NOMATEN

CEA NCBJ VTT

ANNUAL REPORT 2021

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

PROJECT PARTNERS

NCBJ

Narodowe Centrum Badań Jądrowych w Świerku

National Centre for Nuclear Research

Poland

CEA

Commisariat à l'energie atomique et aux énergies alternatives

Alternative Energies and Atomic Energy Commission

France

VTT

Teknologian tutkimuskeskus VTT Oy

Technical Research Centre of Finland

Finland

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PARTNERS AND FUNDING

NATIONAL CENTRE FOR NUCLEAR RESEARCH

NCBJ (Narodowe Centrum Badań Jądrowych) combines fundamental and applied research profile combines nuclear power-related studies with various fields of sub-atomic physics (elementary particle physics, nuclear physics, hot plasma physics etc.). The Centre is strongly involved in developing nuclear technologies and promoting practical applications of nuclear physics methods. Major market products manufactured in the Centre include radiopharmaceuticals and a range of particle accelerators for science, various industry sectors and medicine.

The Centre is an IT and R&D background infrastructure indispensable to provide expert support for decision-makers in the project to develop in the coming years nuclear power industry in Poland. National Centre for Nuclear Researchis the largest research Institute in Poland. We are also the only Polish research institution operating a nuclear reactor (the MARIA reactor). Currently we are hiring over 1000 employees. Our research staff includes about 70 Professors and holders of the Dr hab. post-doctoral degree, as well as over 150 PhDs.

ATOMIC ENERGY AND ALTERNATIVE ENERGY COMMISSION

CEA (Commissariat à l'Énergie Atomique et aux Énergies Alternatives) is a public establishment devoted to scientific, technical and industrial research and development, under the authority of the Ministries of Energy, Research, Industry and Defence. The CEA is today a major player in research, development and innovation in four areas: defense and security, low-carbon energies (nuclear and renewable), technological research for industry and fundamental research (sciences matter and life sciences). conducts a part of its research in the framework of the French nuclear deterrent programme. It also provides technology to strengthen security in the face of new hazards such as terrorism and cyber attack, and to upgrade response to earthquakes and tsunamis.

As a key player for energy research, the CEA mobilises its expertise and multidisciplinary competencies to propose innovative technological solutions to address major

societal challenges, such as energy transition, nuclear and renewable energy, and understanding the mechanisms of climate change. The CEA follows a research strategy encompassing the whole energy system, focusing simultaneously on means of electrical power production, both nuclear and renewable (solar), improving energy efficiency and dynamic adjustment of supply and demand through energy storage (batteries), the use of hydrogen as an energy vector, or smart power grids.

Beside challenges associated with energy and climate changes, the CEA also mobilises its expertise and multidisciplinary competencies to biotechnologies and biomedical innovations. Challenges linked to personalized medicine and technologies for the medicine of the future are priorities, and dedicated research are conducted in the field of in vivo molecular imaging probes, diagnostic tools and molecules for therapeutic or theragnostic uses. Methodologies devoted to isotopic labelling remains a specificity of the CEA, both serving drug development and radiopharmaceutical development.

TECHNICAL RESEARCH CENTRE OF FINLAND LTD

Teknologian tutkimuskeskus VTT Oy is a leading research and technology company in the Nordic countries. We use our research and knowledge to provide expert services for our domestic and international customers and partners, and for both private and public sectors. We use 4,000,000 hours of brainpower a year to develop new technological solutions. We have over 2,000 experts. VTT Group turnover is approximately EUR 270 million yearly. VTT's mission is to help customers and society to grow and renew through applied research. We have 75 years' experience supporting our clients growth with top-level research and science-based results. We develop new smart technologies, profitable solutions and innovation services. We cooperate with our customers to produce technology for business and build success and well-being for the benefit of society. A brighter future is created through science-based innovations.

NOMATEN'S FUNDING

This project has received funding from the European Union Horizon 2020 research and innovation programme under grant agreement No 857470 and from European Regional Development Fund via Foundation for Polish Science International Research Agenda PLUS programme grant No MAB PLUS/2018/8. Additional NOMATEN activities are funded from the ORIENT-NM (Organization of the European Research Community on Nuclear Materials) grant (Horizon 2020 Framework Programme, grant agreement No. 899997) and the GOSPOSTRATEG-HTR project financed by the National Centre for Research and Development.

NOMATEN'S VISION AND NEXT YEAR'S TARGETS

The Center of Excellence has now become an actual center, with several (five) research groups in action. The second year of our existence has been one of quick growth in spite of the global pandemic crisis, which has affected research very much. The lack of international mobility and exchanges has so to speak been substituted with hard work in the offices and laboratories. For NOMATEN, this is a well-working recipe as the steps to build up a real research environment do depend on the individual and joint effort of our staff. We should also acknowledge the institutional support of the National Center for Nuclear Research, hosting us as an operationally independent department. Likewise, the Teaming partners CEA (France) and VTT (Finland) have been – however virtual – supportive and encouraging external "team members". The CoE is firmly backed by the funding of the Foundation for Polish Science and is under the umbrella of an International Scientific Committee headed by prof. Sergio Bertolucci.

NOMATEN CoE Director
prof. Mikko Alava

In hard science our work has been about the establishment of the scientific profile of a "newly minted" CoE. Materials science needs laboratories and facilities and we have busily been setting up our own ones. A crown jewel in this sense is the acquisition by a leasing contract of a most modern Scanning Electron Microscope with additional analysis and sample preparation capabilities such as a Focused Ion Beam one for complex manipulations. We have also a heavy effort in materials modelling, and the NCBJ computing center CIS with its considerable resources is invaluable to us. Whereas in 2020 our scientific production may be considered a cross-over from the past research activities of the scientific workforce of the CoE 2021 has seen the first true NOMATEN papers published. These range from modelling the nanoindentation of metals to a review of material informatics as a discipline – very important in modern materials science – to applications of machine learning in detecting the onset of plastic yielding.

