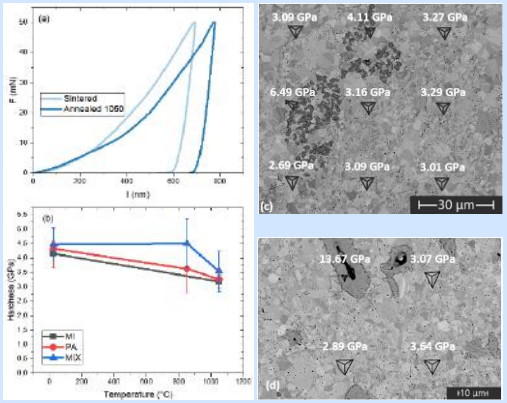
NOMATEN CoE, NCBJ, Functional Properties Group

NATIONAL CENTRE FOR NUCLEAR RESEARCH ŚWIERK

Process parameters

	Milling speed [rpm]	Milling intervals [min:min]	Pre-alloying process	BPR / PCA
MI (one-milling cycle)	250	15:15	No	**5:1 / C_7H_{18}**
PA (+Cr-Ni prealloying)	250	15:15	**10 h**	
MIX	**350**	**15:5**	**10 h**	

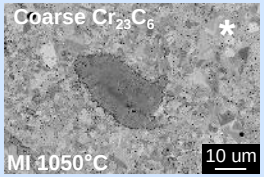
Hardness tests

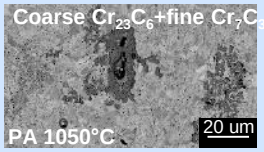


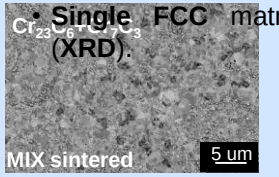
- Significant hardness stability of MIX sample;
- Nanohardness of reinforment phase up to 15 GPa and ~7 GPa for agglomerates (weighted average of matrix and precipitates);
- Results are consistent with microhardness

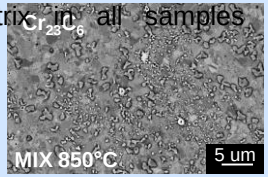
Microstructure observation

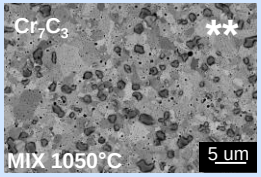
- Coarse **Cr-rich particles** formation after **one-milling cycle**;
- **Pre-alloying** process caused **Cr refinement** and **carbides clusters** formation;
- **Increased milling speed and intervals** caused almost **even distribution** of carbides;
- **Different carbides** are forming depending on **annealing temperature** and **process parameters (XRD/TEM)**;
- **Single FCC** matrix in all samples (**XRD**).











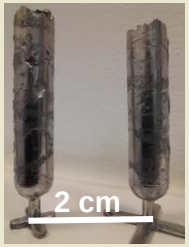
Process evolution

Annealing temperature

Conclusions

Process improvement -> Cr particles refinement during MA;
Annealing temperature -> carbides evolution (PCA addition);
Both together -> hardness improvement.

Arc melting – very soon



Ingots

After melting

After HT

* Starting point from previous research: A. Olejarz et al JAC 168196 ** Already submitted to Materials & Design

Julie Patissou

Synthesis and evaluation of new supramolecular receptors for molecular imaging and therapy

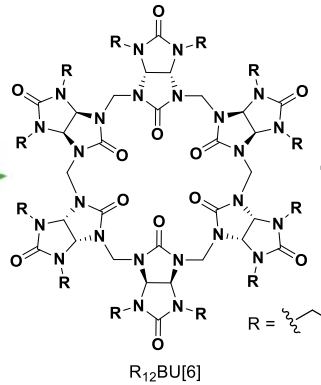
CEA / DRF / JOLIOT / DMTS / SCBM

In collaboration with :

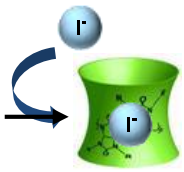
(ADI UPSaclay 2023 laureate, but JP choose the Doctoral School bursary for her thesis)

Synthesis and evaluation of new supramolecular receptors for molecular imaging and therapy

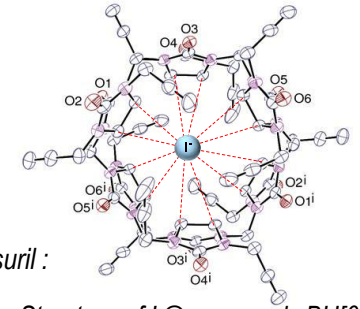
Bambusurils



$R_{12}BU[6]$



Structure of bambusuril : $I^-@R_{12}BU[6]$



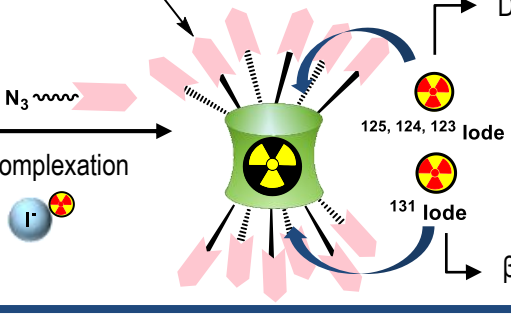
Structure of $I^-@propargyl_{12}BU[6]$

12 bonds C-H- - I^-

Functionalisation

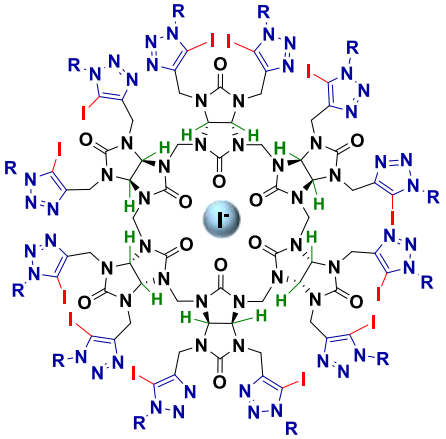
1) N_3

2) Complexation

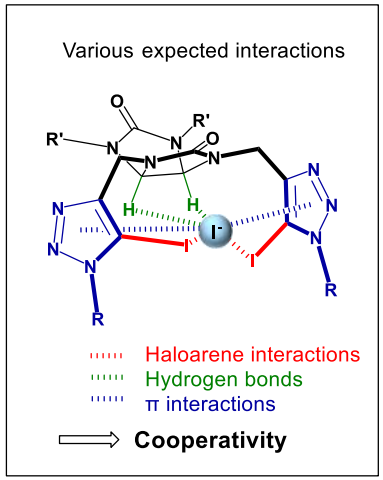


➢ Improve complexation by acting on the portal

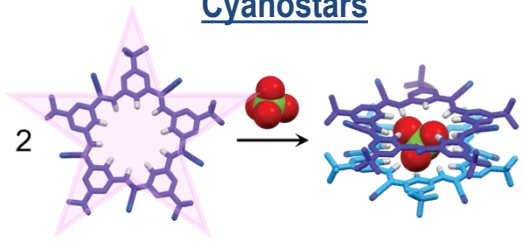
Haloarenes | π interactions | Hydrogen bonds



12 bonds C—I- - - I^-



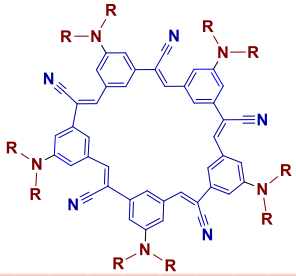
Cyanostars



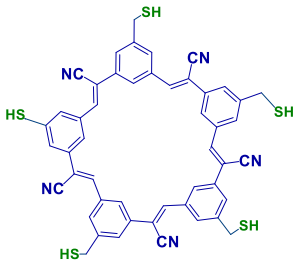
Complexation : BF_4^-, ClO_4^-, PF_6^- et I^-

➢ Designing new cyanostars

- Fluorescent cyanostars



- Sulfurcyanostars



Mathilde Ponchelle

Theranostic micellar nanocarriers for imaging, targeted radiosensitization and internal radioisotope therapy

CEA / DRF / JOLIOT / DMTS / SCBM, Nanosciences group
NOMATEN CoE, NCBJ, Radiopharmaceuticals group

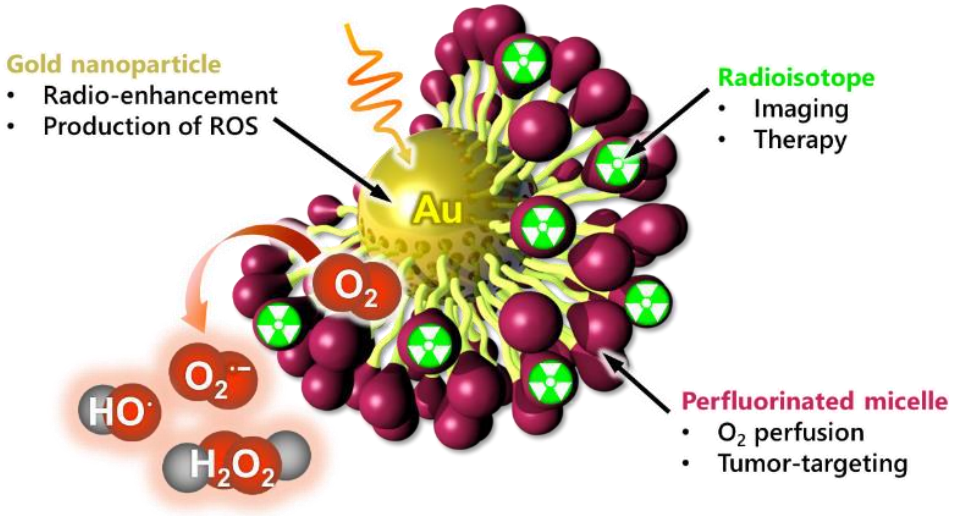
ADI UPSaclay 2022 laureate ! MP choose the co-tutelle program for her thesis

Context

Radiotherapy is widely used for the treatment of cancer.
Effectiveness of radioisotope therapy can be hampered by hypoxia.

Project

Develop “two-in-one” nanoscale carriers to locally enhance the production of reactive oxygen species (radio-enhancement) and re-oxygenate tumour tissues to counterbalance hypoxia.



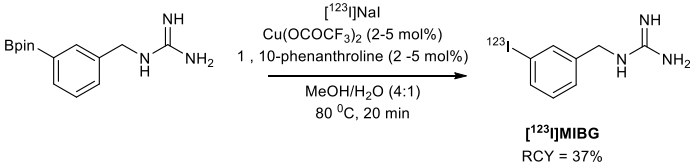
Ihab Shokair

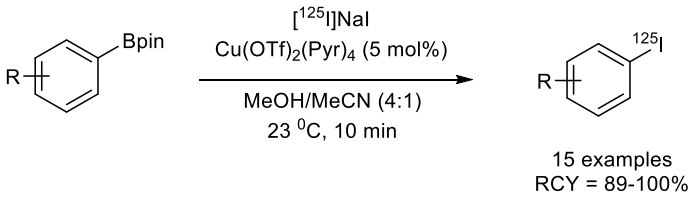
Copper-mediated nucleophilic approach for the radioiodination of various prosthetic groups

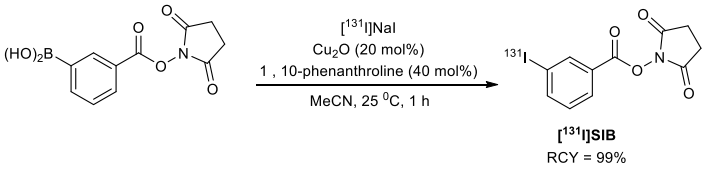
NOMATEN CoE, NCBJ, Radiopharmaceuticals group

In collaboration with :

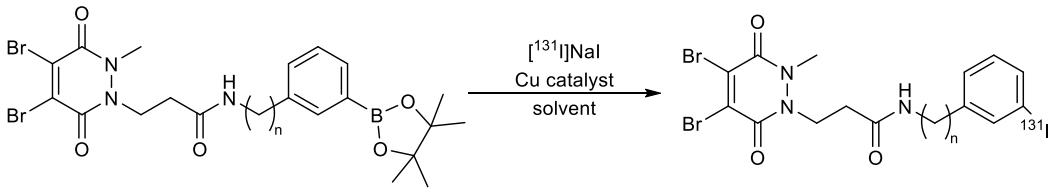
Introduction:







Method and results:



n = 0 → **B(0C)**
n = 1 → **B(1C)**

Copper catalyzed reactions: 1- $Cu(py)_4(OTf)_2$, [^{131}I]NaI, MeOH:MeCN (4:1), RT, 20 min

2- Cu_2O, [^{131}I]NaI, 1,10-phenantroline, MeCN, RT, 1 h

3- $Cu(OCOCF_3)_2$, [^{131}I]NaI, 1,10-phenantroline, MeOH:H_2O (4:1), 80 ^{0}C, 20 min

Precursor	Catalyst	RCY (TLC)	RCY (HPLC)	Number of reactions
B(0C)	$Cu(py)_4(OTf)_2$	87 ± 2 %	96 ± 2 %	3
B(1C)	$Cu(py)_4(OTf)_2$	86 ± 9 %	96 ± 4 %	3
B(0C)	$Cu(OCOCF_3)_2$	70 ± 11 %	89 ± 9 %	3
B(1C)	$Cu(OCOCF_3)_2$	73 ± 12 %	72 ± 28 %	3
B(0C)	Cu_2O	0 %	0 %	1
B(1C)	Cu_2O	0 %	0 %	1

Wilson, T. C.; McSweeney, G.; Preshlock, S.; Verhoog, S.; Tredwell, M.; Cailly, T.; Gouverneur, V. Radiosynthesis of SPECT Tracers via a Copper Mediated 123I Iodination of (Hetero)Aryl Boron Reagents. Chem. Commun. 2016, 52 (90), 13277−13280

Reilly, S. W.; Makvandi, M.; Xu, K.; Mach, R. H. Rapid Cu-catalyzed [211At]Astatination and [125I]Iodination of Boronic Esters at Room Temperature. Org. Lett. 2018, 20 (7), 1752−1755

Zhang, P.; Zhuang, R.; Guo, Z.; Su, X.; Chen, X.; Zhang, X. A Highly Efficient Copper-Mediated Radioiodination Approach Using Aryl Boronic Acids. Chem. - Eur. J. 2016, 22 (47), 16783−16786

Kinga Suchorab

Understanding oxidation of zirconium and its alloys in air and water vapour operating conditions - high temperature Raman studies

NOMATEN CoE, NCBJ, Functional Materials group

Zr alloys - nuclear fuel cladding material:

- Constitute the first barrier against the release of fission products into the primary circuit

GOAL

Comparison of corrosion kinetics of different Zr-alloys

MATERIALS AND CONDITIONS

Zr

E110

Zircaloy-2

OXIDATION

Temperatures:

500 °C | 600 °C

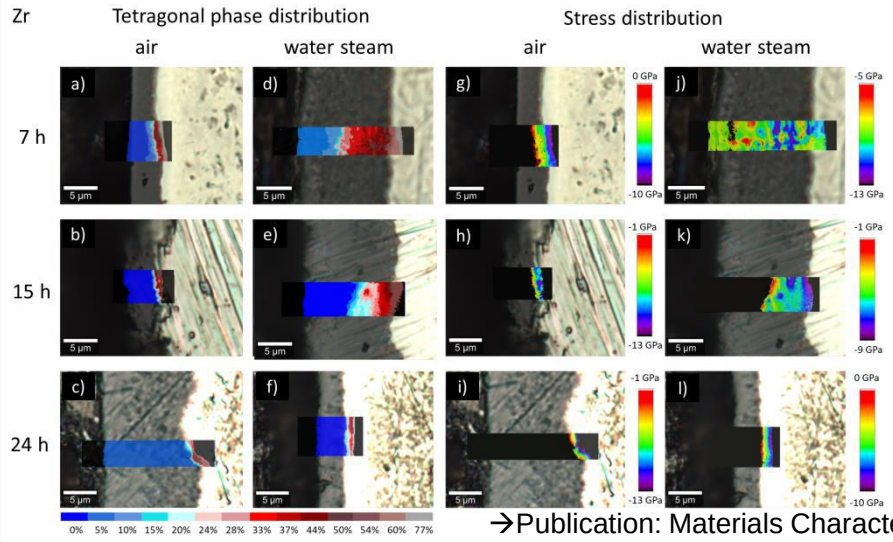
Durations:

7 h | 15 h | 24 h

Atmospheres:

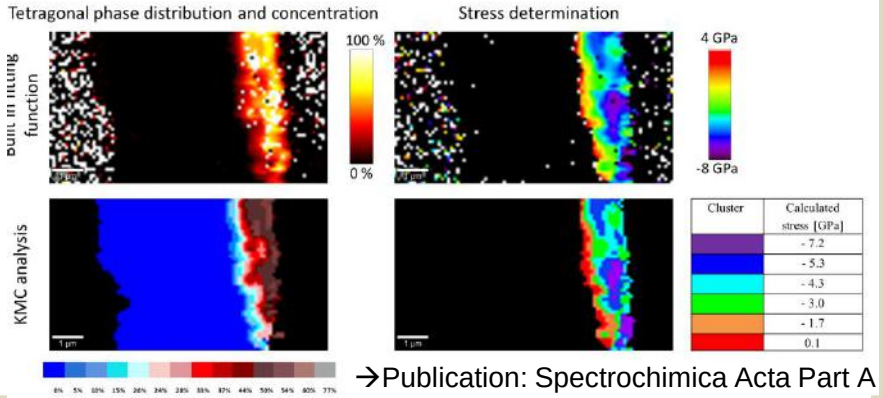
Air | Water vapour

PHASE CONTENT AND STRESS ANALYSIS √



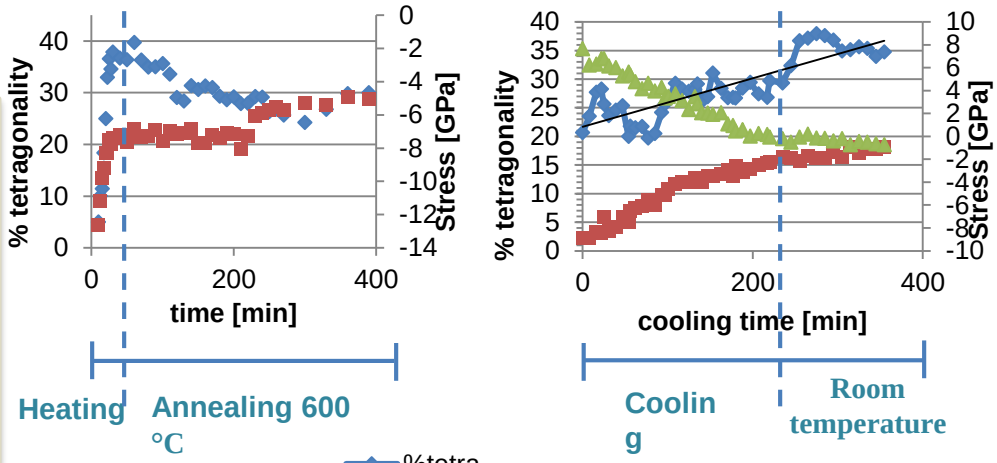
→Publication: Materials Characterization

RAMAN ANALYSIS METHODOLOGY COMPARISON √



→Publication: Spectrochimica Acta Part A

HIGH TEMEPERATURE IN SITU RAMAN ANALYSIS



Edyta Wyszkowska

Impact of radiation damage on the structural and mechanical properties of fcc Ni_xFe_{1-x} single crystal alloys

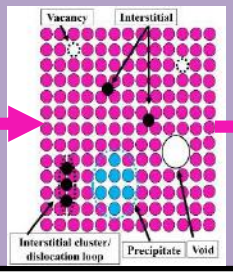
CoE NOMATEN, NCBJ, Functional Properties Group

NATIONAL CENTRE FOR NUCLEAR RESEARCH ŚWIERK

1

Formation of radiation defects!!!

Harsh working environment in nuclear reactors:
- **Temperature**
- **Neutron irradiation**



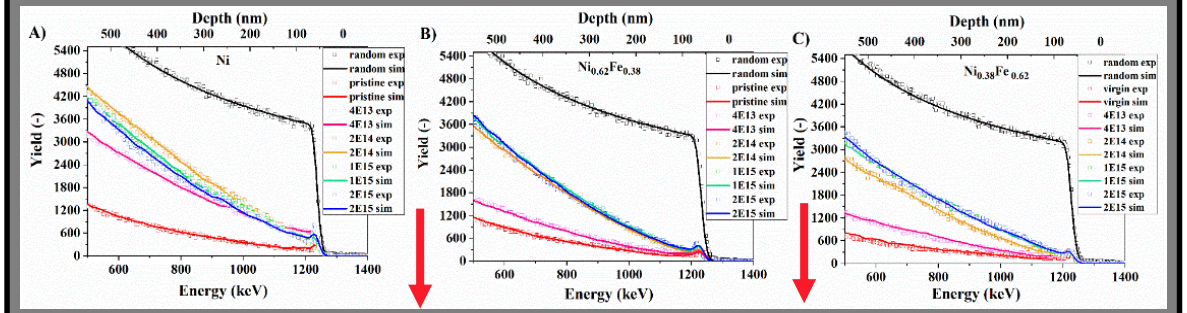
- Degradation of mechanical properties
- Structural changes
- Swelling of the material - change in volume
- Reduction in material lifetime

There is evidence that tuning the chemical composition of a single-phase alloy may significantly change the features of defect clusters and overall characteristic of the material, which needs to be elaborated.

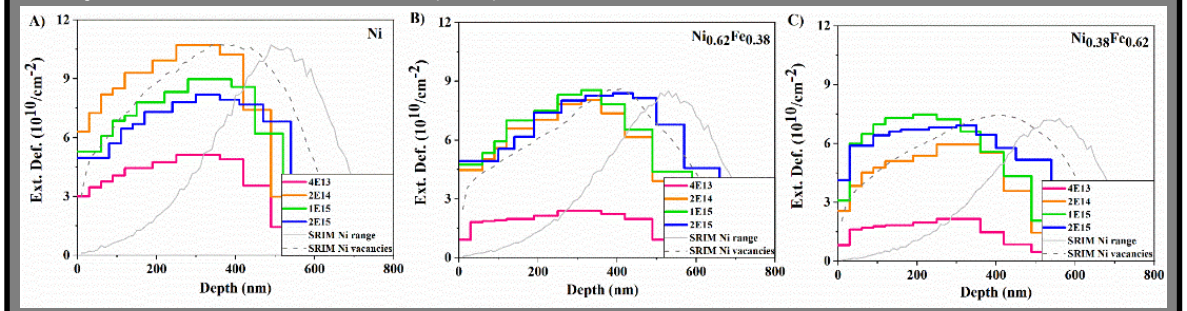
Ni_xFe_{1-x} (Fe – 0, 12, 38, 62 at%) single crystals seem to be a good candidates to understand such mechanisms!

2

RBS/C ion channeling and damage distribution profiles

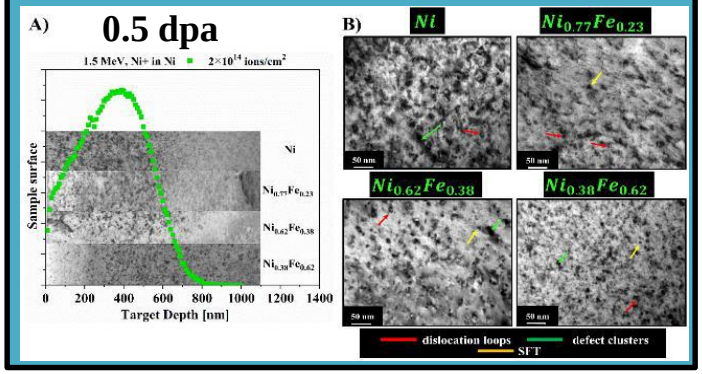


E. Wyszkowska et al, *Nanoscale* 15 (2023) 4870



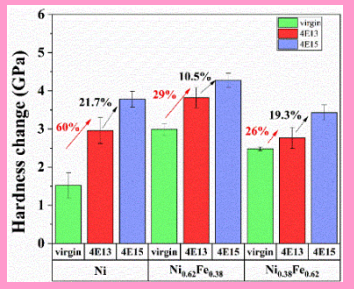
3

TEM observations



4

Irradiation induced hardening



E. Wyszkowska et al., **J. Nucl. Mater.** 584 **(2023)** 154565

1 – Motivation; **2 -** RBS/C ion channeling and damage distribution profiles; **3 -** TEM observations of irradiated materials; **4** – Hardness change

NOMATEN Winter school
November 27-30, 2023
NCBJ, Otwock-Świerk, Poland

NOMATEN
Centre of Excellence in Multifunctional Materials for Industrial and Medical Applications

PhD poster session

Wednesday November 29th, 2023 16h30-18h00

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Chair : Christophe Gallé (CEA) | Łukasz Kurpaska (NCBJ)

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 857470

Mechanical characteristics of ITER-grade tungsten: small punch test and crystal plasticity modelling

Authors: Brahim Dif, Janne Heikinheimo, Juhani Rantala, Abhishek Biswas, Matti Lindroos, VTT Technical Research Centre of Finland

Background and Introduction

Within the ITER reactor, critical components like the divertor are required to function in extreme conditions. For this plasma-facing application, tungsten (W) has been the preferred material of choice, owing to its remarkable heat resistance, high melting point, and low hydrogen retention, consequently, making a comprehensive understanding and modeling of the mechanical behaviour of great significance. However, W mechanical behavior, particularly under hydrogen exposure, remains a critical area of study. Additionally, a clear link between plasma-induced morphology changes and evolving macroscopic mechanical properties is still unclear.

Methodology and Material

This research combines experimental small punch testing (SPT) with crystal plasticity modeling. The studied material is the ITER-specification tungsten referred to as IGW which is used in the divertor's monoblocks of ITER. The plate sample (Fig.1.) has been supplied by A.L.M.T. Corp (Japan).

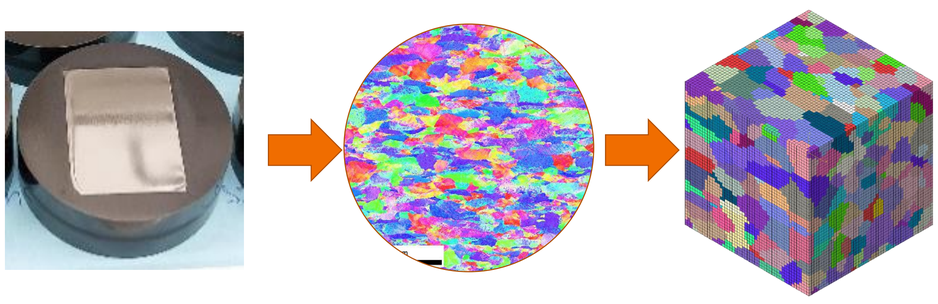

Figure 1: From left to right: ITER-specification W sample supplied by A.L.M.T corp, Japan. SEM EBSD maps in the longitudinal direction, a representative volume element.

Crystal plasticity modelling

A representative volume element is constructed based on SEM EBSD maps of different surfaces of the sample. Crystal plasticity modeling is used to simulate dislocation behavior, stress and strain distribution at the microscale, which enables to predict macroscopic material responses. Fig. 2. shows a comparison of numerical and experimental stress-strain curves.

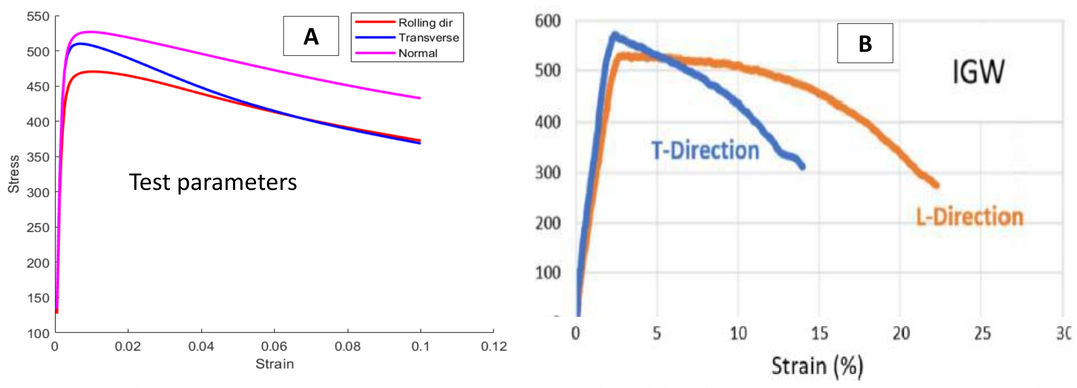

Figure 2 A) Stress vs strain curves obtained from numerical modeling for IGW at 500 °C . B) Experimental tensile stress vs. strain curves at 500 °C for IGW [1]

Small punch testing

Small punch testing is inherently biaxial, where a disc-shaped specimen is subjected to indentation, enabling a localized assessment of mechanical properties such as yield strength and tensile strength. The tests were conducted on standardized disc specimens (8 mm in diameter, 0.5 mm thick) at room temperature, 300°C, 500 °C, and 600 °C in accordance with the EN10371 standard (2021).

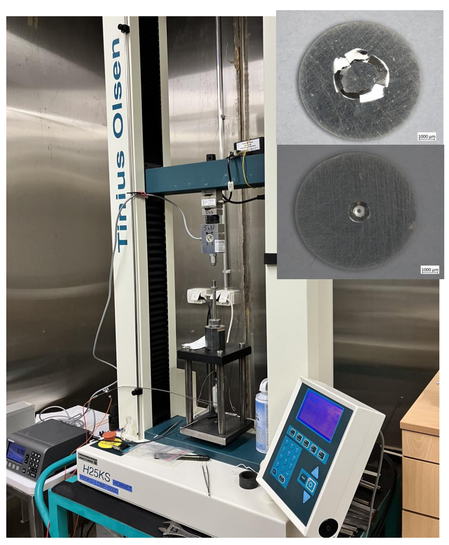

Figure 3. Small punch test set up, and a close-up magnification of IGW specimens tested at room temperature.

	Tensile test (L-direction)	Tensile test (T-direction)	SPT
Ultimate tensile strength at 500°C (MPa)	545	533	527

Table 1: Comparison of UTS results from tensile testing and small punch testing. Tensile experimental values are averaged from data published in [1].

Discussion

From the crystal plasticity percpective, the elongated polycrystalline morphology of IGW, gives initial results in the right direction for plastic behaviour of the material when compared with experimental data.
Based on the experimental results, tungsten exhibits a brittle fracture behaviour at low temperatures (< 300 °C) which makes the use of SPT quite challenging. Nevertheless, at elevated temperatures, the extracted results closely align with values derived from conventional tensile testing (Table 1). It's worth noting however that the biaxial stress makes a direct comparison with tensile values quite complex (elongated morpholgy). The simplicity of the SPT method and small amount of sample material used, makes it a viable method for assessing materials properties in fusion applications.

Summary and future continuation

- **Preliminary results from crystal plascicity modelling correlate well with tensile data even without parametrization. Full field simulation of SPT test to be carried out at a later stage.**
- **Small punch test provide relatively comparable results with tensile data available in the literature.**
- **Small punch test rig in hydrogen environment is under development. The test should provide new insights into hydrogen embrittlment mechanisms.**

References:
[1] J.-H. Yu, H. Tanigawa, D. Hamaguchi, and T. Nozawa, "Mechanical properties of three kinds of Iter-grade pure tungsten with different manufacturing processes," Fusion Engineering and Design, vol. 157, p. 111679, 2020)

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Tel. +358 40 123 4567, brahim.dif@vtt.fi

beyond the obvious

Green Aromatics From Lignocellulosic Biomass Via Catalytic Aromatization

Bibesh Gauli[1], Aitor Arandia[1], Francesco Sandri[2], Eveliina Mäkelä[1], Johanna Kihlman[1], Matti Reinikainen[1], Narendra Kumar[2], Dmitry Murzin[2], and Juha Lehtonen[1]

[1]*VTT Technical Research Centre of Finland, Espoo, Finland;* [2]*Åbo Akademi University, Turku, Finland*

BACKGROUND

- Monocyclic aromatics such as benzene, toluene, and xylenes (BTX) are important platform chemicals to produce various value-added chemical products (such as rubber, resins, and plastics) [1].
- Sustainable chemical production is becoming increasingly important.
- GreenAro Project funded by Business Finland is developing catalytic solutions for the selective production of BTX from lignocellulosic biomass (Figure 1).

Figure 1: Process scheme to produce BTX from biomass.

EXPERIMENTAL

- **Reactor:** 4 parallel fixed bed reactors (Figure 2)
- **Model compounds**: Methylcyclohexane, octane, and 4-propylphenol
- **Catalysts:** 2 wt.% Zn-modified ZSM-5 zeolites synthesized by evaporation impregnation method
- **Catalyst characterization**: Nitrogen physisorption, FTIR, XRD, SEM, and TEM
- **Analysis**: GC-FID/TCD and GC-MS for hydrocarbons identification and quantification

Figure 2: Reactor setup for catalytic aromatization tests

CATALYST CHARACTERIZATION AND TESTING

- Catalysts with 2 wt.% loading of Zn on H-ZSM-5 zeolite with different silica/alumina ratios (Si/Al = 30, 50, and 80) were synthesized and characterized with different techniques.
- Reactor setup was designed for the catalytic tests.

SEM AND TEM IMAGES

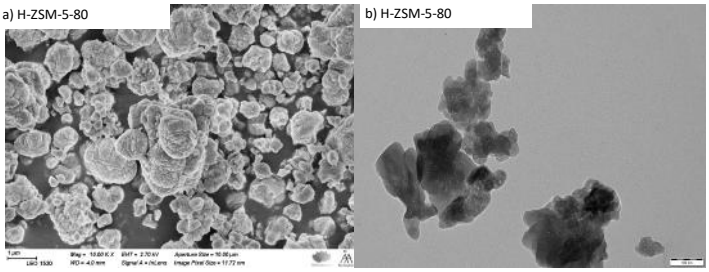

Figure 3: SEM image a), and TEM image b) of H-ZSM-5-80 zeolite.

NITROGEN PHYSISORPTION

Table 1: Textural properties of pristine H-ZSM-5 and 2 wt.% Zn-doped ZSM-5 catalysts (synthesized by evaporation impregnation)

Sample	S_{BET} / $m^2.g^{-1}$	V_p / $mL.g^{-1}$ total	V_p / $mL.g^{-1}$ micropore	Si/Al
H-ZSM-5-30	317	0.174	0.150	30
2 wt. % Zn- ZSM-5-30	295	0.165	0.142	30
H-ZSM-5-50	356	0.197	0.170	50
2 wt. % Zn- ZSM-5-50	329	0.180	0.155	50
H-ZSM-5-80	338	0.179	0.163	80
2 wt. % Zn- ZSM-5-80	320	0.184	0.147	80

CONCLUSIONS

- 2 wt.% Zn loaded ZSM-5 found to be a promising candidate for the catalytic aromatization of fast pyrolysis bio-oil [2],[3] based on the literature.
- Synthesized Zn-modified ZSM-5 catalysts retained their specific surface area, porosity, and morphology.
- Next steps: Catalytic aromatization tests

FUNDED BY BUSINESS FINLAND

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beyond the obvious

References

1. Che, Q., Yang, M., Wang, X., Yang, Q., Rose Williams, L., Yang, H., Zou, J., Zeng, K., Zhu, Y., Chen, Y., Chen, H., **2019**. *Bioresource Technology* 278, 248–254.
2. Yan, K., Li, H., **2021**. *Energy Fuels* 35, 45–62.
3. Zheng, Y., Wang, F., Yang, X., Huang, Y., Liu, C., Zheng, Z., Gu, J., 2017. *Journal of Analytical and Applied Pyrolysis* **126**, 169–179.

Understanding the corrosion mechanisms of zirconium alloys and studying the influence of the electric field on the oxidation rate and hydrogen absorption.

Dina GNICHI
CEA Paris-Saclay/DES/ISAS/DRMP/SEMI/LM2E
Doctoral School: SMEMAG Paris-Saclay University

Context

Study of the corrosion phenomenon of zirconium alloy fuel cladding under the primary conditions of Pressurized Water Reactors (PWRs).

→ Understanding the mechanisms of zirconium oxide and hydride formation.

→ Evaluation of oxygen and hydrogen concentration for modeling purposes in PWR scenarios (such as normal operation).

State of the art [1],[2],[3]

Oxide formation follows a parabolic law e(ox) = k√t in the first months (pre-transition), where e(ox) is the oxide thickness, k is the kinetic reaction constant, and t is the time (see Figure 2).

Two pathways for hydrogen reduction (see Figure 1 & 3).

Initiation of hydrogen uptake starting from an oxide thickness of 2.5 µm (see Figure 4).

Hypothesis I There would be an electrochemical process responsible for triggering hydrogen intake, possibly linked to a decrease in the Nb content at the metal/oxide interface, reducing the metal potential and promoting interface reactions.

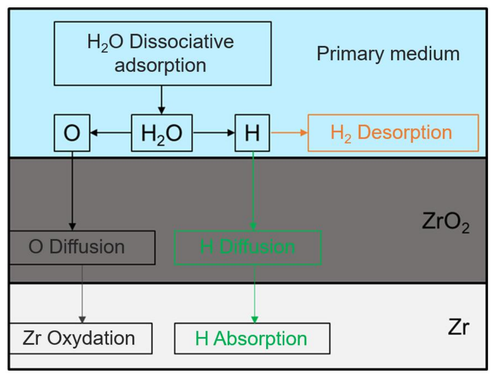

Fig 1. *Pathways of elements transport in corrosion conditions.* [3]

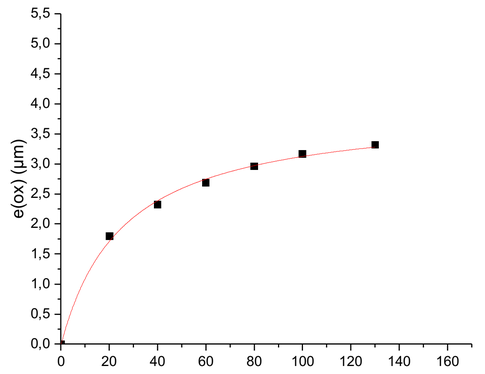

Fig 2. *Evolution of Zr-1Nb oxide thickness over time in PWR conditions P = 186 bar, T = 366°C, [Li] = 2 ppm; [B] = 1000 ppm.*

$$Zr \rightarrow Zr^{4+} + 4e^-$$
$$2H_2O \rightarrow 2O^{2-} + 4H^+$$
$$Zr^{4+} + 2O^{2-} \rightarrow ZrO_2$$
$$4H^+ + 4e^- \rightarrow 2H_2 \text{ or } 4H^+ + 4e^- \rightarrow 4H_{i\text{-}m}$$

Fig 3. *Oxidation mechanism of zirconium.*

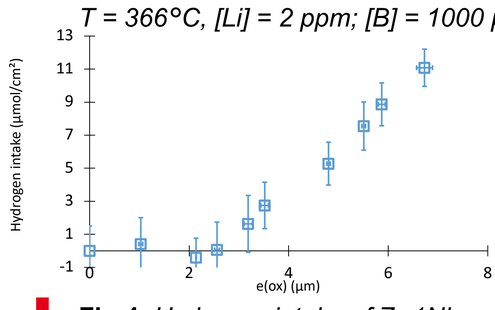

Fig 4. *Hydrogen intake of Zr-1Nb over time in PWR conditions P = 186 bar, T = 366°C; [Li] = 2 ppm, [B] = 1000 ppm.* [3]

Objectives & experimental approach

- Studying the effect of the electric field on the migration of species (O & H) through anodic polarization (in-situ PEIS) and SIMS analysis.
- Evaluating the influence of the conductivity variation of Zr-1Nb on hydrogen intake (in-situ EIS at open circuit potential) at different oxide thicknesses.
- Assessing the role of niobium in various phenomena (electric field, conductivity, species migration) through an analysis of its distribution and oxidation state before and after hydrogen intake initiation (performed via SIMS and XPS).