Our build-up phase is now finishing in that the core research of the CoE is in place with radiopharmaceutical research and materials

> **NOMATEN Center of Excellence has now become an actual center with five research groups in action**

science represented both experimentally and from the modelling side. In 2022, I foresee a strong growth of our scientific productivity, with works published from collaborations within the CoE – demonstrating cohesion and synergy – and from novel collaborations with external partners, including the Teaming ones. Our target is getting 20 articles published on CoE key research in materials and radiopharmaceuticals in addition to other secondary ones. The structural developments of the CoE will tackle those ones concerning key infrastructures (CERAD, PolFEL, neutron diffraction equipment installation) by key investments in personnel. This, getting additional research strength by now-starting calls, and other research support staff hirings will get our key staff numbers to more than 40 or so from the current 27 An example is the MCSA project of Aleksandra Baron-Wiechec (MagnifiCor grant) which is expected to start in June 2022, run for two years, and in addition to developing our capabilities in corrosion research will develop into a collaboration with Guangdong Technion-Israel Institute of Technology. Other collaborations are starting with U. Tennesse-Knoxville (Kurpaska, with Y. Zhang, also at Oak Ridge National Laboratory), with Harvard (Papanikolaou), with CEA – RG Papanikolaou with the SRMP team (C. Marinica, A. Goryaeva) on the identification of defects in HEA for multiscale modeling, "Functional Properties" on radiation damage in complex alloys, and finally on radiopharmaceuticals – and with VTT in early 2022.

These advances and the growth of the recently started collaborations and research lines plus those already on starting line will lead in addition to substantial and high-quality research output also to a comparable effort for gaining further funding by various calls. I expect strong participation in Horizon Europe and in national calls (NCN, NCBR) with at least 20 proposals submitted with several getting funded. A natural expectation is that these are often done with strong collaborators and an example is given by two so-called Twinning ones under preparation (submission in early 2022). Likewise, the growth will be visible by the formation of the NOMATEN "graduate school", that is to say a cohort of new PhD students who apart from doing a regular PhD either at the NCBJ Graduate School or one of Warsaw area universities – depending on the subject – will be formed. We should have of the order of 10 by the summer of 2022 depending on the success of the on-going calls in our both key fields.

Our visibility will gain from the lifting of the pandemic-related restrictions and the ability to visit and host visitors and take part in conferences where our work will be presented. In particular, the CoE will organize in June 2022 an international conference on material informatics, supported by a generous NAWA (Polish National Agency for Academic Exchange) grant. We are also investing significant effort into applied research, where the newly established NOMATEN Network of Advisors is helping us to identify potential openings. The first industrial contacts have actually been established, and we will move in 2022 into concrete collaborations with an economic impact.

> **NOMATEN Network of Advisors is helping us to identify potential openings**

> **"Our research team grew from 7 to almost 30 people in 2021**

OPERATIONS SUMMARY

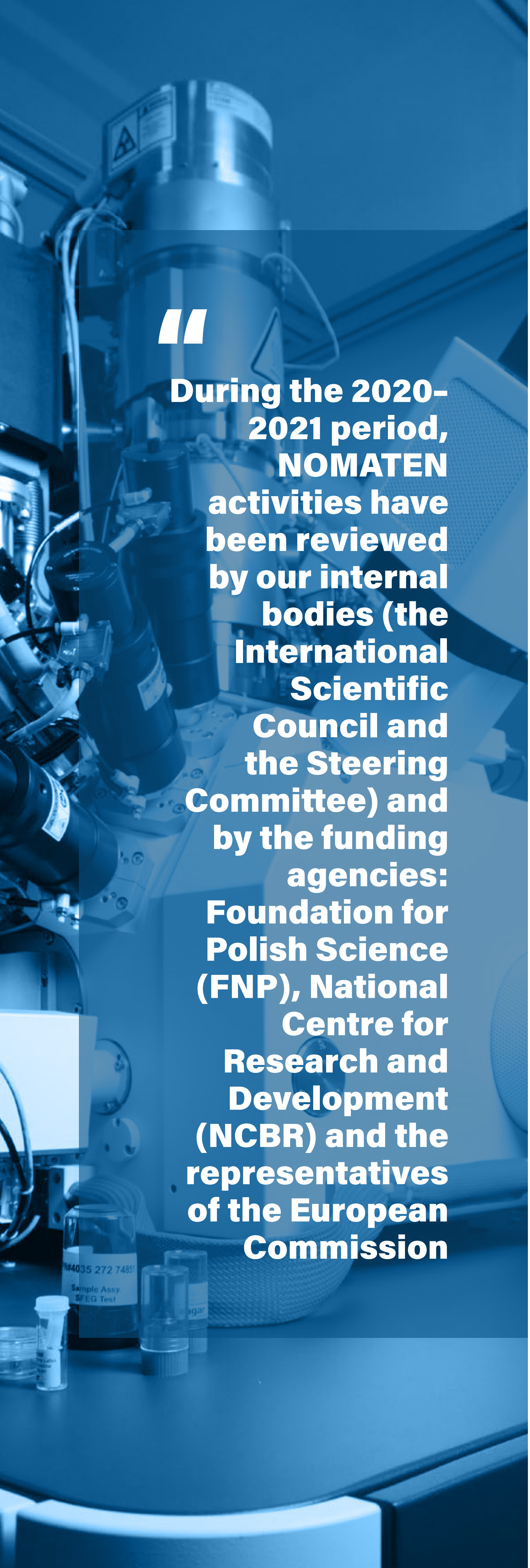
Director for Scientific Operations
prof. Paweł Sobkowicz

The past 12 months, from October 2020 to September 2021, have been a period of dynamic growth and activities. Despite the COVID-19 pandemic (in partcular the travel restrictions) we have been able to successfully conduct multiple searches for researchers and support personnell. These searches were executed in full concordance with the European Charter for Researchers and the Code of Conduct for the Recruitment of Researchers, open to any nationality. As a result, our research team grew from 7 to almost 30 people. About half of them came from abroad, creating a lively, multinational team. The details of the recruitment are described in Chapter 5. The research groups led by prof Mikko Alava, prof Łukasz Kupraska and dr Stefanos Papanikolaou are not fully functional. We continue our search for talent, expanding the abovementioned groups and filling the new groups led by prof Marek Pruszyński and dr Iwona Jóźwik.

This growth would not be possible without the support of our Hospitality Manager, Barbara Paprocka and HR Manager Magdalena Jędrkiewicz,, who handled such diverse issues as increase paperwork necessary for obtaining work permits during the pandemic, support for researcher families and various on-boaring tasks. The experience gathered at NOMATEN has led to the idea of creating the Hostpitality Centre for the whole National Centre for Nuclear Research. The detailed proposal for such a centre, prepared in part by the NOMATEN HR team, has received recognition (and financing) of the Polish National Agency for Academic Exchange NAWA.

In parallel to building the research teams, we have been expanding the NOMATEN infrastructure, as described in Chapter 9. Combining various sources of funding and employing innovative forms of financing (e.g. long-term financial leasing) has allowed us to build-up the experimental capacities – as well as the computational ones, via purchases of dedicated software licenses.

In addition to research activities (described in detail in Chapter4) which led to several publications in leading journals (Chapter 13),



"During the 2020-2021 period, NOMATEN activities have been reviewed by our internal bodies (the International Scientific Council and the Steering Committee) and by the funding agencies: Foundation for Polish Science (FNP), National Centre for Research and Development (NCBR) and the representatives of the European Commission

we have been working on the increase of cooperation with industrial partners and customers. The Marketing Plan and market analysis, prepared under the Teaming grant with the help of the NOMATEN Partners, VTT and CEA has allowed us to define NOMATEN strong points and relate them to the market needs of specific industries. With the relaxation of COVID-19 related restrictions, we have resumed existing contacts with the industry and started new ones (for details, see Chapter 10). These included direct contacts with specific companies, participation in industry events, and, very importantly, creating the NOMATEN Network of Advisors, composed of representatives of leading companies who agreed to support NOMATN with their expertise and advice.

NOMATEN personnel participated in activities promoting the general recognition of competencies of NOMATEN. For example, we actively participate in the ORIENT-NM (Organization of the European Research Community on Nuclear Materials) project, which focuses on the development of a convincing strategic research agenda on materials for all generations of nuclear reactors foreseen by 2040, with particular emphasis on the plan for the first 5 years. The plan will be consistent with national programmes and industry needs, including supply chain constraints, paying attention to standardisation issues and verifying the availability of appropriate infrastructure.

Another example is our participation in the ATTRACT program (https://attract-eu.com). ATTRACT is an initiative funded by the European Commission under Horizon 2020 programme and co-developed by leading European research institutions forming a programme consortium: Aalto University, European Organization for Nuclear Research (CERN), European Industrial Research Management Association (EIRMA), European Molecular Biology Laboratory (EMBL), ESADE Business School, European Synchrotron Radiation Facility (ESRF), European X-Ray Free Electron Laser Facility (European XFEL), Institut Laue-Langevin (ILL). The role of ATTRACT is to support the emergence of breakthrough technologies for society and the economy through an innovative formula of support for research funding competitions.

During the 2020–2021 period, NOMATEN activities have been reviewed by our internal bodies (the International Scientific Council and the Steering Committee) and by the funding agencies: Foundation for Polish Science (FNP), National Centre for Research and Development (NCBR), and the representatives of the European Commission. These reviews have confirmed the direction chosen for the NOMATEN development and our progress along the path.

NOMATEN SCIENTIFIC ACHIEVEMENTS

1.1. COMPLEXITY IN FUNCTIONAL MATERIALS RESEARCH GROUP

Background of the group is in fracture (publication 1), plasticity, statistical mechanics of materials, and the structure-property relationship. The group has expertise in machine learning and multiscale models and connections to European High Performance initiatives and Centre Européen de Calcul Atomique et Moléculaire, CECAM. Our current work concentrates in the plasticity of complex alloys (HEA, PLC effect), and collaborations with the other groups (plasticity, Machine Learning, multiscale models, mechanical properties across scales). The RG is also working on contributing Non-Destructive Analysis/experimental analysis (DIC, Digital Image Correlation) using also Machine Learning methods to classify data and predict.

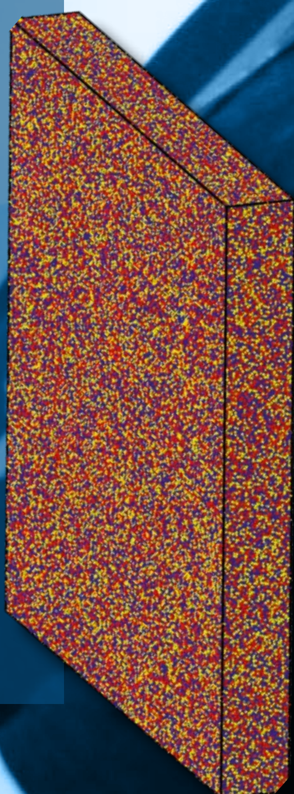
Our strategy is to develop new concepts and tools for multifunctional materials. An example is the concept of yield strength, which is controlled by the properties of dislocations in complex alloys, and by their interactions with precipitates and the complex alloy atomistic structure. Here, expertise from statistical physics and the multiscale models of alloys' plasticity is critical. In many cases we foresee the development of machine learning approaches to understand and classify the yielding of materials, and in particular to develop predictive capabilities for alloys and coatings, and all this including the process-structure-property paradigm. In 2022, we are one of the key organizers of a CECAM workshop in March on artificial intelligence and plasticity, with many keynote speakers from the leading groups in the world. Our group will in the future focus on developing a leading role in this field, on nurturing collaborations with external partners and inside the CoE, and we also plan to develop an activity in applying "problem solving" approaches to more applied materials science problems with the industry, where practical approaches are important including the understanding of data.

The science we have been doing in 2021 has concentrated, to a large degree in interaction with other CoE groups

Research Group Leader
prof. Mikko Alava

and with external partners, on a number of key openings. These include fundamentals of plasticity, studied with nano-indentation: this means comparisons with experiments (at NOMATEN) of complex alloys and basic research on effects of experimental geometry – surface roughness (F. Rovaris, to be published) – and temperature on nano-indentation (publication 2). We have also launched an effort on the physical metallurgy of high-entropy alloys. HEAs are a potential material solution as a multi-functional material. We are developing collaborations and doing modelling of the plasticity of HEAs and how that depends on the local order or segregation. We expect to develop our basic research into dislocation plasticity (publication 3) in this direction in the close future, including the use of machine learning (ML) approaches (publication 4). Several manuscripts are close to being submitted at the time of writing this also in collaboration with Warsaw University of Technology. An important effort is being made in trying work out how HEA-based amorphous materials, or metal glasses, would work out. The complexity of multi-species compositions holds promise in that mechanical, chemical, and irradiation properties might be optimized, as in the case of metallic HEAs, but the thermodynamic stability of the amorphous alloy must be checked. We are also working actively on ML – like ways of approaching experiments, from steels to alloys and to (in the future) HEAs in the sprit of ref. 4.