Selected results

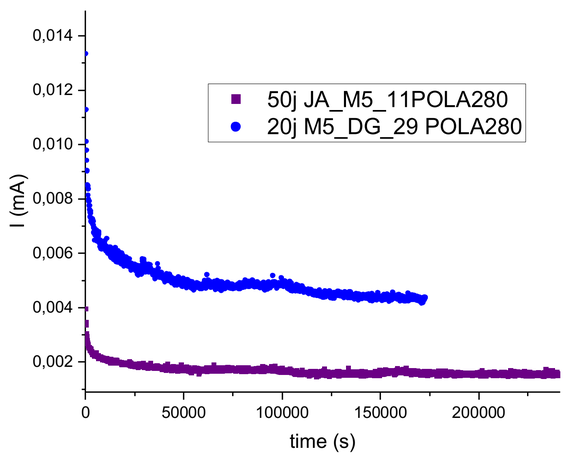

Fig 5. *Chronoamperometry profile with an anodic polarization potential of 280 mV at two different oxide thicknesses 1,8 µm and 2,2 µm (20 days vs 50 days).*

- **Effect of chronoamperometry during anodic polarization:**

→ A higher current signal at 20 days of oxidation than at 50 days due to an increase in the resistance of the oxide layer.

- **Effect of anodic polarization:**
  - Increase in the penetration of ^{18}O isotope.
  - The higher the electrical potential, the deeper the penetration of oxygen.
  - No significant effect on deuterium penetration.

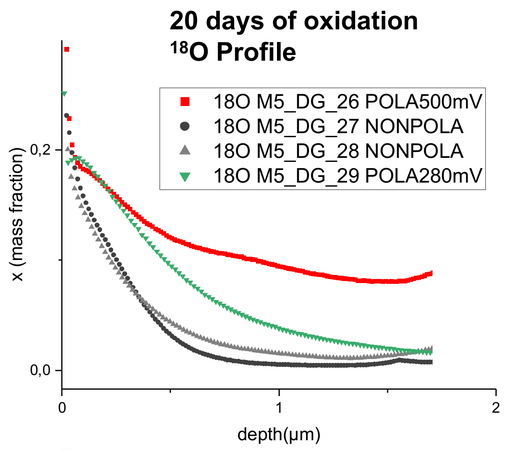

Fig 6. *SIMS profile of ^{18}O mass fraction in function of depth of a 1,8 µm oxide thickness.*

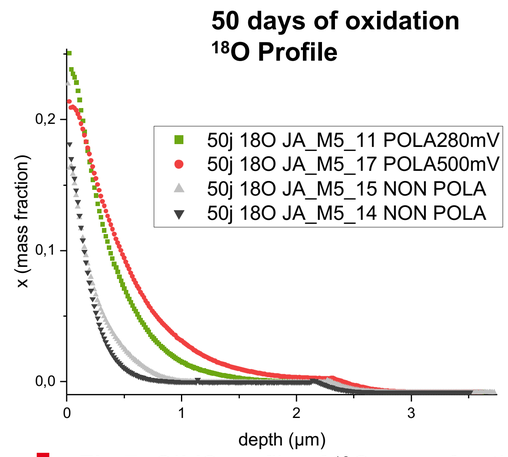

Fig 7. *SIMS profile of ^{18}O mass fraction in function of depth of a 2,2 µm oxide thickness.*

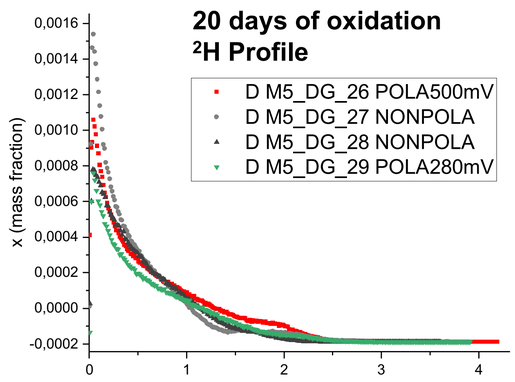

Fig 8. *SIMS profile of ^{2}H mass fraction in function of depth of a 1,8 µm oxide thickness.*

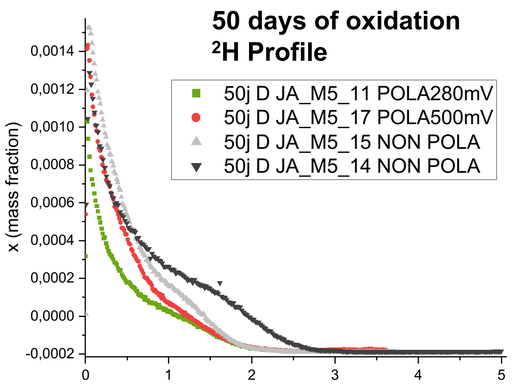

Fig 9. *SIMS profile of ^{2}H mass fraction in function of depth of a 2,2 µm oxide thickness.*

Conclusions & Perspectives

The conductance of the oxidized zirconium alloy (Zr-1Nb) decreases with the thickness of the oxide layer due to the resistive effect of a thicker oxide layer. Furthermore, anodic polarization increases the penetration of oxygen into the oxidized zirconium alloy, as a result of the attraction of O^{2-} ions toward the electric field generated by anodic polarization. Unlike hydrogen, which is assumed to exist as positively charged elements (H^+) or in a molecular form (H_2), where no significant modification of its penetration into the oxide layer is observed after anodic polarization.

These results suggest that the electric field is one of the parameters affecting the kinetic transport of the elements and will be further investigated at other oxide thicknesses, along with an analysis of alloy elements' concentration, distribution, and oxide state related to this phenomenon.

[1]- D.D. Macdonald, "The history of the Point Defect Model for the passive state: A brief review of film growth aspects" Electrochimica Acta, Volume 56, (2011)
[2]- B. Cox, J.P. Pemsler, "Diffusion of oxygen in growing zirconia films", Journal of Nuclear Materials, Volume 28, (1968)
[3]- B. Queylat, "Compréhension de l'évolution de la fraction d'hydrogène absorbé par les gaines en alliage de zirconium", Thèse de l'Université Paris-Saclay (2020)

This study is funded as part of the GAINE project at the tripartite Institute I3P CEA-EDF-Framatome

Synthesis and ^{11}C Isotopic Labeling of Serodolin, a biased ligand of 5-HT_7 receptors

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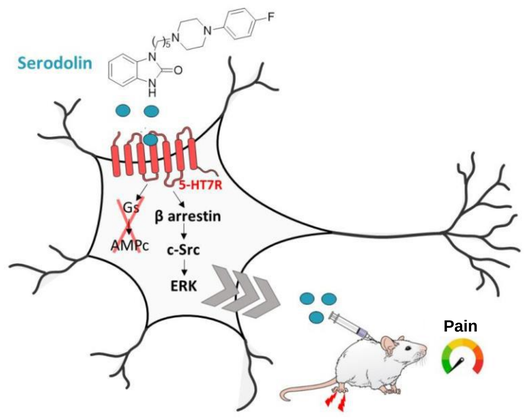
Introduction

Serodolin, a new β-arrestin–biased ligand, showed promising results toward the alleviation of pain related behaviors by targeting the 5-HT_7 receptors. PET imaging using isotopically labeled [^{11}C]Serodolin would be an asset for a complete elucidation of the brain penetration and distribution of this drug.[1]

[1] El Khamlichi C.. et al. Proc. Natl. Acad. Sci. U.S.A. **2022**, 119

Context

5-HT_7 receptors



© Séverine Morisset-Lopez

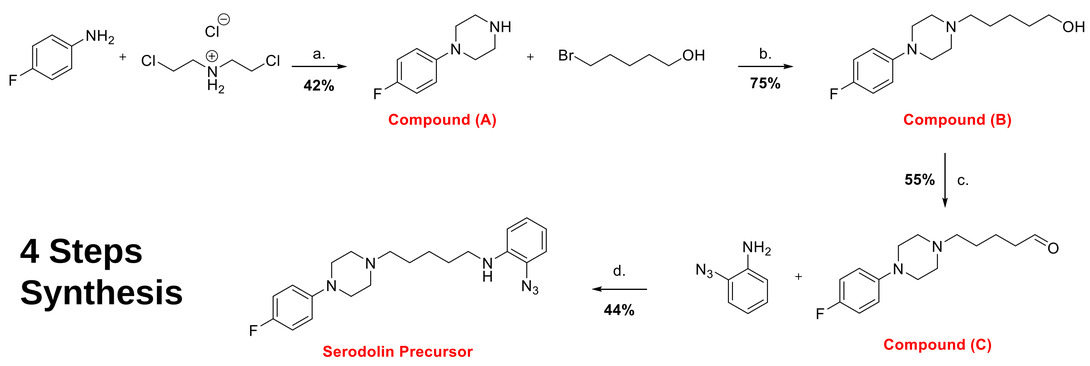
5-HT_7 belongs to the GPCR superfamily of cell surface receptors and gets activated through the neurotransmitter serotonin.

Although the physiological functions of the 5-HT_7 receptors are not fully understood, it has become a promising target for the treatment of many pathologies such as mood disorders, anxiety or schizophrenia and it is involved in the pain circuit.

A biased ligand?

A biased ligand, is a type of ligand that selectively activates certain signaling pathways or responses while avoiding others. It "biases" the cellular response by preferentially activating one pathway over another. This selectivity can be useful in developing drugs that target specific receptors to achieve desired therapeutic effects.

Synthesis



Inspired by literature[2], we were able to syntesize the Serodolin precursor for carbon-11 labeling in 4 steps and 7.6% overall yield.

This compound can now be used for radiochemistry studies.

a. 4-fluoroaniline (1 equiv), bis(2-chloroethyl)amine hydrochloride (1 equiv), DGMME, 150 °C, 3 h ;

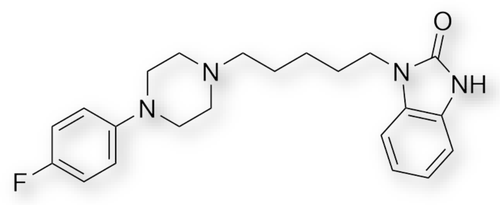
b. Compound (A) (1 equiv), K_2CO_3 (2.2 equiv), 5- bromopentan-1-ol (1.4 equiv), MeCN, 80 °C, 48 h ;

c. DMSO (5.7 equiv), oxalyl chloride (2.4 equiv), -78 °C, 30 min then, 5-Compound (B) (1 equiv), -78 °C, NEt_3 at 0°C for 15 min

d. Compound (C) (1 equiv), 2-azido-aniline (1 equiv), AcOH (4.0 equiv), NaOAc (2.0 equiv), MeOH, r.t., 20 min, then $NaBH_3CN$ (1.1 equiv), 4 h

[2] Del Vecchio, A *et al. Angew. Chem. Int. Ed.* **2018**, *57*, 9744–9748

Serodolin

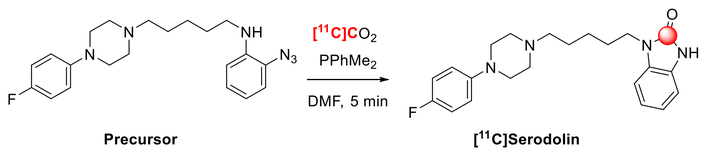


Having unique pharmacological properties and therapeutic potential of a new synthetic ligand, Serodolin is a promising molecule for the treatment of inflammatory pain.

Our aim : Pursue the ongoing researches by performing PET imaging using isotopically labeled [^{11}C]Serodolin to better understand the distribution of this drug.

Radiochemistry

Staudinger/Aza-Wittig



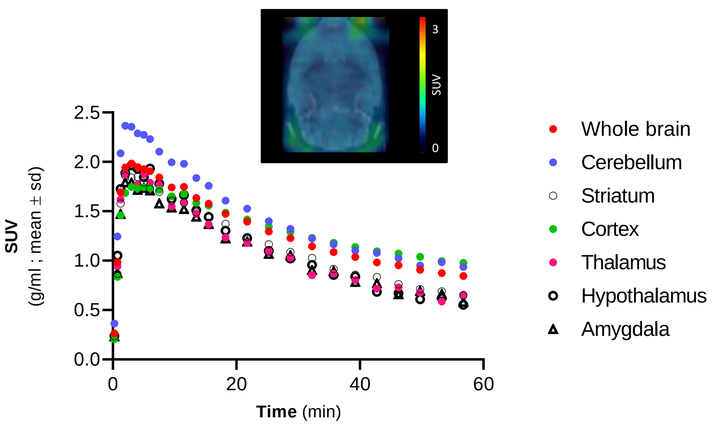
Preleminary radiolabeling results

Starting Activity	Final Activity	RC Yield	RAS (EOB)
1140 mCi @ 6min	60 mCi @ 44min	24%	51.8 GBq/µmol
1088 mCi @ 6min	71 mCi @ 31min	20%	62.9 GBq/µmol

Early experiments were encouraging. We can now perform *in vivo* PET imaging.

Each syntheses were operated on a modified Synthra MeI_{plus} research module for automation of the direct CO_2 bubbling

PET Imaging



In the initial investigative studies of Serodolin, PET imaging using rats was conducted to elucidate its ability to permeate the blood-brain barrier and its affinity towards 5-HT_7 receptors. Preliminary labeling experiments employing radiolabeled [^{11}C]Serodolin demonstrated a perceptible penetration through the BBB, signifying its accessibility to the central nervous system. However, the anticipated binding specificity to 5-HT_7 receptors did not manifest in the initial trials. Furthermore, investigations into the neuropharmacological profile of Serodolin have revealed a notable binding affinity within the cerebellum, despite the recognized absence of 5-HT_7 receptors in this region. Further exploration into alternative molecular targets and mechanistic pathways of Serodolin are thus needed.

Conclusion

In this study, we report an efficient synthesis of the Sedololin precursor making use of a Staudinger/Aza-Wittig sequence for the late-stage addition of [^{11}C]CO_2 into the cyclic urea. With these conditions, we were able to access to [^{11}C]Serodolin in 20% radiochemical yield and 62.9 GBq/µmol molar activity. PET imaging with [^{11}C]Serodolin has been performed in rats and showed interesting first results. Further studies are now needed.

Acknowledgment: The authors thank the CEA and the FOCUS BIOMARQUEUR program for financing this research

NOMATEN

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NOV 28-30 2023

Designing cobalt-free high-entropy alloys for radiation resistant applications: a strategy using d-orbital energy level

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Introduction

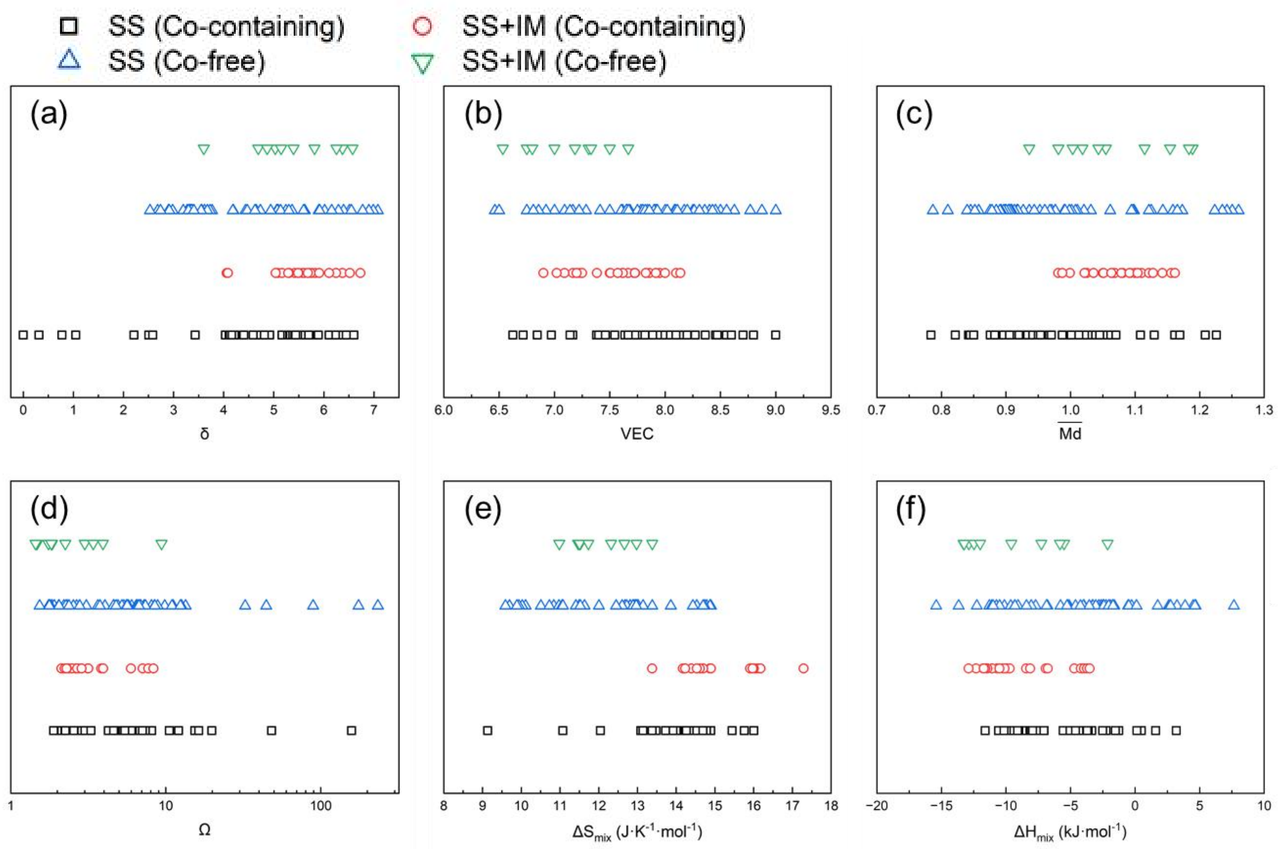
High-entropy alloys (HEAs) are promising materials for high-temperature structural applications such as nuclear reactors due to their outstanding mechanical properties and thermal stability [1]. Instead of the trial and error method, it is efficient to design and prepare single-phase face-centered cubic (FCC) structured HEAs through semi-empirical phase formation rules. However, the HEAs containing cobalt are unsuitable for nuclear applications because of the long-term activation of cobalt [2]. Here, six parameters, d-orbital energy level ($\overline{Md}$), valance electron concentration (*VEC*), entropy of mixing (ΔS_{mix}), enthalpy of mixing (ΔH_{mix}), atom size differences (δ), and parameter of the entropy of mixing (Ω) were calculated based on 133 existing high-entropy alloy compositions to determine the solid solution phase, especially the FCC phase formation rules in cobalt-free HEAs. HEAs of 4 components were arc melted to verify the newly developed phase formation rules.

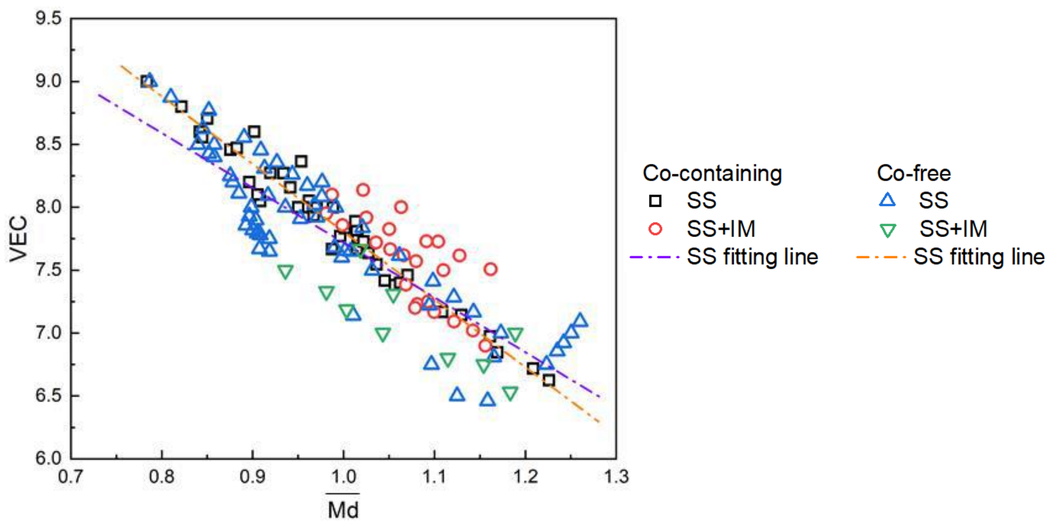
Methods

The collected multi-component systems were carried out using reported literature. The parameters of $\overline{Md}$, *VEC*, ΔS_{mix}, ΔH_{mix}, Ω and δ were used to predict the formation rules of solid solution phase, in particular FCC phase, in Co-free alloys. Three multi-component systems of CoCrFeNi, CoCrFeMnNi, $V_{10}Co_{10}Cr_{15}Fe_{35}Mn_5Ni_{25}$ and a new alloy system of $V_{10}Cr_{20}Fe_{30}Mn_{10}Ni_{30}$ were manufactured to verify the formation rules. And the nanomechanical properties were obtained using nanoindentation.

Solid Solution Formation Rules

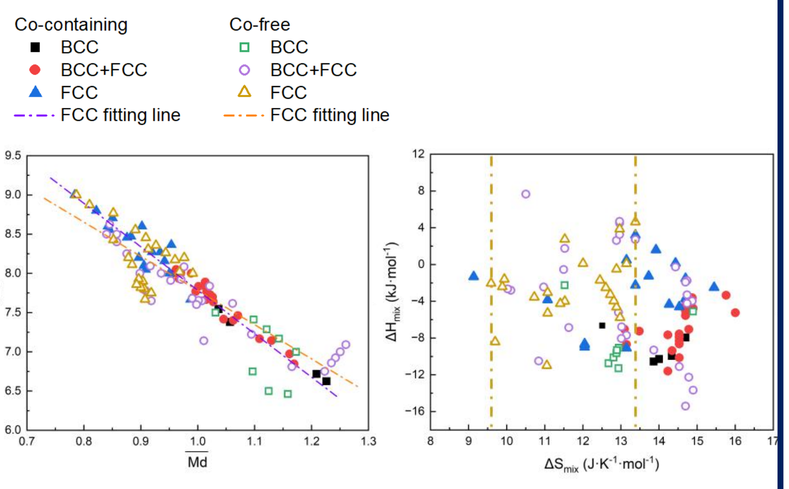
The effect of each parameters on multicomponent alloys in the plot shows that the ranges of δ and ΔS_{mix} for solid soluiton phase formation in Co-free alloys are very different from that of Co-containing alloys. Conversely, the ranges of *VEC* and $\overline{Md}$ for Co-free alloys are slightly wider. A interesting linear correlation between *VEC* and $\overline{Md}$ can be observed, when superimposing the two parameters together. This indicates a physical similarity between *VEC* and $\overline{Md}$. When $\overline{Md}$ < 1.08, a higher *VEC* is needed to form stable SS phases in Co-free alloys, and when $\overline{Md}$ > 1.08, the formation of SS phases in Co-free alloys requires less *VEC* than in Co-containing alloys.





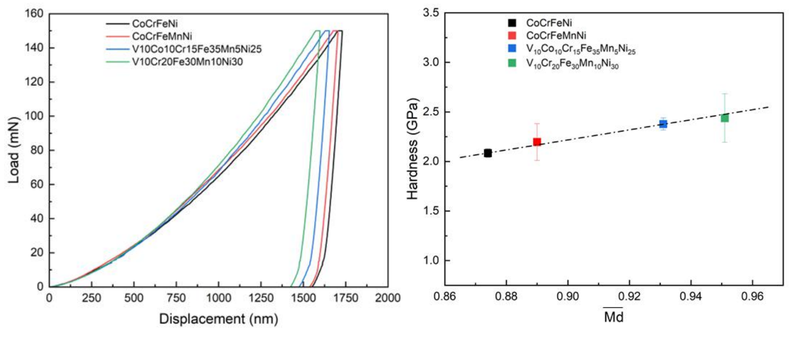
FCC Phase Formation Rules

The smoother slope of the FCC fitting curve for Co-free alloys indicates a reduced susceptibility to modifications in the VEC and $\overline{Md}$, which may contribute to enhanced FCC phase stability in these materials. The FCC phase stable regions in Co-free alloys are smaller than those in Co-containing alloys, as indicated by the two sets of parallel dash-dotted lines in ΔH_{mix} - ΔS_{mix} *map*.



Mechanical Properties

The hardness of the HEAs increases from 2.08 GPa to 2.44 Gpa without a decrease in the elastic modulus. The correlation between the mechanical properties and $\overline{Md}$ inspires us to design the composition in such a way that the $\overline{Md}$ value can be increased as much as possible to obtain a Co-free alloy with high strength while maintaining the single FCC phase.



Conclusions

(1) The formation of the FCC phase in Co-free alloys is contingent upon satisfying specific criteria: 0.787 ≤ $\overline{Md}$ ≤ 0.992, 7.67 ≤ *VEC* ≤ 9.00, 9.59 ≤ ΔS_{mix} ≤13.38, -11.00 ≤ ΔH_{mix} ≤ 4.64, δ ≤ 5.30%, and Ω ≥ 1.77.

(2) Among the six parameters, the d-electron related $\overline{Md}$ and *VEC* are the critical factors that determine the FCC phase stability in Co-free alloys and $\overline{Md}$ can alone used as a benchmark for developing mechanical properties.

(3) The newly designed alloy exhibits good mechanical properties with a hardness of 2.44 GPa and an elastic modulus of 162.88 GPa obtained by nanoindentation.

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[2] N.A.P.K. Kumar, C. Li, K.J. Leonard, H. Bei, S.J. Zinkle, Microstructural stability and mechanical behavior of FeNiMnCr high entropy alloy under ion irradiation, Acta Mater. 113 (2016) 230-244.

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European Union

Detecting Material Properties with Digital Image Correlation and Principal Component Analysis

NOMATEN
Centre of Excellence in Multifunctional Materials for Industrial and Medical Applications

PhD. Student: Bakhtiyar Mammadli Supervisor: Prof. Stefanos Papanikolaou

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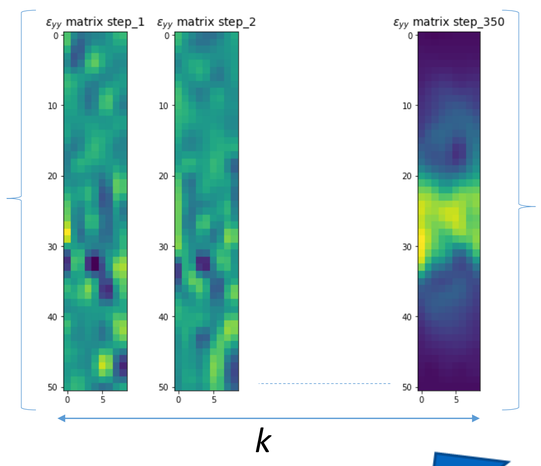
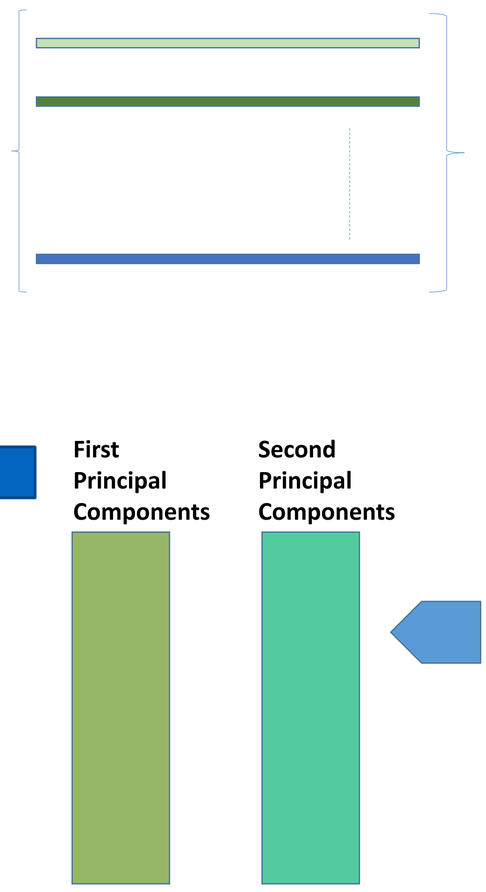
Machine Learning Methodology

$$\tilde{E}_k = \frac{E_k - \langle E_k \rangle}{\sqrt{\langle E_k^2 \rangle - \langle E_k \rangle^2}}$$



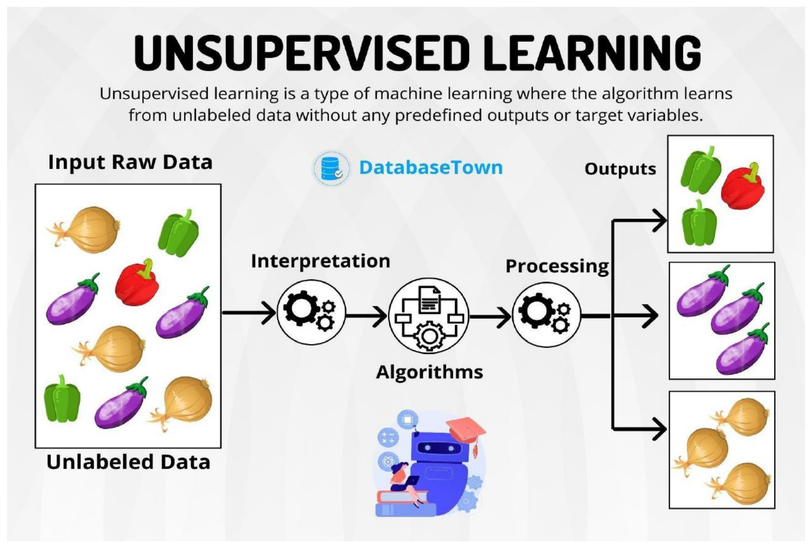
Principal Component Analysis

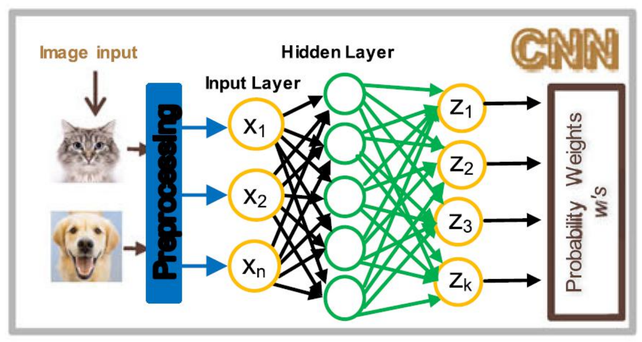


$$X = \{E_k\}$$

Singular Value Decomposition

$$U \Sigma W^T$$



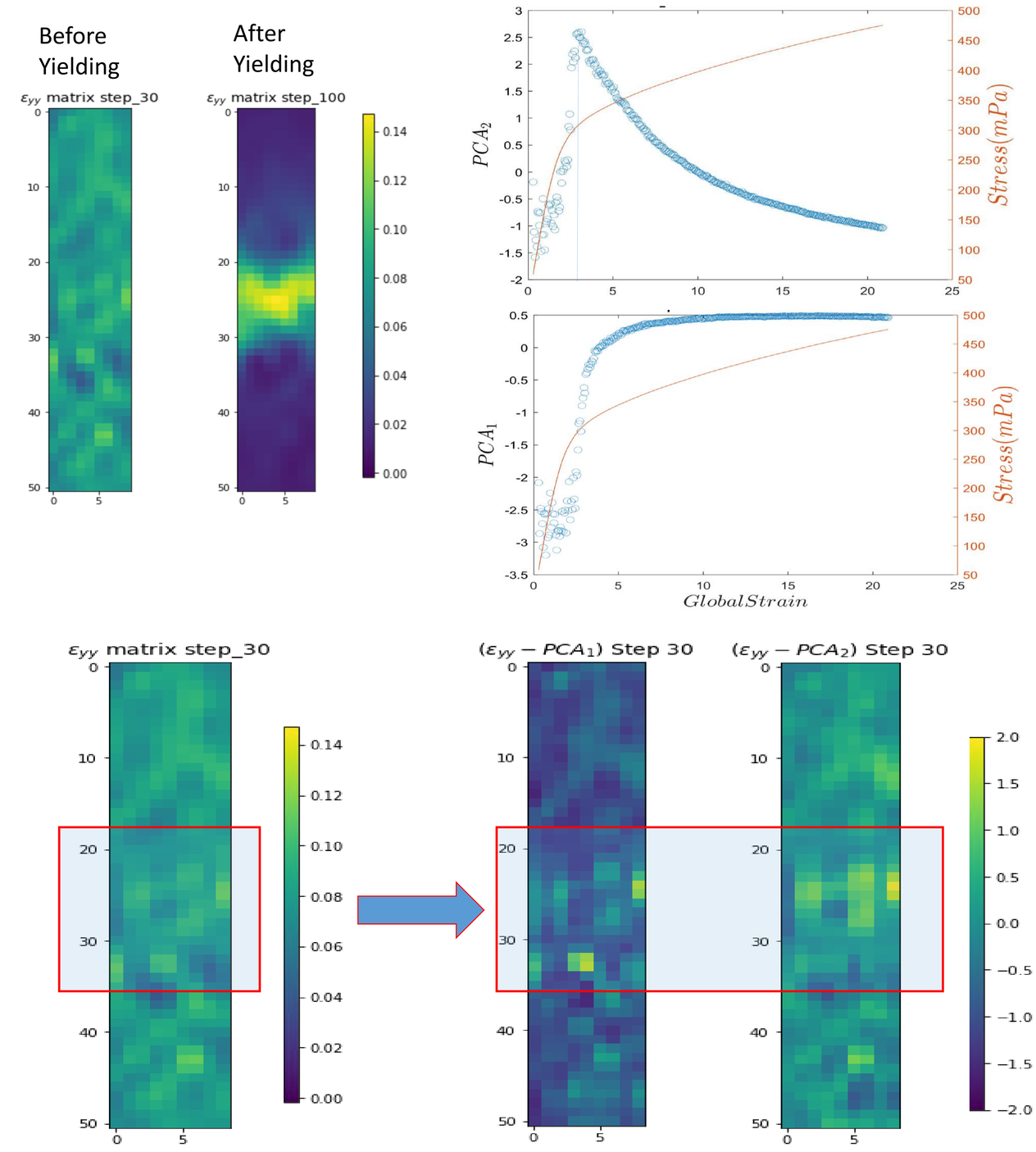


[1] S. Papanikolaou and M. Alava, Direct detection of plasticity onset through total-strain profile evolution, Phys. Rev. Mater., 2021

Detection of Yielding and Necking Instabilities

DIC test of $(FeMnNiCo)_{100-x}Mo_x$,*x=5*

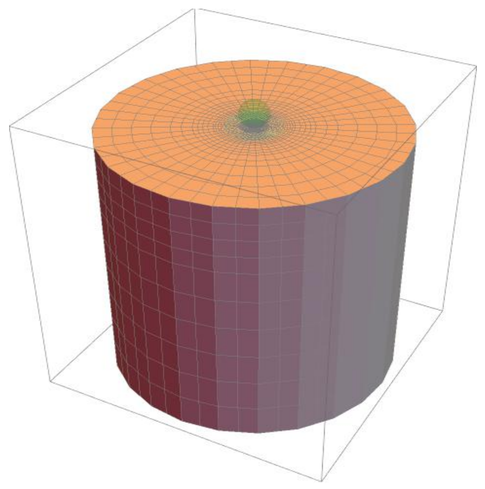
In collaboration with Dr. Krzysztof Muszka's team at AGH University of Science and Technology in Krakow, Poland

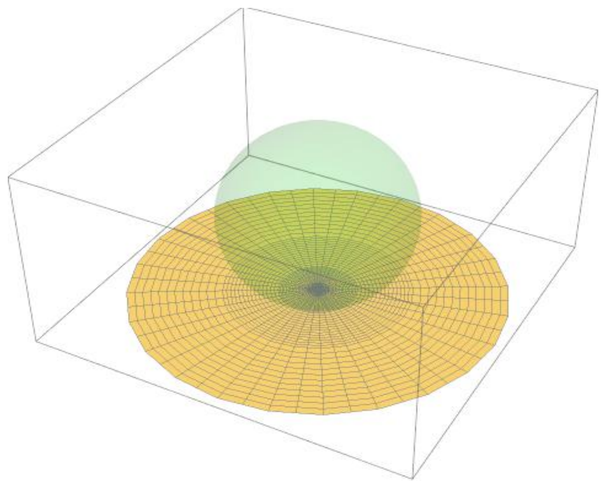


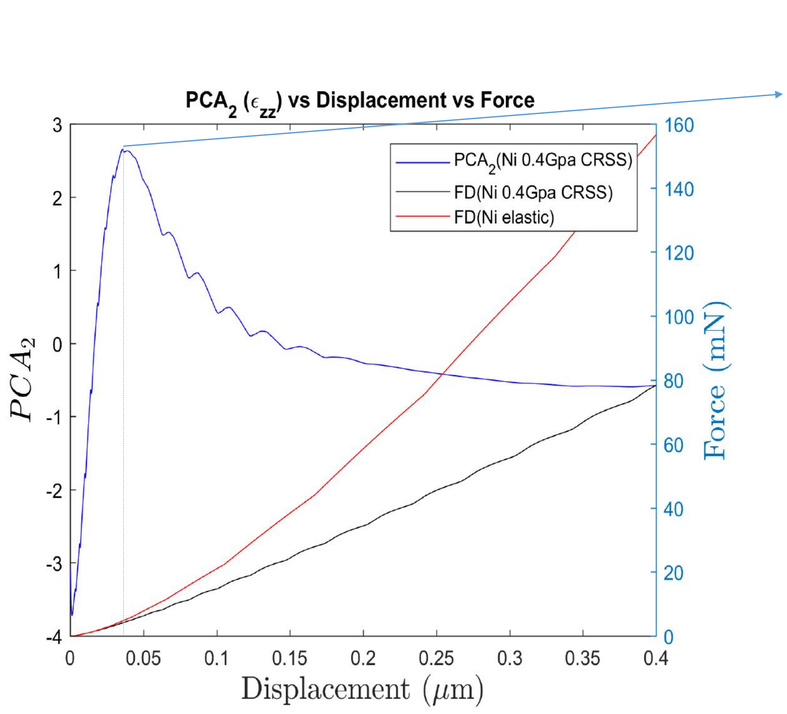
[2] Cichocki, K. *et al.* Effect of Mo on Phase Stability and Properties in FeMnNiCo High-Entropy Alloys. *Metall Mater Trans A* **53**, (2022).