"The complexity of multi-species compositions holds promise in that mechanical, chemical, and irradiation properties might be optimized, as in the case of metallic HEAs, but the thermodynamic stability ofthe amorphous alloy must be checked

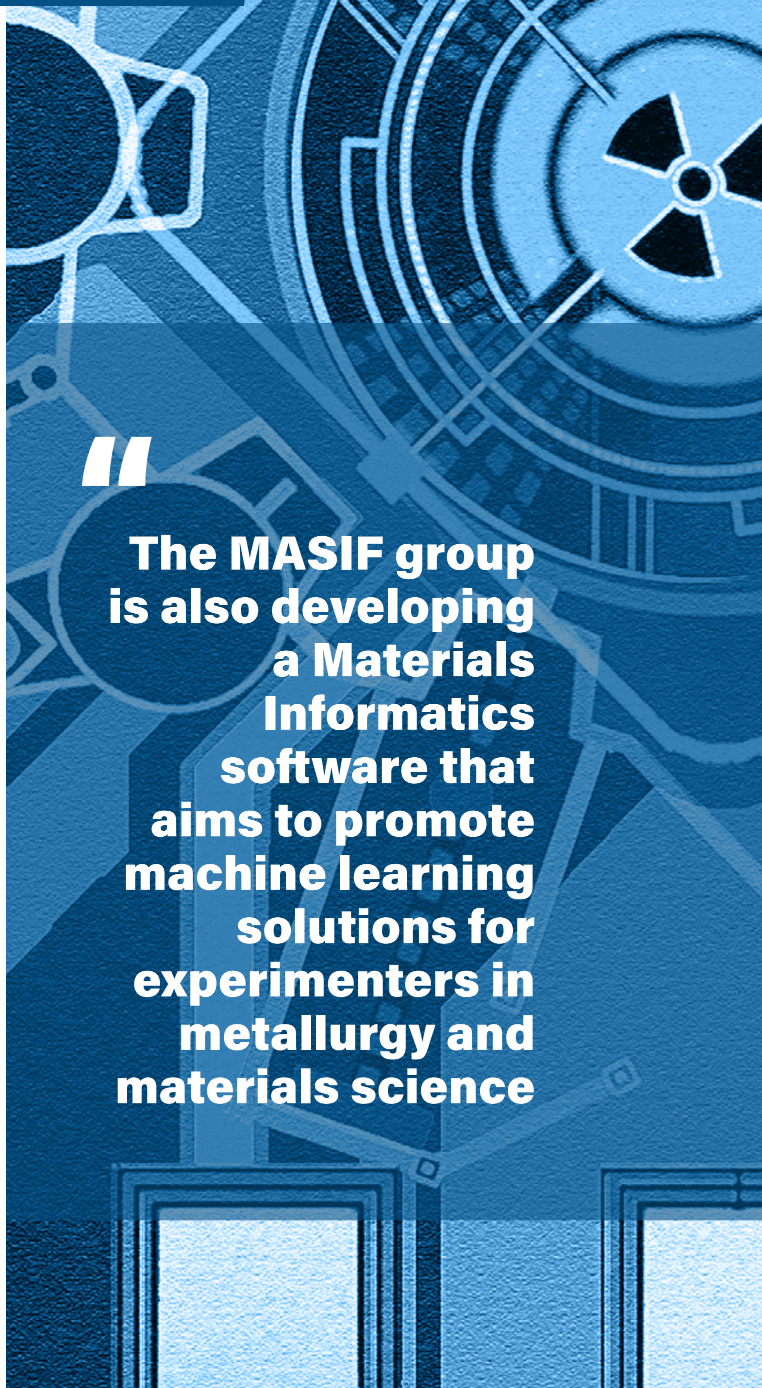


1.2. MATERIALS INFORMATICS - STRUCTURE AND FUNCTION RESEARCH GROUP

Modern metallurgy of metals for extreme conditions is not much different than the methods used for Damascus steel 1000 years ago. Through trial and error, metallurgy has stumbled upon and settled into few excellent materials, that have been used consistently in extreme condition applications, such as nuclear reactors. The MASIF group, a world leader in Materials Informatics for mechanical deformation applications, focuses on the development of similarities, analogies and multiscale modeling, and aims at developing process-structure-property relationships in novel material classes, for identifying cheap, lightweight, strong and ductile materials at extreme conditions, namely high temperature or/and irradiation. Recent highlights include the development of deeper, multiscale understanding of deformation mechanisms in pure metals and the development of a novel method for identifying yield points in materials through the use of camera-obtained surface map sequences.

Research Group Leader
Stefanos Papanikolaou PhD

The group's plan is to further establish and strengthen leadership in Materials Informatics, in Poland and worldwide. For this purpose, a book on "Materials Informatics" will be written (to be published in 2023–24) with modern approaches and insightful methods, with actual programming codes included, for handling data and promoting physics-informed machine learning in materials science. The MASIF group is also developing a Materials Informatics software that aims to promote machine learning solutions for experimenters in metallurgy and materials science. Moreover, the MASIF group aims to produce more than 5 PhD graduates that will be experts in materials informatics, machine learning, multiscale modeling and data science. Research-wise, the MASIF group will focus on a multi-threaded approach, that primarily includes deep understanding of the interplay between thermo-kinetic processes and mechanical deformation in the extreme conditions of high temperature and irradiation. The key for making progress is the development of efficient multiscale materials modeling approaches and interatomic potentials, by using machine learning methods. In addition, the focus will be on the use the long-developed rules-of-thumb in metallurgy to promote novel, automatically identified, analogies for materials informatics solutions and process-structure-property relationships that shall promote novel pathways in manufacturing.



"The MASIF group is also developing a Materials Informatics software that aims to promote machine learning solutions for experimenters in metallurgy and materials science

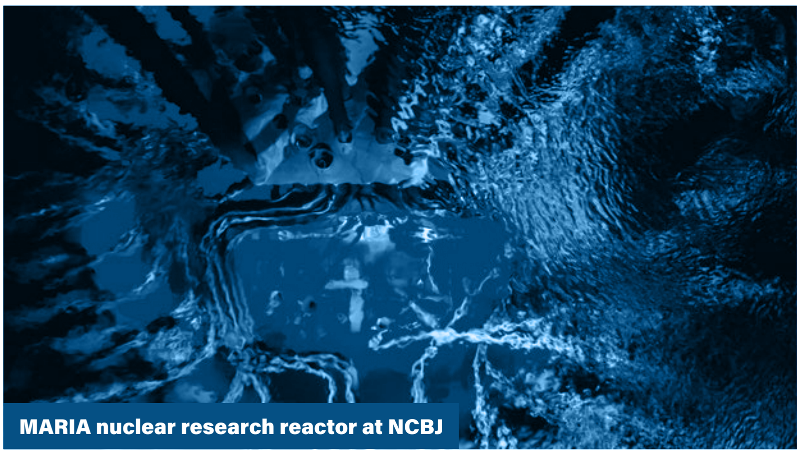
1.3. FUNCTIONAL PROPERTIES RESEARCH GROUP

Research group headed by Lukasz Kurpaska is composed of 7 researchers. 5 people are employed on a PhD positons and 2 persons have been selected for post-doc positons. Due to the COVID-19 restrictions, post-doc's will arrive to NOMATEN CoE at the end October 2021 and at the beginning of 2022. They orginate from India and China.