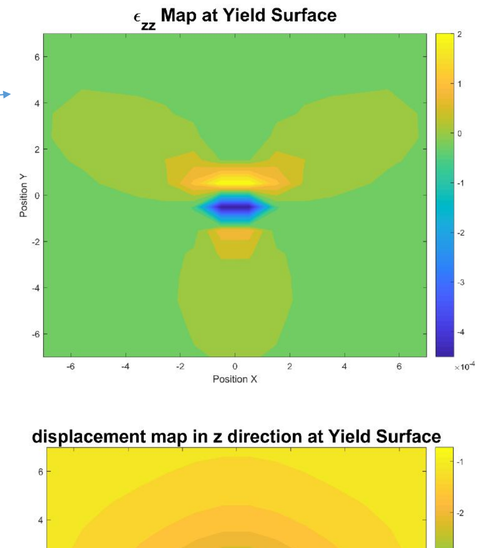
Detection of Indentation (CP-FEM) Yielding

CP-FEM (Crystal Plasticity – Finite Element Method)
Indentation simulation of pure Nickel with spherical indenter









[3] Frydrych, K.; Papanikolaou, S. Unambiguous Identification of Crystal Plasticity Parameters from Spherical Indentation. Crystals 2022

Compositional Search of Stable Crystalline Structures in Multi-Component Alloys Using Generative Diffusion Models

Grzegorz Kaszuba*[,1], Amirhossein D. Naghdi*[,1,2], Stefanos Papanikolaou[2], Andrzej Jaszkiewicz[3], Piotr Sankowski[1]

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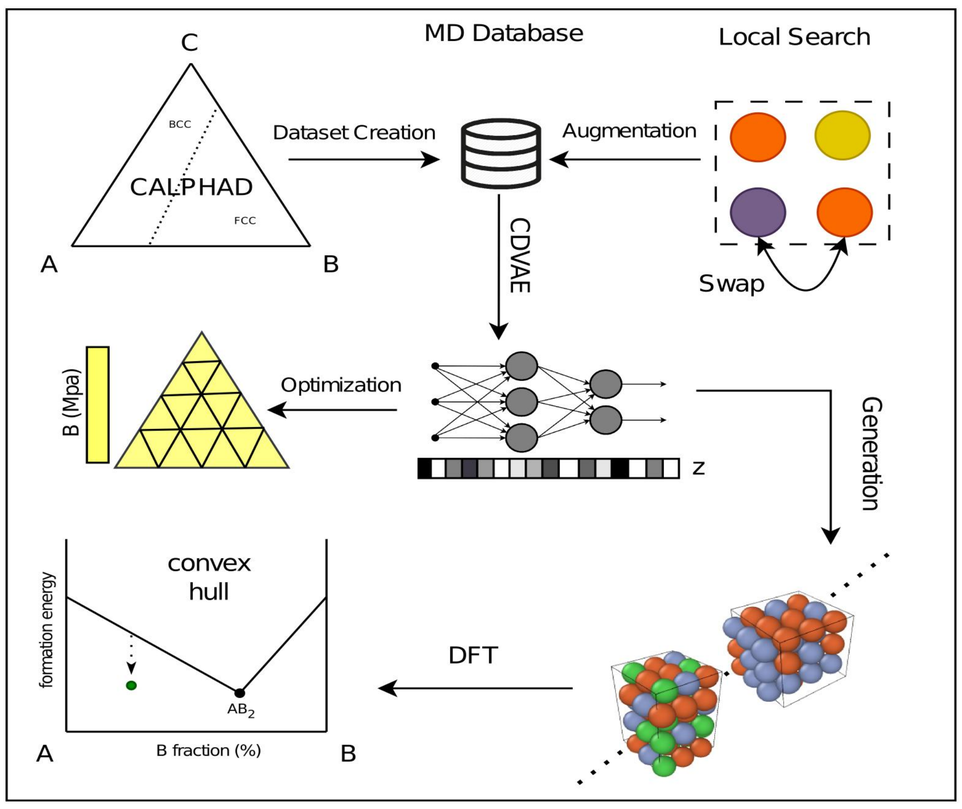
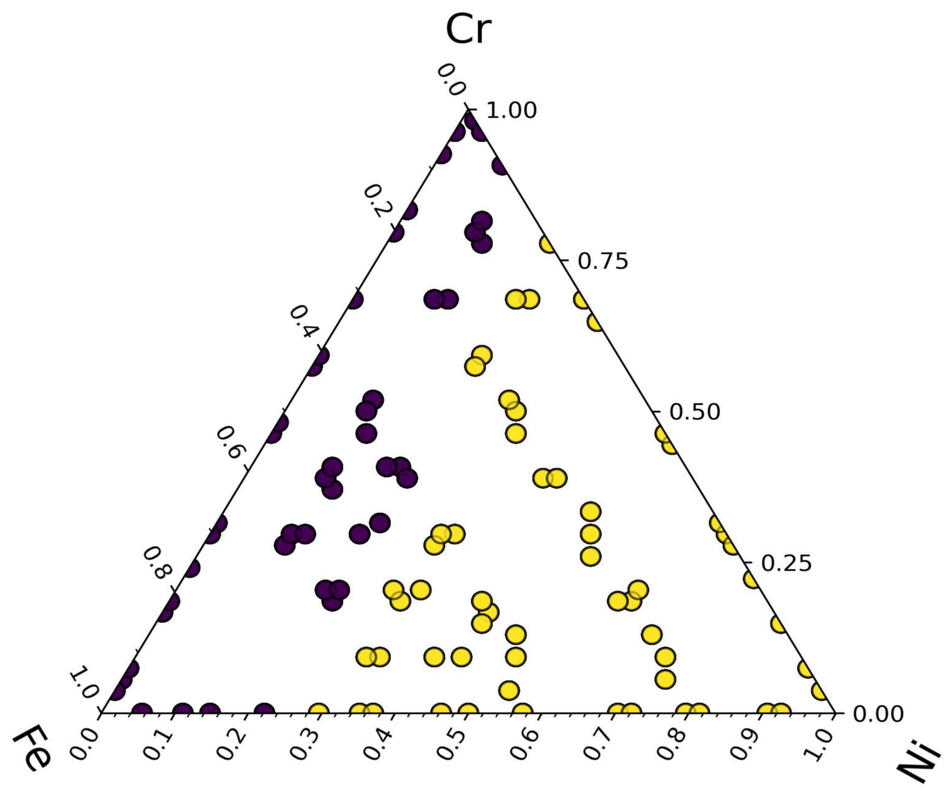
2) NOMATEN Centre of Excellence, National Center for Nuclear Research, 05-400 Swierk/Otwock, Poland
3) Technical University of Poznan, Poland

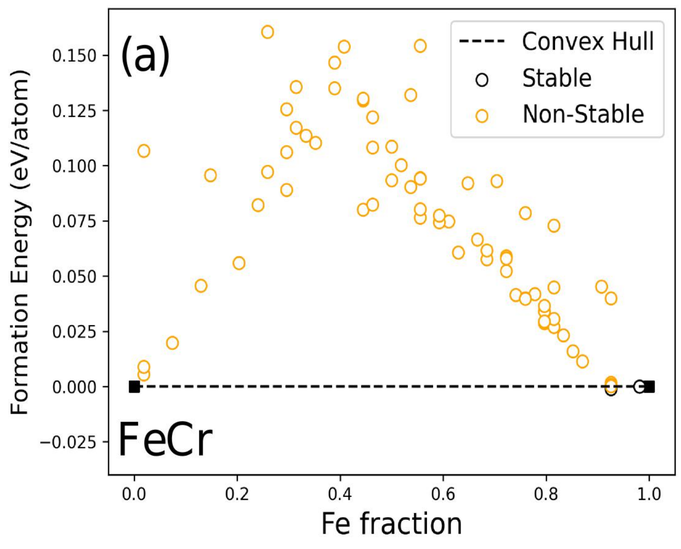
*These authors contributed equally.

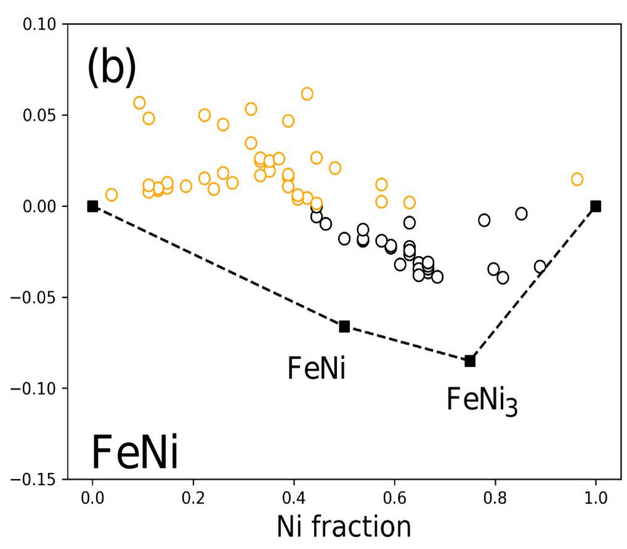


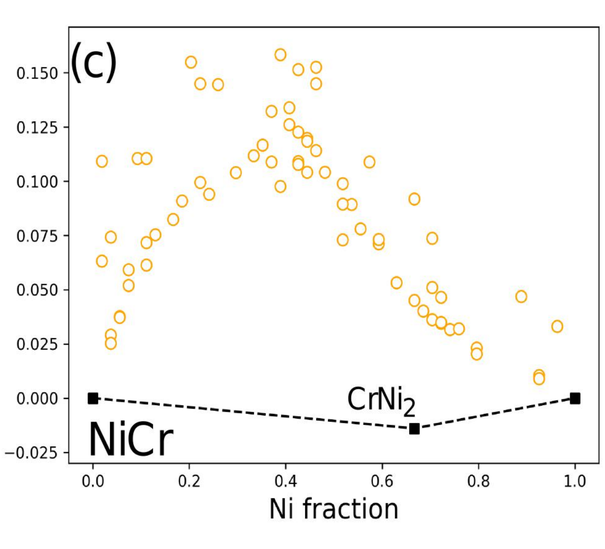
Composition Search Workflow: The dataset is created based on CALPHAD and using generative diffusion models (CDVAE) [1] new materials were created. The new materials were validated by DFT and then were used for optimization of materials properties.

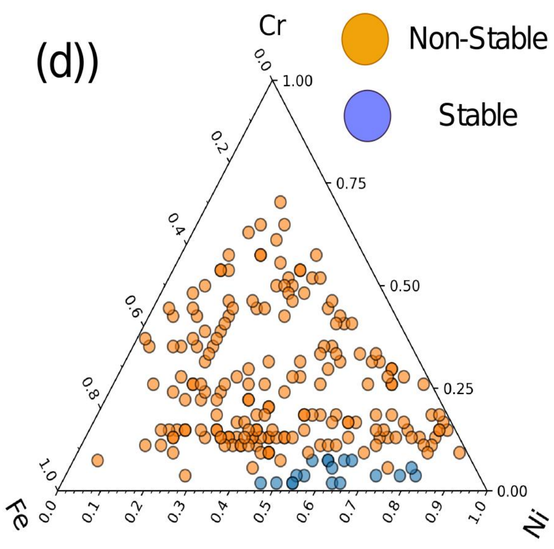


Dataset: The initial database is curated for specific stable compositions of NiFeCr based on CALPHAD calculations [2]. The left section of the phase diagram is in BCC (purple) phase and the right part FCC (yellow).



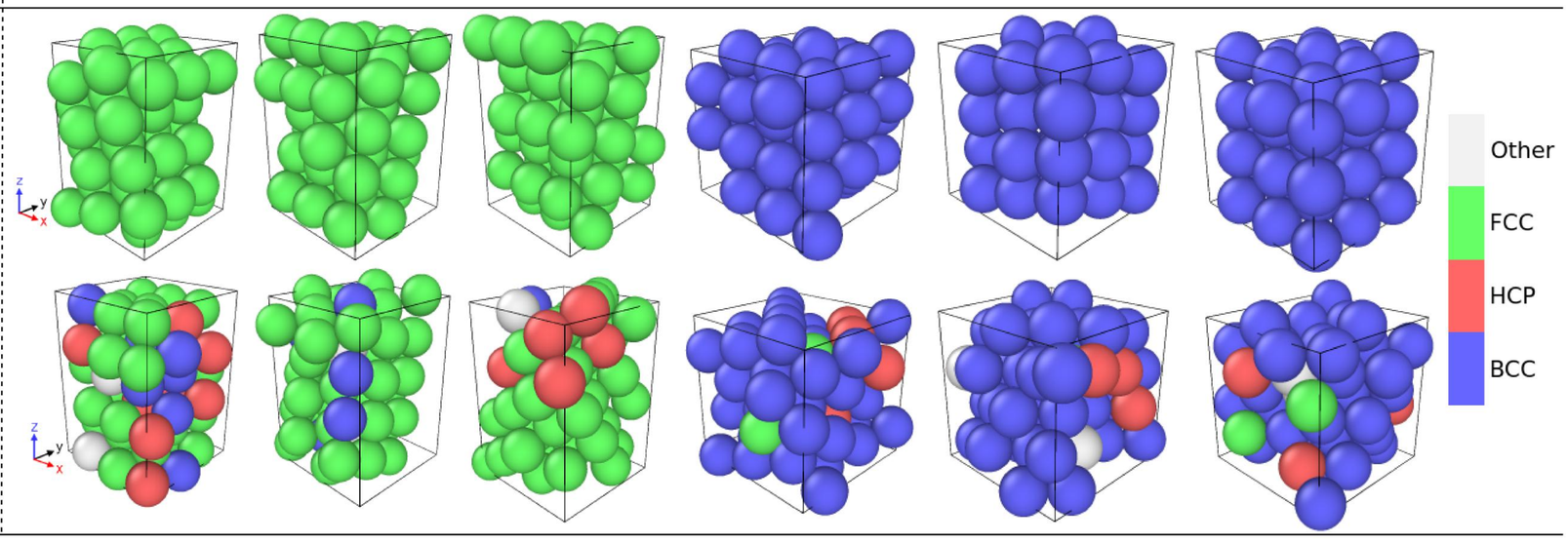






DFT Validation: New materials were generated with the phase-aware CDVAE model (P-CDVAE). Upon validation through DFT, our findings aligned with those obtained through the cluster expansion method for the same problem [3]. This concordance establishes the reliability of our P-CDVAE model, positioning it as a robust tool applicable to other high or medium entropy alloys.

Chemical Formula	$Cr_{28}Fe_{41}Ni_{31}$	$Cr_{31}Fe_{46}Ni_{23}$	$Fe_{85}Ni_{15}$	$Cr_{29}Fe_{38}Ni_{33}$	$Cr_{63}Fe_{37}$	$Cr_{20}Ni_{80}$
CP	FCC	FCC	FCC	BCC	BCC	BCC
P-CDVAE						
CDVAE						



Reconstruction of P-CDVAE: The diffusion model must possess the capability to predict and effectively (re)construct generated materials into the correct crystalline phase. Notably, our Phase-aware P-CDVAE model surpasses the performance of the standard CDVAE by **30%** in accomplishing this task.

REFERENCES

[1] Crystal Diffusion Variational Autoencoder for Periodic Material Generation. https://doi.org/10.48550/arXiv.2110.06197

[2] Modified embedded-atom interatomic potential for fe-ni, cr-ni and fe-cr-ni systems. https://www.sciencedirect.com/science/article/pii/S0364591616302048

[3] Phase stability of ternary fcc and bcc fe-cr-ni alloys. Phys. Rev. B, 91:024108, https://link.aps.org/doi/10.1103/PhysRevB.91.024108

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NOMATEN
Centre of Excellence in Multifunctional Materials for Industrial and Medical Applications

Low ball-to-powder-ratio sintered CoCrFeNi high entropy alloys: Cr-rich structure evolution and enhanced mechanical properties

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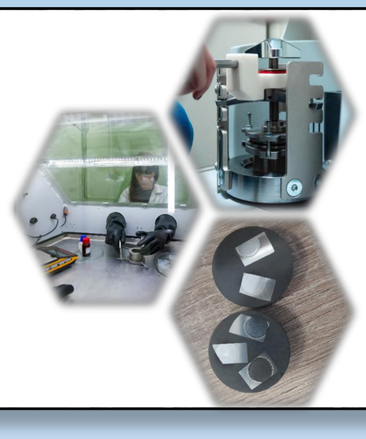
NOMATEN Centre of Excellence, National Centre for Nuclear Research, A. Sołtana 7, 05-400 Otwock, Poland

ABSTRACT

Powder metallurgy is a promising alternative for manufacturing of modern alloys including high-entropy alloys. The main assumption of this group of techniques is to mix all the desired elements in a proper composition and then synthesized to obtain a bulk material. Beside many advantages of these methods the biggest disadvantage is the scale of obtained pieces. In order to overcome difficulties we decided to reduced ball-to-powder ratio (BPR) to find the possibilities to make this process more industrially scalable.

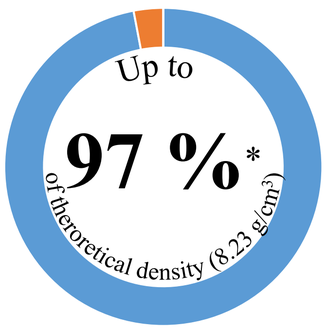
Our goals

- Process productivity improvement with efficiency maintain simultaneously.
- Choosing the best manufacturing conditions based on well known composition (CoCrFeNi).
- Manufacturing of the unique high entropy alloys composition with high mechanical properties, corrosion and radiation resistance (based on the work of simulations groups) using arc melting and powder metallurgy techniques.



Process parameters

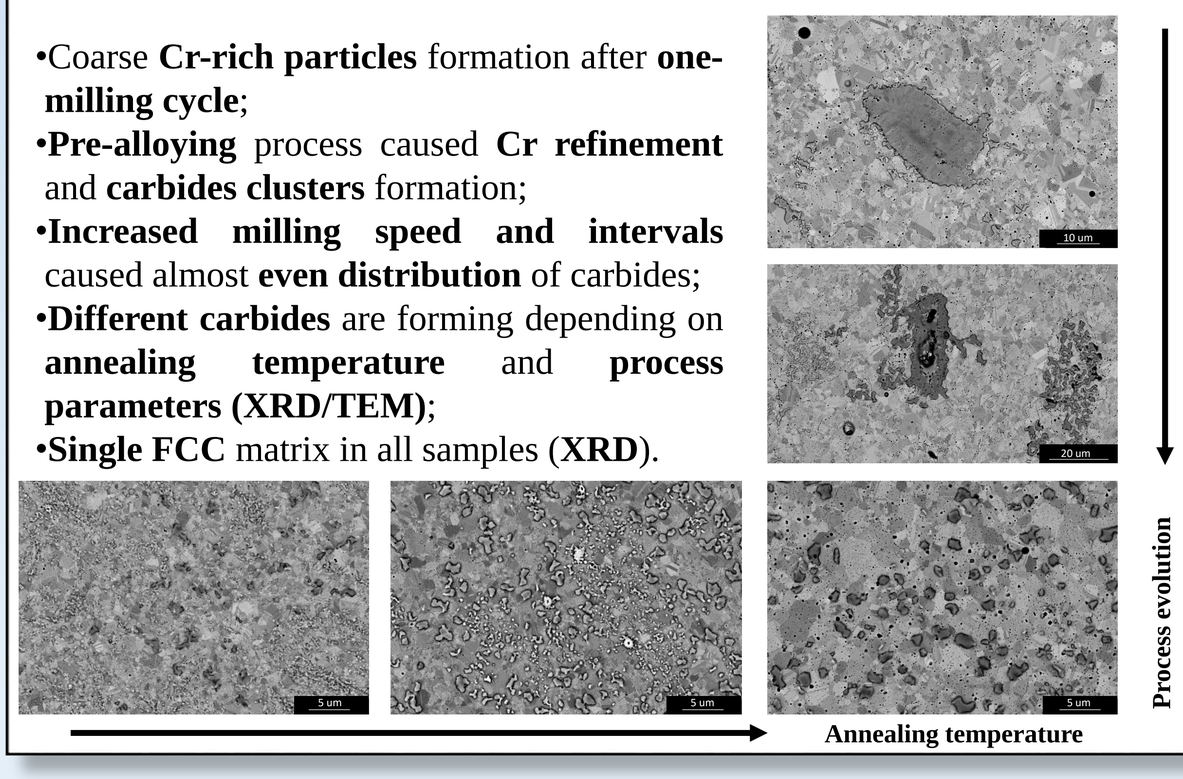
	Milling speed [rpm]	Milling intervals [min:min]	Pre-alloying process	BPR / PCA
MI (one-milling cycle)	250	15:15	No	5:1 / C_7H_{18}
PA (+Cr-Ni prealloying)	250	15:15	10 h	
MIX	350	15:5	10 h	



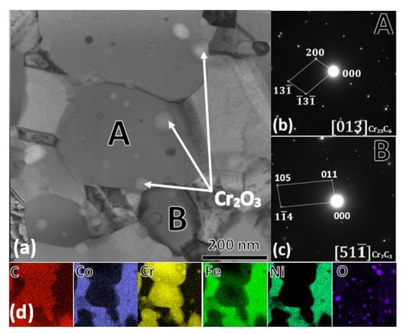
Sintering: **950°C/10 min**; Annealing: **850°C/1050°C for 12 h**

Microstructure observation

- Coarse **Cr-rich particles** formation after **one-milling cycle**;
- **Pre-alloying** process caused **Cr refinement** and **carbides clusters** formation;
- **Increased milling speed and intervals** caused almost **even distribution** of carbides;
- **Different carbides** are forming depending on **annealing temperature** and **process parameters (XRD/TEM)**;
- **Single FCC** matrix in all samples (**XRD**).

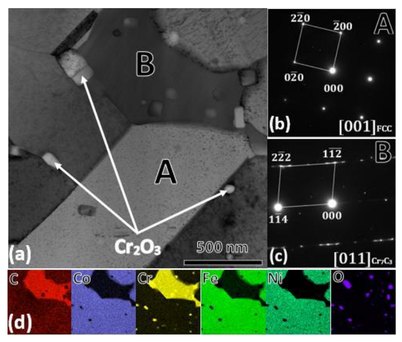


TEM



MIX sample after **sintering**:

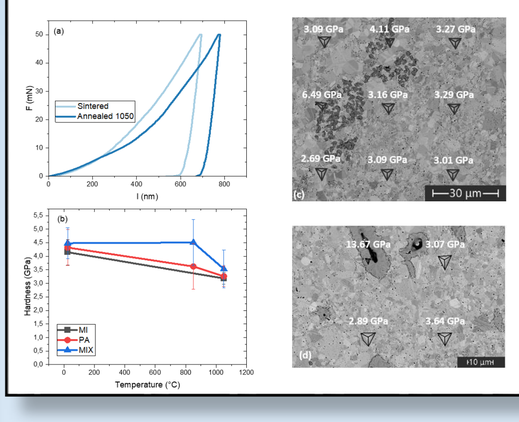
- Two types of chromium carbides: $Cr_{23}C_6$ (A) and Cr_7C_3 (B) – dark grey and light grey particles;
- Small chromium oxides formation.



MIX sample after **annealing at 1050°C**:

- One type of chromium carbide – Cr_7C_3 – dark grey particles;
- Small chromium oxides remains.

Hardness



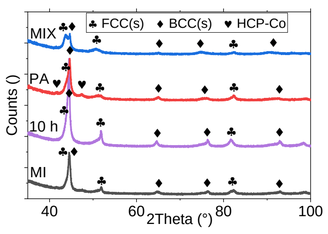
- Significant hardness stability of MIX sample;
- Nanohardness of reinforment phase up to 15 GPa and ~7 GPa for agglomerates (weighted average of matrix and precipitates);
- Results are consistent with microhardness.

Conclusions

- Chromium **carbides refinement** after **two-steps process** implementation;
- Chromium carbides' **even distribution** after further **process optimization**;
- The **evolution of carbides** as a function of annealing **temperature**: **$Cr_{23}C_6$/Cr_7C_3** → **$Cr_{23}C_6$** (transformation at ~650°) → **Cr_7C_3** (reverse transformation after long term high temperature annealing + water quenching);
- **Hardness improvement** after process improvement.

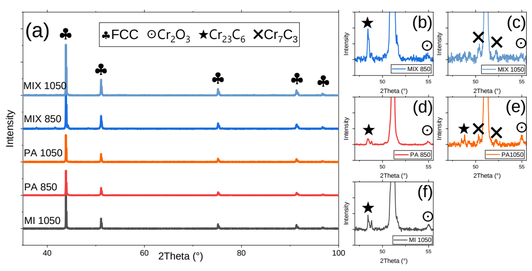
Paper already submitted to ***Journal of Materials Research and Technology***

Structural studies



Powder diffraction:

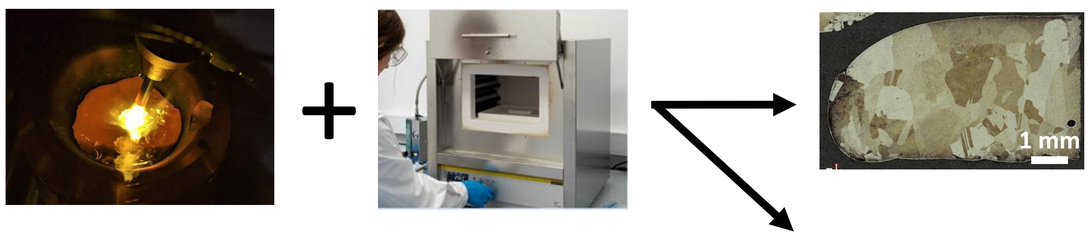
- FCC, BCC, HCP peaks can be observed;
- Mechanical alloying did not provide the fully alloyed powder.



Sintered and annealed samples:

- Single FCC peak represent single FCC phase;
- XRD pattern is free of BCC peaks;
- Different carbides formation depending on the manufacturing process and annealing temperature;
- No correlation between process and the amount of chromium oxides.

Arc melting



Observations:

- No dendrites – grains structure;
- Coarse grains and uneven grain growth;
- Negligible elements loss;
- High chemical composition stability in both XRF and EDS scale;
- Plastic deformation + recrystallization process needed.

Cantor alloy	Wt. % Co	Cr	Fe	Mn	Ni
Nominal	21	19	20	19	21
Via XRF	22	19	22	17	20
Via EDS	23	18	21	16	22

European Funds
Republic of Poland
FNP Foundation for Polish Science
European Union

Synthesis and evaluation of new supramolecular receptors for molecular imaging and therapy

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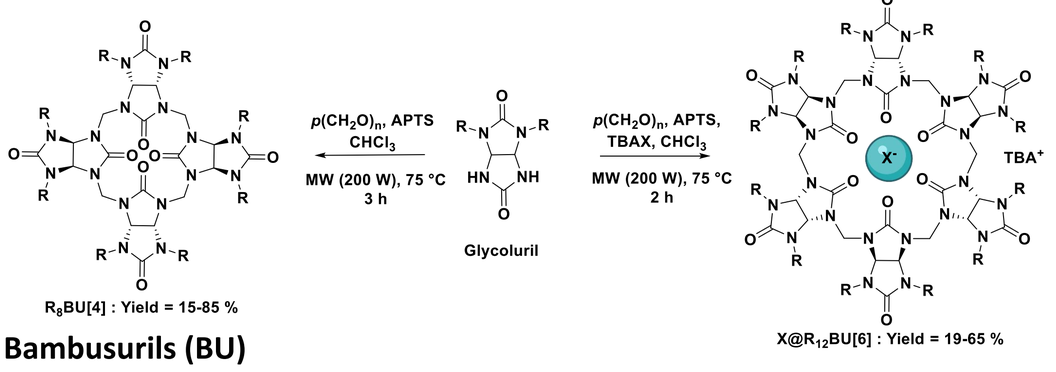
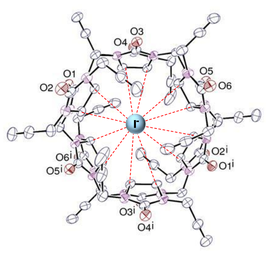
History of Bambu[4,6]surils

Synthesis and properties of Bambu[4,6]surils



Bambusurils (BU)

- Synthetic cage molecules discovered in 2010 [1]
- Soluble either in organic or aqueous media depending on R substituents
- Two sizes: BU[4] and BU[6]



Crystal structure of I^-@propargyl$_{12}$BU[6].TBA$^+$

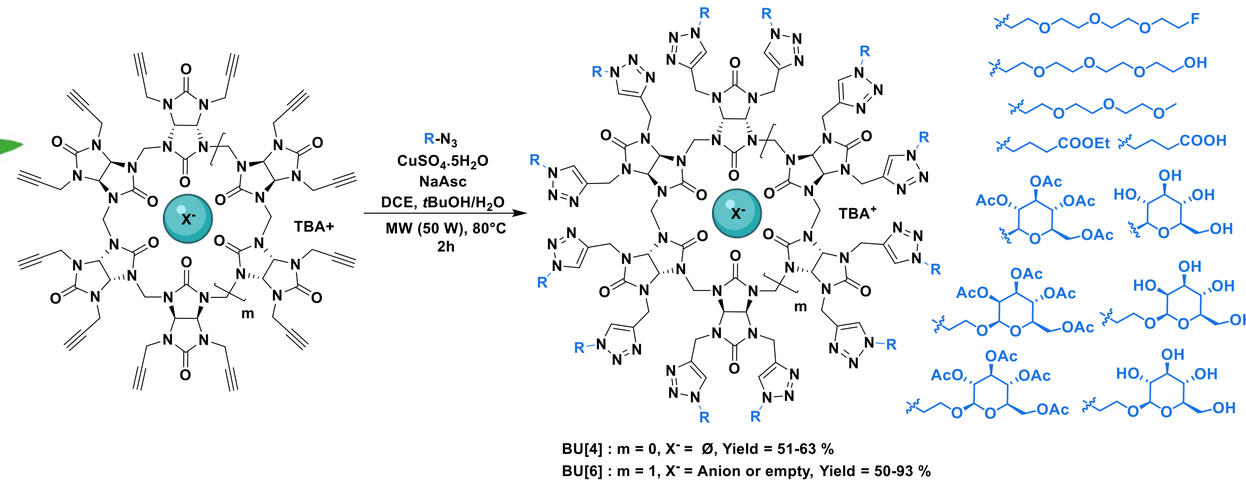
Complexation properties

- BU[6] can encapsulate anions with strong affinity
- 12 C-H bonds pointing inside the cavity of BU[6], creating a positive potential
- High affinity for I^- (10^7 – 10^{10} M^{-1}) in organic solvent or water
- K_a : I^- > Br^- > Cl^- > F^- :4400:1200:12:1
- BU can be used as a multivalent platform

[1] J. Svec, M. Necas, V. Sindelar, *Angew. Chem., Int. Ed.* **2010**, *49*, 2378.

Previous work

Post-functionalisation of PropargylBU[4,6] by CuAAC reaction



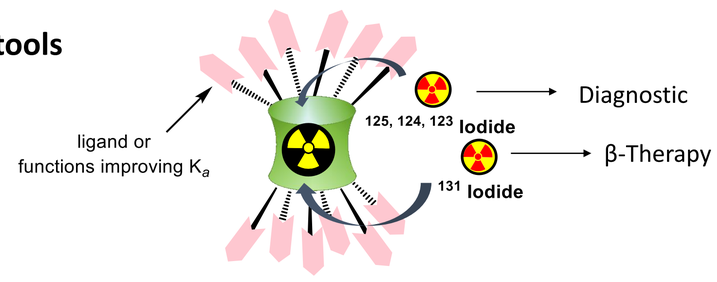
- Perfunctionalisation [2]
- Access to organosoluble and hydrosoluble BUs
- Affinity constants K_a with I^- measured by ITC 10^4 – 10^5 M^{-1} (H_2O) [3]
- Dual scaffolds for iminosugars presentation [4]

[2] M. Lafosse, E. Cartier, K. Solmont, J. Rivollier, D. Azazna, P. Thuéry, Y. Boulard, A. Gontier, J.-B. Charbonnier, B. Kuhnast, M.-P. Heck, *Org. Lett.* **2020**, *22*, 3099 ; [3] Unpublished results ; [4] M. Lafosse, Y. Liang, J. P. Schneider, E. Cartier, A. Bodlenner, P. Compain, M.-P. Heck, *Molecules* **2022**, *27*, 4772.

Goal of the PhD work

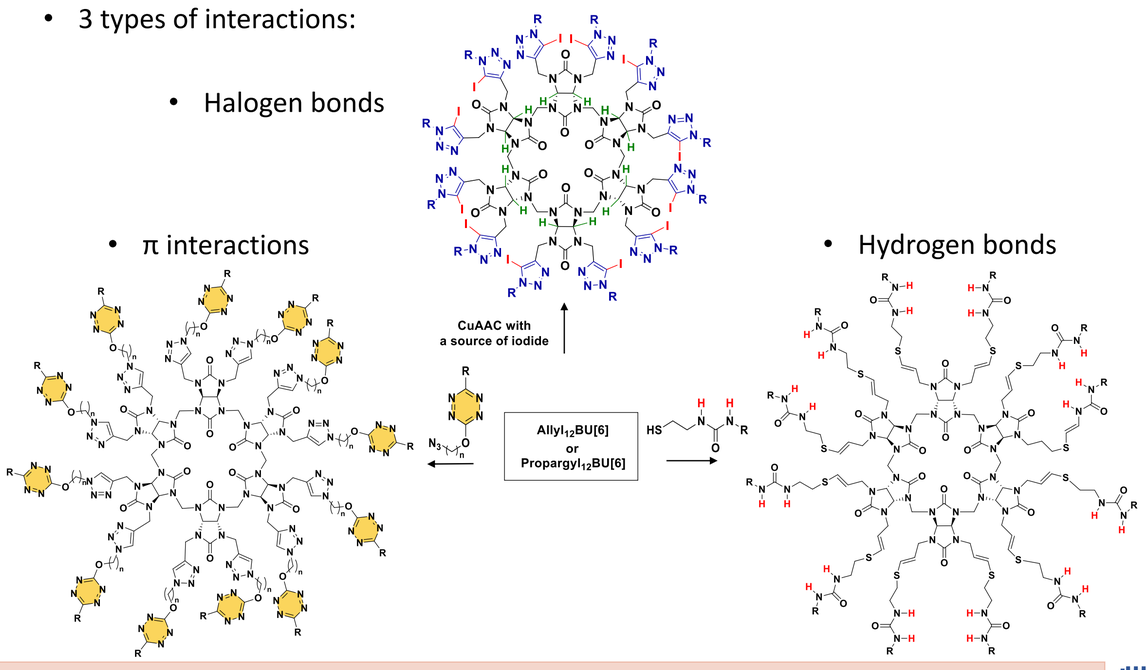
1) To synthesise new theranostics tools

- Based on BU skeleton
- More selective
- More efficient for targetting



2) To improve complexation efficiency by adding weak interactions on the portal

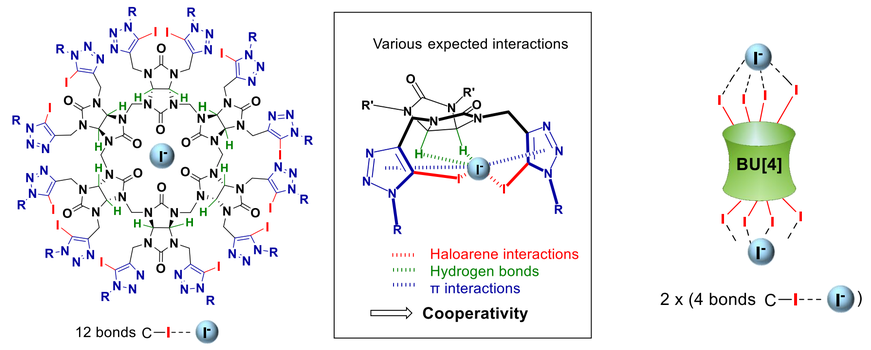
- 3 types of interactions:
  - Halogen bonds
  - π interactions
  - Hydrogen bonds



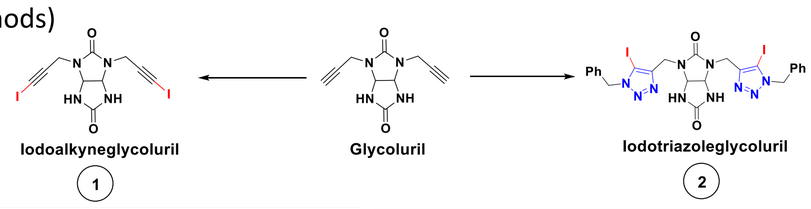
Working Plan 1

➢ Synthesis of BU functionalised with iodotriazoles [5]

- Increase the affinity constant through a cooperative effect
- Find the first application of BU[4] as an anionic complexing agent



The study initially focused on propargylated glycoluril, which was functionalised with iodoalkynes and iodotriazoles. Complexation studies must be carried out soon (NMR, ITC, UV methods)

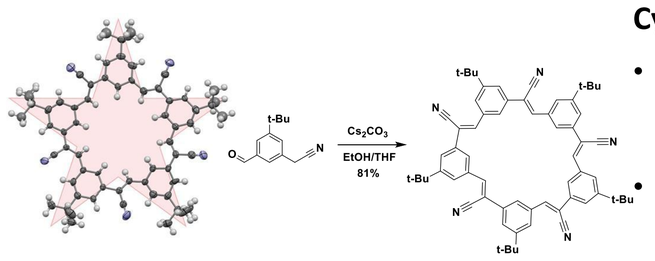


Conditions	Yields (1)
KI, TBHP, MeOH	67 %
nBuLi, I_2, THF	/
NIS, AcOH, CH_3CN	/

Conditions	Yields (2)
NaAsC, $CuSO_4.5H_2O$, H_2O/*t*-BuOH	/
CuI, NBS, DIPEA, THF	/
$Cu(ClO_4)_2$, NaI, DBU, TBTA, CH_3CN	74 %

[5] In progress

History of Cyanostars

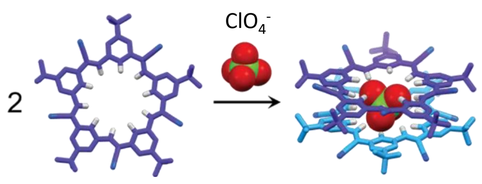


Cyanostars (CS)

- Macrocyclic star-shape receptors having an electrophilic cavity surrounded by H–bond donors discovered in 2013 [6]
- First fluorescent CS having remarkable spectral properties (Stokes shift of 15000 cm^{-1}) discovered in 2020 [7]

Complexation properties

- CS can encapsulate anions in 2:1 π-stack sandwich complex
- The most efficient 2:1 receptors so far known for I^-



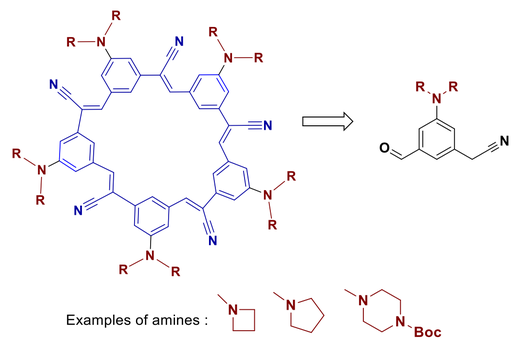
[6] S. Lee, C.-H. Chen, A. H. Flood, *Nat. Chem.*, **2013**, Vol. 5 ; [7] A. Dhara, T. Sadhukhan, E. G. Sheetz, A. H. Olsson, K. Raghavachari, A. H. Flood, *J. Am. Chem. Soc.* **2020**, *142*, 12167.

Goal of the PhD work

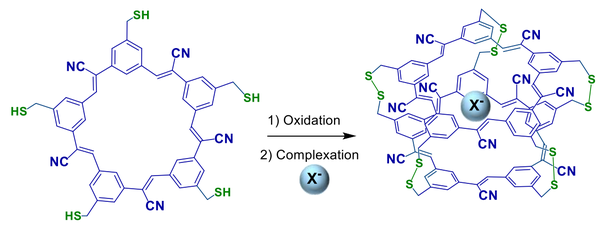
➢ To design new cyanostars

- To increase the affinity for iodides
- New CS with new photophysical properties
- To be used in water media

- Fluorescent cyanostars



- Sulfurcyanostars



Conclusion and perspectives

- Synthesis of propargyl$_8$BU4 and X^-@propargyl$_{12}$BU6
- Synthesis of functionalised glycoluril
- Functionalisation of BU4 and BU6 by click reaction
- Study of the affinity constant of functionalised glycoluril
- Polyfunctionalisation of BU
- Synthesis of new anion receptors

Theranostic Micellar Nanocarriers for Imaging, Targeted Radiosensitization and Internal Radioisotope Therapy

Mathilde Ponchelle[1,2], Edmond Gravel[2], Izabela Cieszykowska[3], Marek Pruszyński[1,4], Eric Doris[2]

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[4]Institute of Nuclear Chemistry and Technology, Warsaw, Poland

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Introduction

The effectiveness of internal radioisotope therapy is hampered by a number of radioresistance-inducing phenomena, such as hypoxia. Selective re-oxygenation of the target tissues can potentiate the local effect of the irradiation by enhancing the production of altering reactive oxygen species (ROS).
We designed a micellar nanocarrier combining re-oxygenation properties, thanks to a perfluorinated core, and dose potentiation of ^{177}Lu, thanks to encapsulated gold nanoparticles (AuNPs).