Research Group Leader
prof. Łukasz Kurpaska

In addition to that, two people responsible for maintenance and operation of newly created XRD lab and TEM support specialist have been employed in 2021. These experts support young researchers employed in the Research Group in conducting tests and processing specific experimental data. Among many activities which took place in the past year, the research group managed to establish new manufacturing line composed of: stainless steel chamber with controlled atmosphere (Ar) equipped with laboratory scale and small lab tools. In 2021 we installed new planetary energy ball mill (Retsch) equipped with 2x stainless steel vessels, one additional vessel covered with TiC type coating and steel balls. We prepared several chemical compositions of ODS and HEA specimens. Among many one can name NiCoCrFe and (bal.)Fe 9%Cr 5%Al 0.3%Y_2O_3 0.5 and 1%Ti specimens. Mixing of the materials is performed via powder metallurgy method while sintering process is conducted in the collaborating institution (IMiF, Warsaw) by using Spark Plasma Sintering technique. In order to stabilize obtained structures, sintered specimens are annealed at high temperature under Ar-atmosphere. High temperature muffle-type furnace have been purchased and installed for this purpose. Finally, the group was involved into setting up a completely new

"Members of the group help to purchase and install new research devices (Charpy impact machines, microhardness tester, thermal analysis equipment ect.)



MARIA nuclear research reactor at NCBJ

sample preparation laboratory. Together with other instruments, purchased via complementary fundnig, new, fully equipped metallographical lab has been established. It includes sample cutting, polishing (including vibro and electropolishing) and mounting specimens in the resine. New fume hoods have been installed in the lab, and they are available when using acids or volatile substances. Prepared in such a way samples are tested via XRD, SEM or nanoindentation techniques. There are our prime tools to understand impact of radiation damage, structural integrity and corrosion resistance of the studied materials.

Among many topics which are currently of our interest we are particularly interested in:

- "Manufacture of HEA via powder metallurgy and SPS technique and studies of radiation damage resistance mechanism in these materials". In this project the main objective is to manufacture a multifunctional, state-of-the-art material based on Cr-Ni-Co-Fe elements. Some data indicate that the most promising HEAs contain additions of V and Ti (up to 0.5 in wt.%). It is planned that the targeted material will have chemical composition suggested by numerical group headed by S. Papanikolaou. HEA specimens are beeing prepared via mechanical alloying of elemental Fe, Cr, Co and Ni powders. Afterwards, CoCrFeNi HEA ingots are produced via SPS technique, this process is followed by annealing. This investigation will allow identification of a correlation between mechanical parameters measured in nano and micro-scales with chemical and structural properties of newly produced HEA ingots.

- "Studying corrosion mechanism in zirconium and its alloys". The main objective of this work is to develop a general understanding about the stress state developed at the metal/oxide interface and to study corrosion resistance of model pure zirconium and its commercial alloys: E110 and zircaloy 2 and 4. This approach will be realized by combining structural (Raman, SEM/EBSD, XRD) and mechanical (indentation) methods in order to determine properties and stress in thin film on metal substrate, formed during high temperature treatment. Corrosion tests will be performed at high temperature, in water vapor atmosphere (special stove have been purchased for this purpose). The aim of this work is to simulate the situation reproducing the behavior of zirconium in nuclear reactors and develop predictive models of material behavior at high temperature.

- "Impact of radiation damage on mechanical and structural properties of amorphous alumina coatings". Goal of the work is to understand physicochemical and functional properties of amorphous alumina coatings. These materials are inert to very corrosive media like liquid lead, and possess remarkable mechanical properties and radiation resistance. The current state of knowledge indicates that as a result of radiation damage and high temperature, the microstructure of the coating evolves, resulting in changes in the material properties. However, this transformation occurs at very high temperature and dpa, suggesting, that this material can be successfully used in LFR (Lead-cooled Fast Reactor) type reactor.

- "Investigation of the plasticity effect and radiation damage resistance via nanoindentation in Fe-Cr alloys". The goal of the work is to understand complex phenomena associated to the formation and evolution of irradiation induced defects and their role on the deformation behaviour in ferritic/martensitic (f/m) steels, incl. Fe, Fe9%Cr, Fe9%Cr-NiSiP and Eurofer 97.

- "Fabrication of ODS steels strengthened by refractory oxides like alumina Al2O3 and/or zirconia ZrO2". These are foreseen to be used as alternative strengthening elements in new type of ODS alloys. These compounds have been chosen due to theirs similar behavior to yttria – both of selected oxides are characterized by similar to yttria thermal stability at high temperature. Planned works include conducting mechanical alloying process, consolidation of powders by Spark Plasma Sintering (SPS) technique and characterization of microstructural and mechanical properties of the manufactured materials.

Described topics represent full spectrum of PhD works which are currently on-going in the research group. At the same time, members of the group help to purchase and install new research devices (Charpy impact machines, microhardness tester, thermal analysis equipment ect.).

Detail research plan for new post-doc's will be prepared upon their arrival to NOMATEN. However, based on the CVs and their bacground, it is expected that they will be working in the area of manufacturing of HEA via arc melting, radiation damage resistance and plastic deformation of steels.

1.4. MATERIALS CHARACTERIZATION RESEARCH GROUP

The main goal of the Materials Characterization Group, lead by Dr Iwona Jozwik, is to conduct the advanced characterization of novel multifunctional materials on the atomistic level using state-of-the art equipment. Development of new materials to be implemented in harsh environment (radiation, temperature, corrosion – such as present in nuclear, energy and chemical industry applications) must be preceded by the detailed understanding and prediction of their long-term behavior in extreme conditions. This can be only achieved via carefully designed and executed scientific experiments, working in the closed loop between the multiscale modelling effort and experimental data, based on the structural and mechanical studies performed in the frame of this project. The main concept of the research processes conducted in the context of the NOMATEN CoE project is the circulation of the information derived from computer modeling, structural characterization and functional properties studies with the role of the Materials Characterization Group as an inevitable part of the self-sustaining core. It is obvious, that theoretical modelling of material structure must be massively validated by advanced experimental works.

Research Group Leader
Iwona Jóźwik PhD

Despite the number of RGs created, they must stay in close collaboration with each other to successfully define and study new materials. The modelling outputs must be supported, explained and confirmed by detailed microstructural characterization, which in turn will be verified by experimental mechanical studies at nano – micro – and macro-scales. The structural characterization of the studied materials under extreme conditions fills the gap between simulations and functional properties of the material, by verification of the structural model, analysis of material response on various conditions occurring in real environments, analysis of mechanisms of damage accumulation and studies of microstructure influence on the mechanical properties.

The Group will actively collaborate with external partners. Among them, strategic partners of the project (CEA and VTT) are of prime importance, as well as national laboratories: L-IMiF, WIM PW and AGH should be mentioned as the most important partners. A special attention will be put on Transnational Access program, ensuring European researchers use top equipment available in the European Research Area, such as RADIATE and ESTEEM3.

The Group's activities focus is on studying impact of high temperature, oxidizing atmosphere and radiation on the structural properties of materials by the implementation of experimental techniques, such as scanning electron microscopy (SEM), focused ion beam (FIB), electron backscattered diffraction (EBSD), energy dispersive X-ray spectroscopy, transmission electron microscopy (TEM), and structural studies by using X-ray diffraction (XRD) and Raman spectroscopy (in-situ at high temperatures). The Materials Characterization Group material studies are mainly realized by:

SEM microscope at NOMATEN

- SEM imaging for obtaining information about topography, relative differences in composition (identification of precipitates), conductivity or crystallographic orientation in studied materials;
- EDS analysis for qualitative and quantitative determination of material composition, (including precipitates of different phases in host material);
- EBSD analysis of relative crystallographic orientation of polycrystalline structures (crystal deformation studies, grain size and distribution, grain boundaries statistics);
- FIB preparation of ultra-thin transparent samples for TEM and HRTEM analysis of material microstructure, defects structure and defect formation mechanisms;
- FIB cross-sectioning of the multiphase materials in order to reveal the interface, inner structure, inner-phase in matrix distribution, crack propagation, corrosion propagation and in-situ imaging in SEM (the sectioning may be conducted in a strictly defined area, for example specific grain boundary, precipitate, indent or crack in the material);
- XRD (X-ray Diffraction) phase determination and structural deformation studies;
- Analysis of strain in materials, including correlation between damage and stress, stress distribution in layered structures, corrosion-altered layers formation etc. These studies will involve mainly GID XRD and HR XRD techniques, including in-situ analyses at high temperatures.

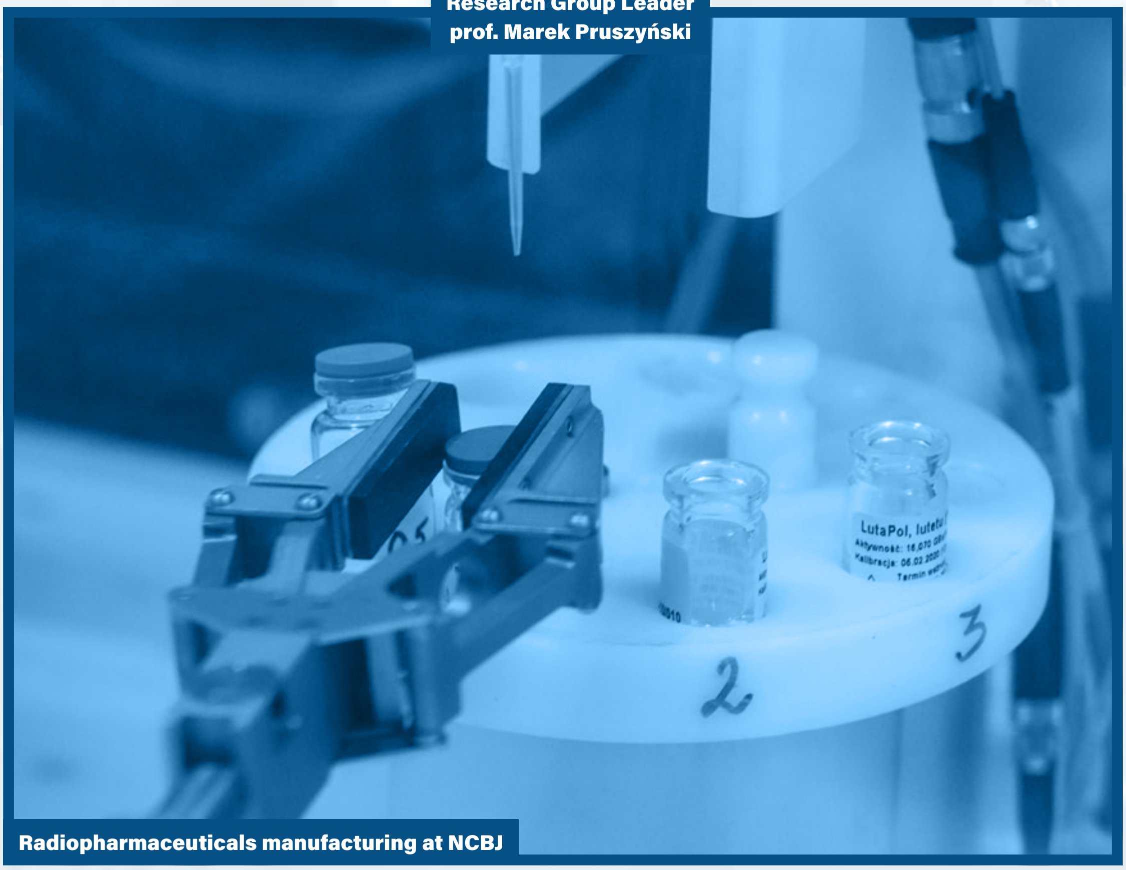
1.5. NOVEL RADIOPRHARMACEUTICALS RESEARCH GROUP

Cancer is one of the leading causes of human deaths in the world, and its incidence has been steadily increasing. Therefore, one of the major challenges of modern medicine is the development of effective diagnostic methods enabling early detection and determination of the character of cancer, which allow further selection of an appropriate therapeutic path. The discovery of the presence of certain biomarkers on cancerous cells enables the development of appropriate biomolecules targeting them. These biomolecules might be carriers of diagnostic and therapeutic radionuclides, and thus can be used as molecular radiopharmaceuticals. Hence, the major goal of the Radiopharmaceuticals Group is to design, synthesize and preclinically evaluate novel molecular radiopharmaceuticals which might be used further as diagnostic probe, and/or therapeutic agent when theranostic is concerned, both relative to the so-called, targeted, personalized medicine.