Methods

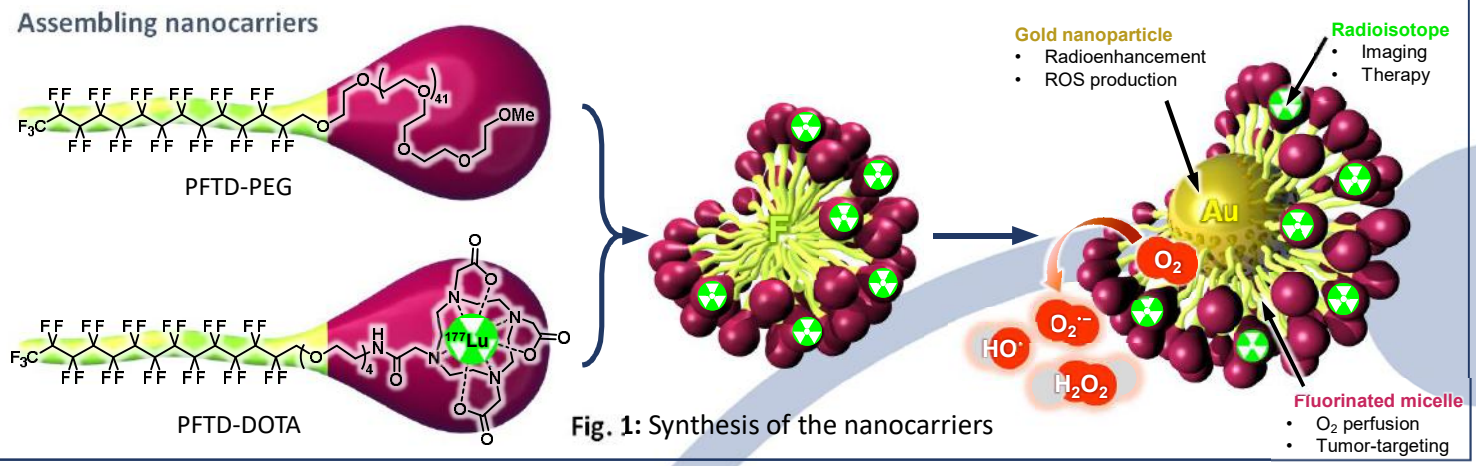


Fig. 1: Synthesis of the nanocarriers

Results

^{175}Lu complexation

- pH 5 (NaOAc buffer)
- 1 equiv. ^{175}Lu
- RT, overnight or
- 100 °C, 30 min

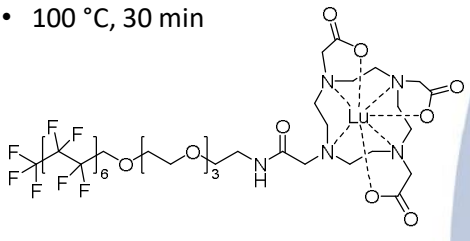


Fig. 2: Complexation of ^{175}Lu

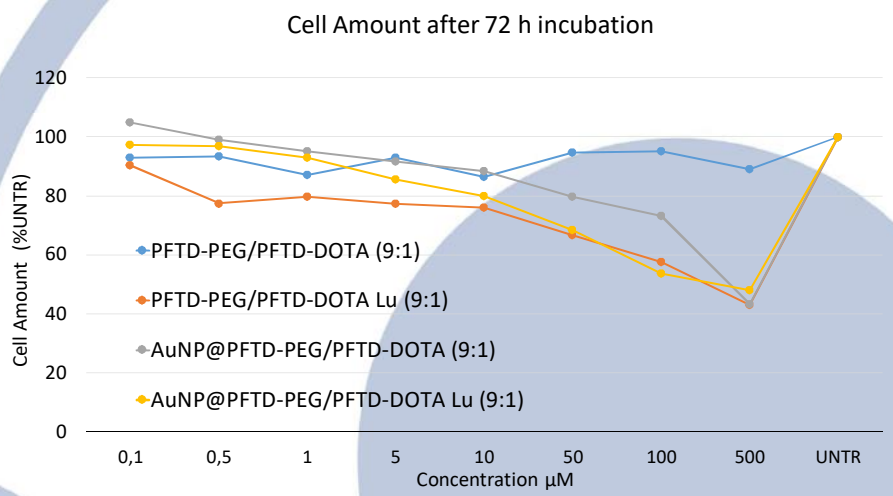


Fig. 3: Toxicity of the nanocarriers ; cell line SKBR3 – HER2 positive

Conclusion

At this stage, complexation with radioactive ^{177}Lu should be implemented to finalize preliminary studies before biodistribution and full *in vivo* evaluation is performed. Dual targeted re-oxygenation of cancer tissues and potentiation of internal radioisotope therapy is expected through the combination of a fluorinated reservoir (O_2 transport) and a gold core (radioenhancement) in the nanohybrid system.

Acknowledgment

We acknowledge support from the European Union Horizon 2020 research and innovation program under grant agreement no. 857470 and from the European Regional Development Fund via the Foundation for Polish Science International Research Agenda PLUS program grant No. MAB PLUS/2018/8. This work is also supported by the "ADI 2022" project funded by the IDEX Paris-Saclay, ANR-11-IDEX-0003-02".

Radioiodination of novel prosthetic groups *via* copper-mediated nucleophilic approach

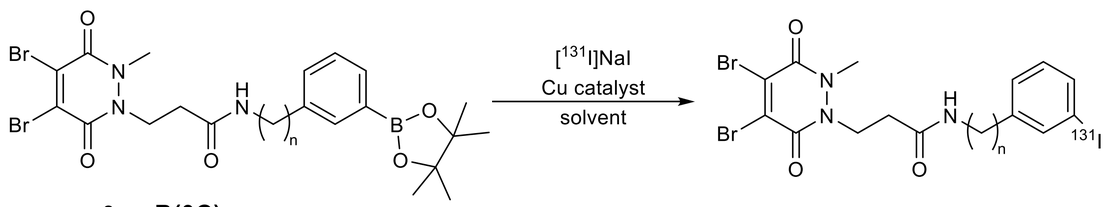
Ihab Shokair*[1], Anna Krzyczmonik[1], Mylène Richard[2], Justyna Pijarowska-Kruszyna[3], Bertrand Kuhnast[2], Renata Mikołajczak[3], Marek Pruszyński[1,4]

[1]NOMATEN Centre of Excellence, National Centre for Nuclear Research, Otwock, Poland [2]Université Paris-Saclay, CEA, CNRS, Inserm, BioMaps, Orsay, 91401, France [3]Radioisotope Centre POLATOM, National Centre for Nuclear Research, Otwock, Poland [4]Institute of Nuclear Chemistry and Technology, Warsaw, Poland

1. Introduction and objective

- A new highly efficient copper-mediated method was developed for the facile radioiodination of aromatic and heteroaromatic boron reagents[1-3].
- This method is efficient, low cost, and unlike electrophilic labeling methods, requires no oxidizing agents.
- **The main objective of this project was to radiolabel two new prosthetic groups using the copper-mediated iododeboronation method and to test three different copper catalysts according to the previously published procedures[1-3].**

2. Methods



n = 0 → **B(0C)**
n = 1 → **B(1C)**

Copper catalyzed reactions: 1- $Cu(py)_4(OTf)_2$, [131I]NaI, MeOH:MeCN (4:1), RT, 20 min

2- Cu_2O, [131I]NaI, 1,10-phenantroline, MeCN, RT, 1 h

3- $Cu(OCOCF_3)_2$, [131I]NaI, 1,10-phenantroline, MeOH:H_2O (4:1), 80 ^{0}C, 20 min

Fig 1. Synthesis of two novel prosthetic groups *via* copper-mediated radioiodination method

3. Results

For precursor B(0C):

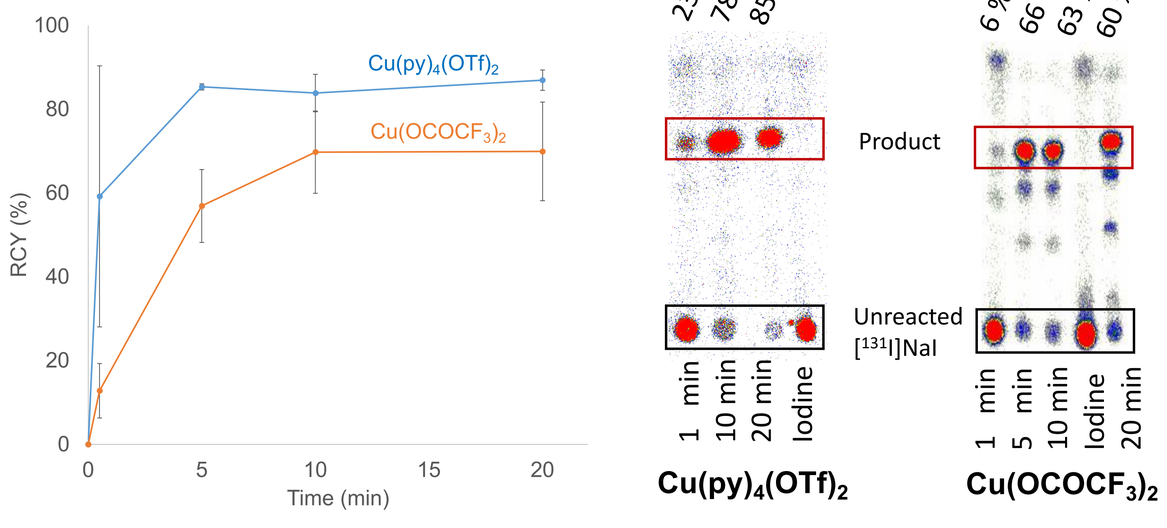


Fig 2. Results of the kinetic studies of the reaction progression and examples of the radio-TLC images from the reactions performed with $Cu(py)_4(OTf)_2$ and $Cu(OCOCF_3)_2$

Table 1. Results of the copper-mediated reactions performed with different copper catalysts

Catalyst	RCY (TLC)	RCY (HPLC)	Number of reactions
$Cu(py)_4(OTf)_2$	87 ± 2 %	96 ± 2 %	3
$Cu(OCOCF_3)_2$	70 ± 11 %	89 ± 9 %	3
Cu_2O	0 %	0 %	1

For precursor B(1C):

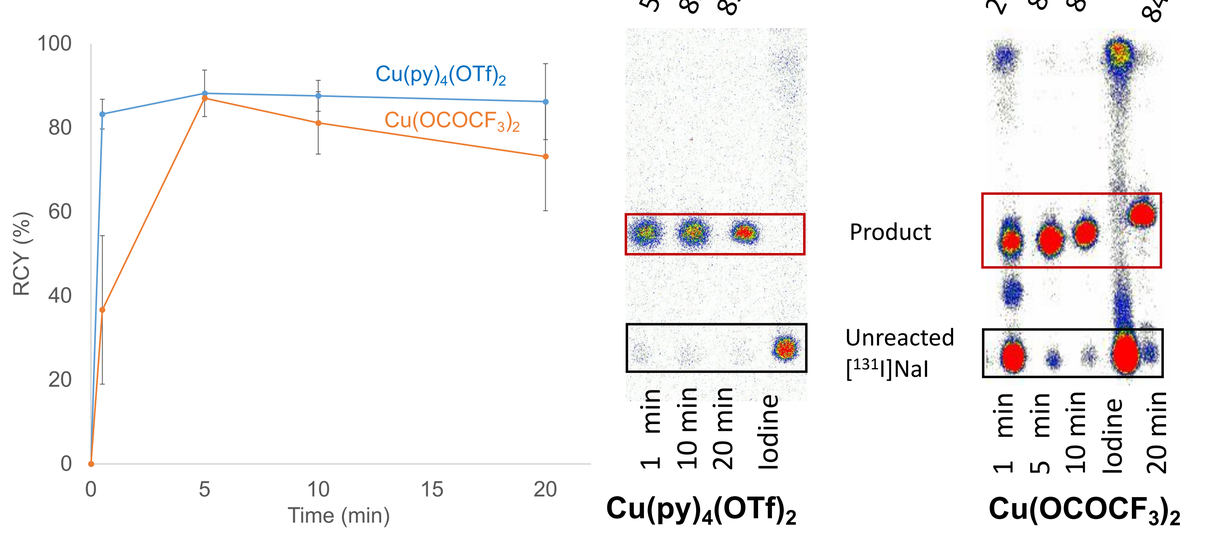


Fig 3. Results of the kinetic studies of the reaction progression and examples of the radio-TLC images from the reactions performed with $Cu(py)_4(OTf)_2$ and $Cu(OCOCF_3)_2$

Table 2. Results of the copper-mediated reactions performed with different copper catalysts

Catalyst	RCY (TLC)	RCY (HPLC)	Number of reactions
$Cu(py)_4(OTf)_2$	86 ± 9 %	96 ± 4 %	3
$Cu(OCOCF_3)_2$	73 ± 12 %	72 ± 28 %	3
Cu_2O	0 %	0 %	1

RCY: Radiochemical yield

4. Conclusions

- The best results for radiolabelling of the two prosthetic groups were obtained when using $Cu(py)_4(OTf)_2$ as a catalyst.
- Good radiolabelling using $Cu(OCOCF_3)_2$.
- No radiolabelling was obtained using the Cu_2O catalyst.

5. Future plan

- The two radiolabeled prosthetic groups will be further used for the conjugation of octreotide *via* disulfide rebridging.

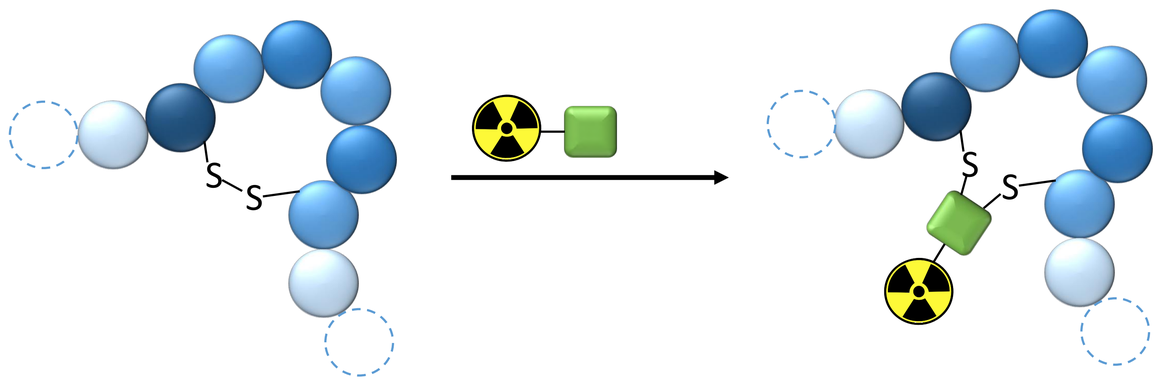


Fig 4. Site-selective modification of biomolecules *via* disulfide rebridging

6. Acknowledgments

This project is supported by the European Union Horizon 2020 research and innovation program under grant agreement no. 857470 and by the European Regional Development Fund via the Foundation for Polish Science International Research Agenda PLUS program grant No. MAB PLUS/2018/8

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NOMATEN

Winter School, Warsaw
NOV 28-30, 2023

Understanding oxidation of zirconium and its alloys in air and water vapour operating conditions – high temperature Raman studies

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INTRODUCTION

Zirconium alloys are used for fuel cladding in nuclear reactors, where they act as a barrier separating the fuel from the coolant [1]. During operation, a cyclic corrosion process occurs due to constant contact with water. At each stage of the cycle, the oxide phases and their physicochemical properties undergo changes [1-2]. High temperature in situ Raman studies enable precise tracking of the evolution of tetragonal phase content and stresses in the oxide during corrosion. The presented work specifically focused on the alternations during heating, annealing, and cooling of the sample.

MATERIALS

Zr

air	up to 600 °C
heating	20 °C/min
annealing	7 h
cooling	3 h

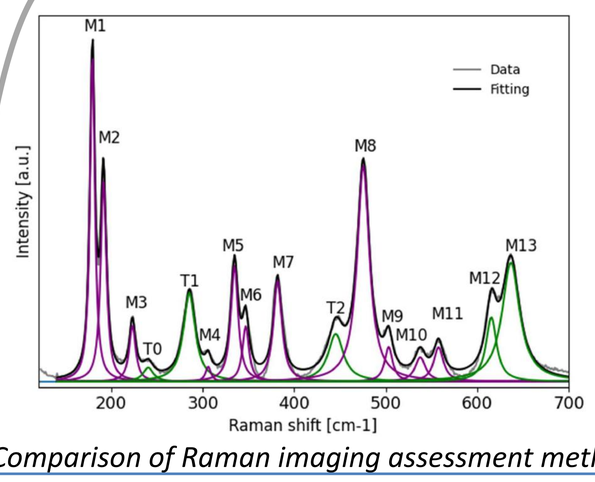
Linkam TS1000

WITec Raman alpha 300R

METHODOLOGY* – HIGH TEMPERATURE RAMAN ANALYSIS

Background substraction → Cosmic ray removal → Fitting

Tetragonal phase percentage calculations [mol%]



Band assignment	M1	M2	T1
Intensity	649.56	447.5	840.78
Raman shift	178.08	190.36	281.88
FWHM	8.14	10.48	10.44

$$\%T_{ZrO_2} = \frac{I(T_1)}{I(M_2) + I(M_1) + I(T_1)}$$

Stress state determination (σ)

$$\sigma = \Delta\vartheta \cdot \pi_{uniaxial}$$

$\pi_{uniaxial}$ [cm^{-1}/GPa] [3]

M1	M2	T1
-0.653	-0.83	1.2

$$\pi_{uniaxial} = \frac{\pi_{hydrostatic}}{3}$$

$\pi_{hydrostatic}$ – Piezospectroscopy coefficient

$$\Delta\vartheta = \vartheta_\sigma - \vartheta_0$$

ϑ_0 [cm^{-1}]

M1	M2	T1
179.1	191.2	285

ϑ_0 – *Raman shift of stress-free sample*

ϑ_σ – *Raman shift of stressed sample*

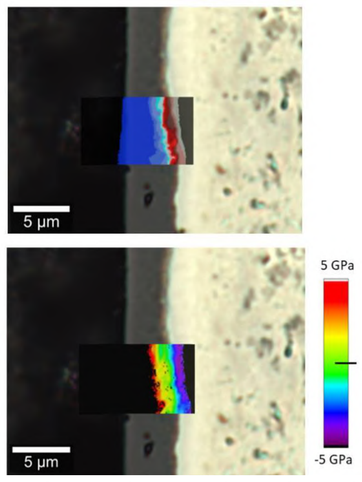
* K. Suchorab et al. *„Comparison of Raman imaging assessment methods in phase determination and stress analysis of zirconium oxide layer”*, Spectrochim Acta A Mol Biomol Spectrosc, 2023

RESULTS – EVOLUTION OF PHASE CONTENT AND STRESSES DURING OXIDATION

Cross section Raman examination**

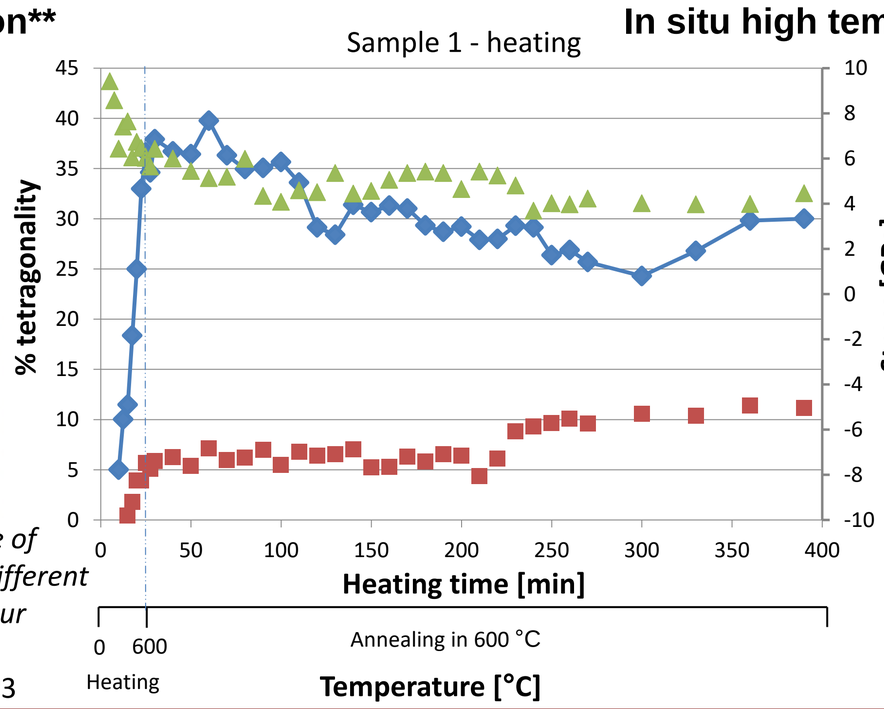
Tetragonal phase distribution

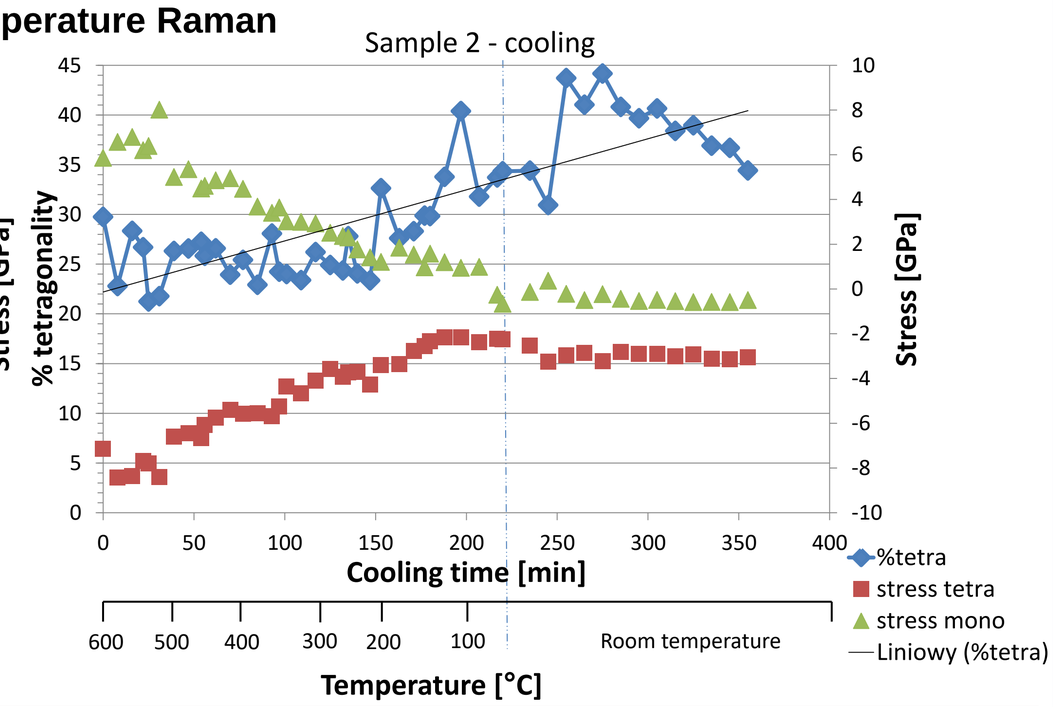
Stress distribution



** K. Suchorab et al. *„Understanding the role of tetragonal phase in oxidation behaviour of different zirconium-based alloys in air and water vapour conditions – phase fraction and stress field distribution”*, Materials Characterisation, 2023

In situ high temperature Raman





Highlights

Heating

- Initially monoclinic zirconium oxide is formed
- Subsequently, tetragonal zirconium oxide creates and its concentration increases with continued heating
- The creation of phases is accompanied by a significant stress level
- The absolute stress values decrease during the heating process for both phases

Annealing

- The tetragonal phase diminishes during annealing
- This is a sign of tetragonal to monoclinic transition
- The decrease in the absolute value of stress slows down

Cooling

- The amount of tetragonal phase oscillates at increasingly higher values, indicating a continuous formation of the tetragonal phase, followed by t→m transitions (with the dominant effect of tetragonal phase formation)
- During cooling, stress in the monoclinic phase fall to zero
- In the tetragonal phase, stress diminished during cooling and stabilises at a level of about 2 GPa

Room temperature

- After reaching room temperature, the creation of tetragonal phase and t→m transitions still take place
- After some time, the tetragonal phase starts oscillating to lower values
- Stabilisation of stresses

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[3] P. Bouvier, *Etude Raman des distributions de phases de contrainte dans des couches d'oxydation d'alliages de zirconium*, **PhD thesis** – Institute National Politechnique de Grenoble, **2000**.

FUTURE PLANS

Stresses and corrosion:

1. ❑ TGA in air and water vapour
   ❑ HT RAMAN with tensile stage
   ❑ HT XRD
   ❑ LIBS – stoichiometry determination
   ❑ TEM – grain size detemination

Hydrogen charging and its influence:

2. ❑ TDS
   ❑ Miniature tensile tests
   ❑ Raman and HT Raman with tensile stage

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NOMATEN Winter School
28-30 of November 2023, Warsaw, Poland

Effect of radiation and temperature on the mechnical and structural properties of fcc NixFe1-x single crystals

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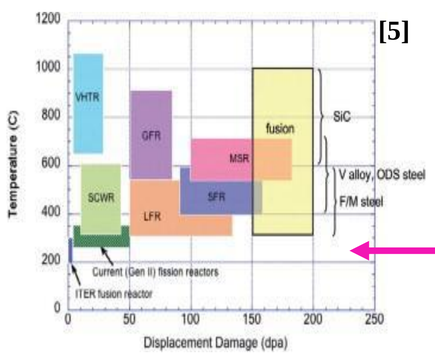
Introduction

The structural materials for Generation IV concept fission reactors will be subjected to exceptional fluxes of high-energy neutrons and extreme operating temperatures [1,2]. Those factors in turn lead to changes in the structure, thermo-mechanical properties, and reduced lifetimes of the target materials [3,4]. To design the material, that can withstand such harsh conditions one needs to understand its properties under extreme conditions. For this reason, in the proposed work, we study the evolution of the defects and their impact on the mechanical properties of *fcc* Ni_xFe_{1-x} single-crystal alloys and the impact of temperature.

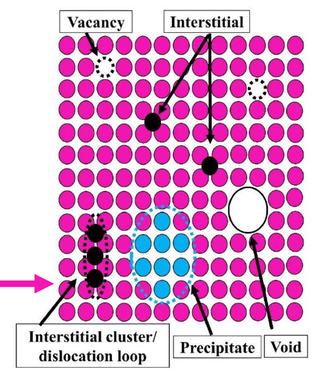
Motivation



[5]

Harsh working environment in nuclear reactors:
- **Temperature**
- **Neutron irradiation**

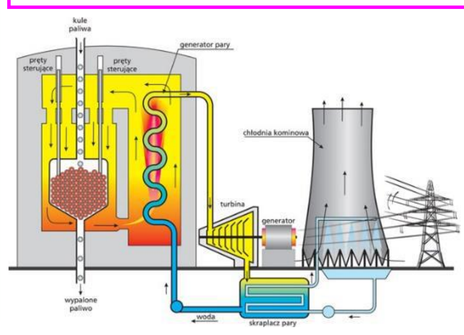
Formation of radiation defects!!!



- Degradation of mechanical properties
- Structural changes
- Swelling of the material - change in volume
- Reduction in material lifetime

There is evidence that **tuning the chemical composition of a single-phase alloy** may significantly change the features of defect clusters **and overall characteristic of the material** [1], **which needs to be elaborated.**

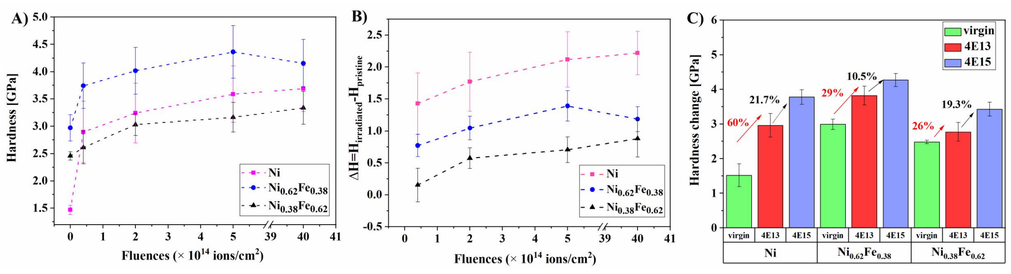
Ni_xFe_{1-x} single crystals seem to be a good candidates to understand such mechanisms!



The outcomes of the performed research of the Ni_xFe_{1-x} single crystals may become the basis for designing a new chemical composition of advanced high-entropy alloys (HEA), which can be used, for example, as an element of the primary cooling circuit in the HTR reactor!

Effect of irradiation

Irradiation-induced hardening of Ni_xFe_{1-x} crystals

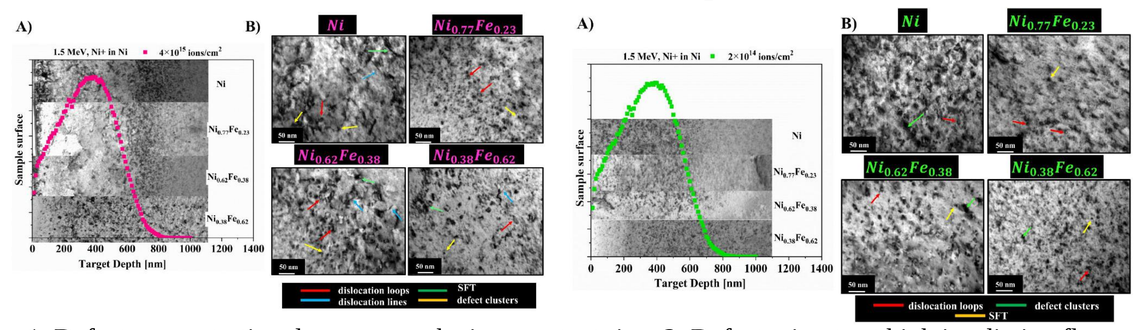


A) Nanoindentation hardness of fcc Ni, $Ni_{0.62}Fe_{0.38}$, and $Ni_{0.38}Fe_{0.62}$ single crystal alloys as a function of irradiation fluence, B) hardness change according to the equation $\Delta H = H_{irradiated} - H_{pristine}$ and C) comparison of hardness change for pristine and irradiated samples of Ni, $Ni_{0.62}Fe_{0.38}$ and $Ni_{0.38}Fe_{0.62}$ between two fluences: 4×10^{13} and 4×10^{15} ions/cm^2.

The hardness of each of presented composition is increasing with increasing ion fluence. The most drastic hardening is visible in Ni, while the smallest hardening occurs in $Ni_{0.38}Fe_{0.62}$

TEM Images

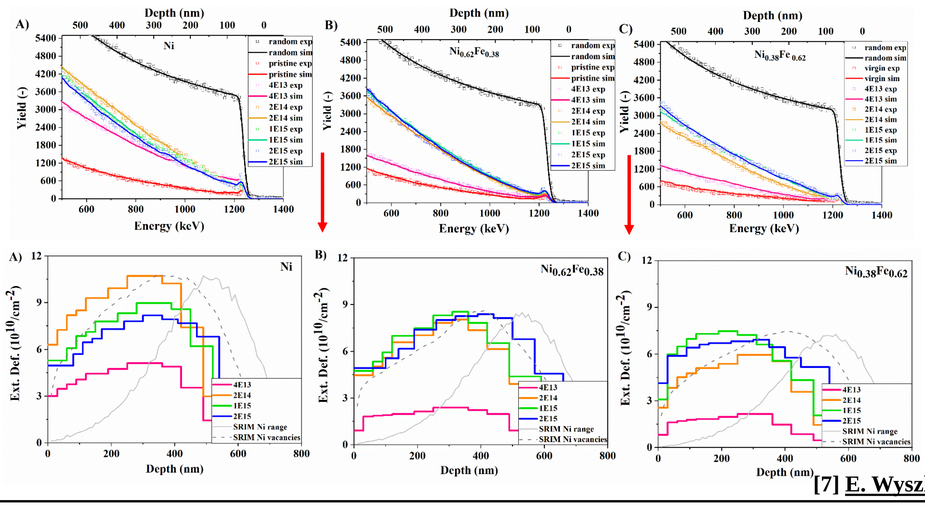
Cross-sectional TEM images of the Ni, $Ni_{0.77}Fe_{0.23}$, $Ni_{0.62}Fe_{0.38}$ and $Ni_{0.38}Fe_{0.62}$ irradiated with a fluence of 2×10^{14} and 4×10^{15} ions/cm^2 compared with SRIM calculations



1. Defect concentration decreases as the iron content rises 2. Defect migrate at high irradiation fluence 3. The migration mechanism could result from a combination of processes such as defect recombination, production, cluster formation etc. 4. In $Ni_{0.38}Fe_{0.62}$, the defects are evenly distributed from the surface into the material.

[6] E. Wyszkowska et al.,, J. Nucl. Mater., 584 (2023) 154565

RBS/C ion channeling and damage distribution profiles

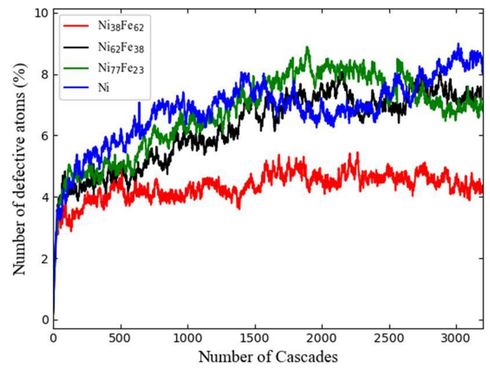


Observations:

- **The number of defects in $Ni_{0.38}Fe_{0.62}$ is about twice smaller compared to pure Ni!**
- Accumulation of defects observed at different depths may indicate defect changes as well as suggest defect migration

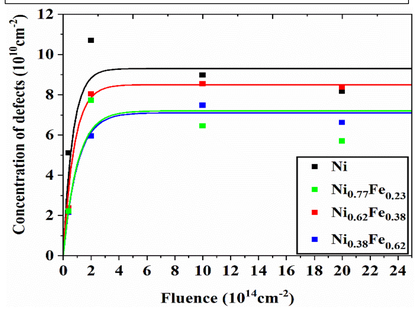
[7] E. Wyszkowska et al,, *Nanoscale* 15 (2023) 4870

MD simulations



The highest numer of defects in Ni and the least defects in $Ni_{0.38}Fe_{0.62}$ have been observed which is consistent with experimental findings [6,7]

Damage kinetics



$$f_d = \sum_{i=1}^{n} (f_{d,i}^{sat} - f_{d,i-1}^{sat})\, G\, [1 - \exp(\sigma_i\, (\Phi - \Phi_{i-1}))]$$

where:

σ_i - cross-section for the formation of a given kind of defect

$f_{d,i}^{sat}$ - level of damage at saturation for i-th kind of defects

Φ_i - fluence threshold for triggering the formation of i-th kind of defects

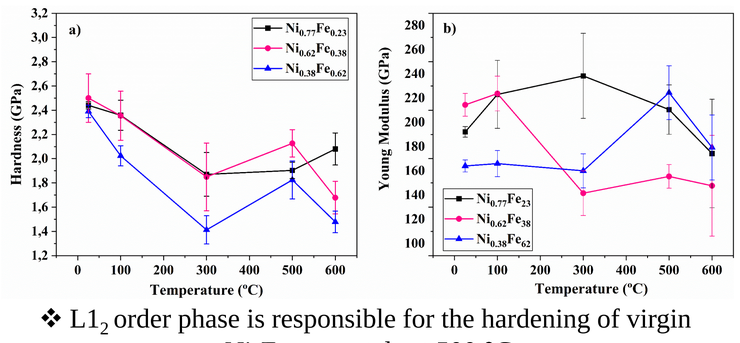
Effect of temperature

High temperature nanoindentation of virgin Ni_xFe_{1-x} crystals

Hybrid MC/MD

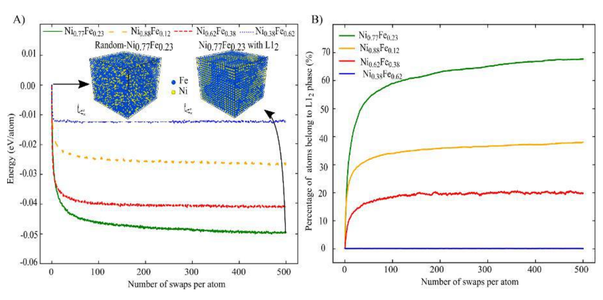
X-ray diffraction of virgin Ni_xFe_{1-x} crystals before and after and annealing

A) The nanoindentation hardness and B) Young Modulus of $Ni_{0.62}Fe_{0.38}$ and $Ni_{0.38}Fe_{0.62}$ measured in a range of temperatures from 25 to 600 °C

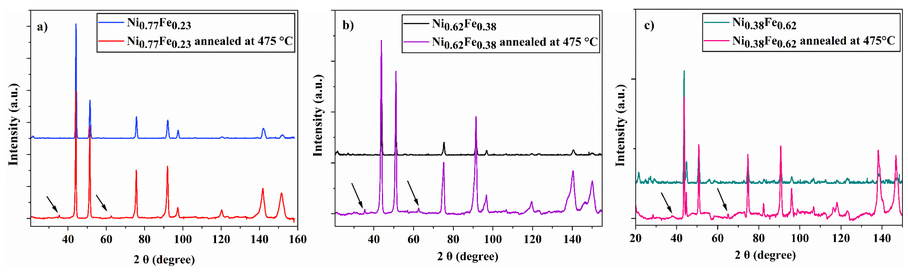


❖ $L1_2$ order phase is responsible for the hardening of virgin Ni_xFe_{1-x} crystals at 500 °C

Simulation of the annealing proces to understand the structure changes at HT



Formation of $L1_2$ clusters in Ni_xFe_{1-x} alloys



❖ Cell size and volume increase with the increasing iron content
❖ The bands shift towards lower angle (to the left side) with increasing iron content
❖ **$L1_2$ phase is visible in three compostions after annealing**

References:
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[7] E. Wyszkowska et al,, *Nanoscale* 15 (2023) 4870

Conclusions

- Depending on the addition of iron in monocrystalline Ni_xFe_{1-x} alloys, we observe a different mechanical reaction, different defects structure and their accumulation.
- Type of radiation-induced defects affects the final hardness of Ni_xFe_{1-x} crystals
- Hardness change with the increase of Fe content is due to different arrangements of Fe atoms in a crystal structure (local atomic environment) which influences the obtained mechanical properties of Ni_xFe_{1-x} in a pristine state and after irradiation.
- $L1_2$ order phase is responsible for the hardening of virgin Ni_xFe_{1-x} crystals at 500 °C

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PhD poster session