The NOMATEN Center of Excellence (CoE) is hosted by the National Center for Nuclear Research (NCBJ) in Świerk, the only institute in Poland operating a nuclear research reactor and involved in the production of radionuclides for the radiopharmaceutical industry, thanks to POLATOM. Moreover, within next 2–3 years at the NCBJ will be installed a modern cyclotron as part of the CERAD project.

The existing and emerging research infrastructures will be unique on a national and European scale. Therefore, the newly created Radiopharmaceuticals Group will have the opportunity to initiate access to the reactor – and cyclotron-produced commercial and potentially applicable new radionuclides. This option requires establishing procedures for targets preparation and later radiochemical separation methods to extract crucial radionuclides from irradiated materials. Next, separated radionuclides will be used for labeling of various biomolecules (monoclonal antibodies or their fragments, peptides and small organic molecules), including those developed by or in cooperation with partner research groups from POLATOM, French Alternative Energies and Atomic Energy Commission (CEA-France, JOLIOT institute), Technical Research Centre of Finland (VTT) and Institute of Nuclear Chemistry and Technology (ICHTJ-Poland). Numerous diagnostic (Short-lived ones (e.g. F-18, Ga-68 for examples) as well as longer-lived (Sc-43–44, Zr-89, Tc-99m etc) and therapeutic (Y-90, I-131, La-135, Lu-177, At-211, Ac-225, Th-227 etc) radionuclides are planned to be used. However, to stably attach them to biomolecules it will be necessary to develop various chelating agents (for metallic radionuclides), prosthetic groups

Research Group Leader
prof. Marek Pruszyński



Radiopharmaceuticals manufacturing at NCBJ

(for non-metallic ones) or nanostructures, e.g. micelles, liposomes, or inorganic/organic nanoparticles. The nanostructures may also play a multimodal function and be used not only as carriers of radionuclides, but also carriers of different chemotherapeutics or compounds which make cancerous cells more sensitive to ionizing radiation, heat through magnetic field (hyperthermia) or light at proper wavelength (photosensitizer). Finally, synthesized radiopharmaceuticals will undergo intensive preclinical in vitro and in vivo evaluation demonstrating their diagnostic potential or therapeutic efficacy.

Currently, were initiated two research topics. One of them is focused on the production of Ac-227 at the Maria reactor at NCBJ for its further application as a generator for alpha-particle emitting therapeutic Th-227. Studies are performed together with the research team of POLATOM and a PhD will be involved in this work. After the development of a procedure for production of Ac-227 and Th-227, experimental studies will be done on radiolabeling of various biomolecules with Th-227. Additionally, Ac-227/Th-227 generator can be used for the elution of Ra-223 the only one alpha-particle radionuclide approved for treatment of metastatic castration-resistant prostate cancer (mCRPC). A second research topic is focused on the application of nanoparticles, particularly micelles, packed with various chemotherapeutics and radiolabeled with Zr-89 to track their biodistribution in mice, either by planar imaging (Cerenkov at POLATOM/NCBJ) or Positron Emission Tomography imaging (PET, CEA/SHFJ). Together with VTT, it is also planned to radiolabel various biomolecules, either already developed or closed to be obtained, like HER2, EGFRvIII and PD/PDL1 antibodies or their fragments.

Our ambition is to build a partnership team composed of world-leading researchers and young, highly motivated people who are passionate about developing of novel diagnostic and therapeutic approaches to defeat cancer disease.

The multidisciplinary nature of this research will be done in close collaboration with the research teams from NOMATEN's partners (CEA, VTT, INCT). Moreover, the cooperation with the scientists from Radioisotope Centre POLATOM at NCBJ, the worldwide known manufacturer of radiopharmaceuticals, will allow translation of developed radiopharmaceuticals into clinical studies and their further commercialization. Achievements in the field of novel molecular radiopharmaceuticals will complement the challenging mission of the NOMATEN CoE to make discoveries that potentially enable patients to reach effective diagnostic or therapeutic regimens and have a significant impact on their survival.

HUMAN RESOURCES POLICY AND HOSPITALITY MANAGEMENT

In the ambition of being a world-class international Centre of Excellence, NOMATEN CoE develops high-impact research portfolio, in fundamental and applied science to become a focal point for collaboration between the research community, industry and government.

Achieving this goal requires the creation of a highly professional, multidisciplinary and motivated team of researchers and staff, and practical and effective implementation of excellence building processes and necessary support.

From the beginning – when the concept of the Centre of Excellence was created – we were sure that people were the most important. Our employees are our strength and are the most important factor of NOMATEN success; therefore, we care about them as much as possible. Our ambition and our goal is to create the best place in the world for the best people – people who want to change the world – brave, creative, with passion.

We are constantly developing. In 2019, our team started from 7 people: 4 scientists and 3 administrators. In 2020, we started building our research and administration teams and we grew to 16 people – 4 Research Group Leaders, 3 postdocs, 3 senior scientis and

6 administration staff. Until October 31st we hired 13 new researchers including: 2 Research Group Leader, 10 researchers (1 senior scientist, 3 postdocs and 6 PhD students) and – 1 scientific and technical specialists.

We hope that up to December 2021 we will finish employment of 2 more postdocs, 3 PhD students and 3 scientific and technical specialists.

Together (on the end of 2021) we will be the team of 34 people in 5 research groups (28 scientists and 6 administration staff). The average NOMATEN employee is 40 years old man with PhD.

We understand science as an endless curiosity and willingness to create. That is why we create conditions that enable continuous development of NOMATEN employees. It is not only about the possibility of sharing knowledge and experience, working on modern infrastructure, but also creating an atmosphere in which it is possible to freely exchange thoughts. Scientists feel that their ideas are being noticed.

Scientific excellence is the goal we want to achieve by many ways, such as by supporting:

- endless curiosity and development (scientific and personal),
- mindful leadership based on respect and trust,
- teamwork built on openness and understanding the autonomy of others,
- individuality creating joint projects,
- creating a safe work environment to share and collaborate,
- diversity is a powerful value and source of our innovation,
- honest feedback as a base of true development,
- building our community by understanding the needs and by the system of career development.

Scientists' autonomy is a value for us. Our researcher have the opportunity to discuss, talk and learn from experienced mentors. Research Group Leaders and independent scientists are mentors, but there is also an opportunity to learn from outstanding scientists – members of the International Science Committee. Thanks to the cooperation between partners – NCBJ, VTT, CEA, employees have access to a unique research infrastructure as well as knowledge and experience of all employees.

"

Diversity is a powerful value for us. Each individual in NOMATEN CoE brings with him or her a unique set of perspectives,work and life experience as well as cultural differences

Diversity is a powerful value for us. Each individual in NOMATEN CoE brings with him / her a unique set of perspectives, work and life experience as well as cultural differences. Diversity is a great opportunity to exchange ideas and points of view. NOMATEN is supposed to gather around people and ideas from various scientific fields from all over the world. Our team consists of experts in the following fields: physics, material science, chemistry, radiopharmaceutical, machine learning, artificial intelligence.

Our scientists are people from Europe (including Poland): 21 (17 from Poland), Asia (6), South America (2), most of them worked in various research centers around the world. We know how challenging is to live in a new country. To make life in a new place easier, we have created the special role in NOMATEN – The Hospitality Manager. She provides continuous practical support to international researchers relocating to Poland to become NOMATEN CoE employees or visiting the CoE for short periods. The Hospitality Manager supports new employees in process of relocation to Poland, assists with residence permits, visas and long-term stay permissions, supports to arrange necessary documents and registrations with local authorities, helps to find accommodation, assists to understand

> **We want NOMATEN to be a place open to everyone, where people can be themselves and really hear themselves**

Polish administrative requirements, local rules and behaviours and eases the transition, reducing stress and interruption.

Communication is an important area for us. Research Group Leaders are people of high sensitivity and empathy. Respect and the atmosphere of cooperation are important to us. We want NOMATEN to be a place open to everyone, where people can be themselves and really hear themselves. They draw from each other's experience. Our employee satisfaction and motivation survey – conducted at the beginning of 2021 show that NOMATEN is the place where people feel good and feel accepted (level of satisfaction in all aspects of work is higher than in NCBJ – average 4.53 in NOMATEN and 4.06 at NCBJ).

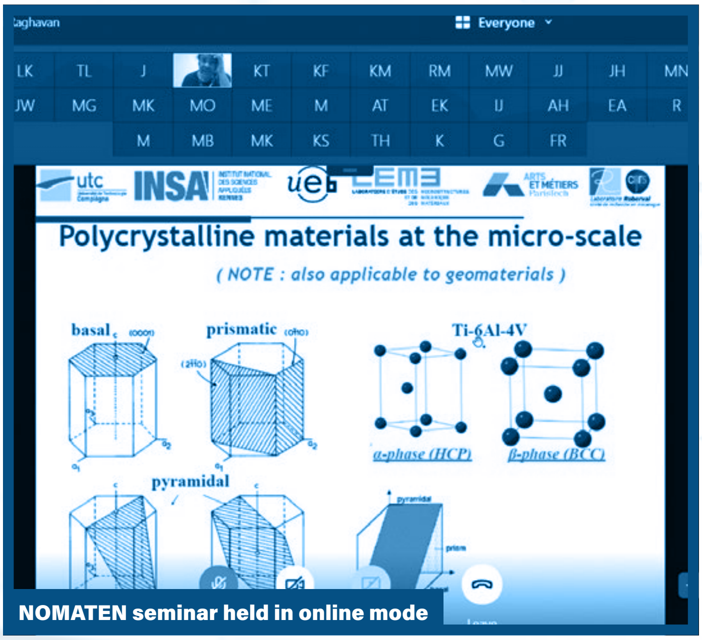
To guarantee the attraction and retention of the best employees, NOMATEN CoE implemented in 2020 a robust human resources strategy for research and administrative staff, encouraging gender equality and covering such key aspects as staff recruitment, evaluation and professional development. For the research staff, all processes must be in line with the European Charter for Researchers and the Code of Conduct for the Recruitment of Researchers. For the support staff, similarly transparent, open and supportive processes should be implemented. In all aspects, the gender equality principles must be obeyed, ensuring appropriate administrative and management capacities for the effective and efficient running of the Centre of Excellence. We constantly improve our HR policy under the influence of our experiences.

NOMATEN study visit at VTT in Finland, including NCBJ and CEA staff

NOMATEN SEMINARS CYCLE. COMMUNITY BUILDING AND SCIENCE DISSEMINATION

In 2021 NOMATEN hosts a series of open scientific seminars devoted to the topics related to materials' design, challenges and trend topics. One goal of these seminars is to share the expertise of the speaker and to be in contact with worldwide scientific leaders. Another goal is to build a network of researchers across different scientific areas related to materials science. In the seminar, the speakers have found a welcoming place where the organizers of the seminar (Dr Javier Dominguez and Maciej Drozd) help with technical support before and during the seminar. We also provide a technical assistance to the speakers when they are not experienced in our gotomeeting platform. In our seminar, we also welcome our speaker online, as a good practice giving us the change to introduce the research groups leader and NOMATEN to the speakers. In this welcoming session several connections and collaborations have been established and strengthen. Due to the pandemic, the following seminars has been set up as online events:

Senior Researcher
Javier Dominguez PhD



NOMATEN seminar held in online mode

"In this welcoming session several connections and collaborations have been established and strengthen

SPRING SESSION			
DATE	**SPEAKER**	**TOPIC**	**AFFILIATION**
January 12	Aleksandra Baron-Wiechec	Materials and technology challenges for nuclear fusion reactors	Guangdong Institute of Technology
January 26	Balaji Raghavan	Indentation-based identification of mechanical properties by mathematical modeling and inverse analysis.	Institut National des Sciences Appliqu´ees de Rennes,
February 9	Elena Akhmatskay	Mathematical methods (efficient HMC samplers, new adaptive numerical integrators	Basque Center for Applied Mathematics
February 23	Albert Bartok	Gaussian Approximation Potential theory and framework	Warwick Centre for Predictive Modelling
March 9	Aneta Ustrzycka	Microplasticity modelling, nanoindentation	Institute of Fundamental Technological Research
March 10	T. Jourdan, L. Dupuy and L. Gélébart	Multiscale approach to predict the mechanical properties of nuclear materials	Commissariat à l'énergie atomique, CEA
March 23	Thomas Schwarz-Sellinger	Experiments in damage in materials	Max-Planck Institute for Plasma Physics
April 6	Marcin Chmielewski	Material sintering and consolidation methods	Łukasiewicz – Institute of Electronic Materials Technology
April 20	Maciej Sitarz	HT corrosion and investigation of the structural properties via Raman spectroscopy	Akademia Górniczo-Hutnicza
May 4	Celine Cabet	Accelerator testing for nuclear materials – JANNuS irradidiation facility	Commissariat à l'énergie atomique, CEA
May 18	Chang Li	Mechanical properties of High entropy alloys at room and elevated temperatures	Max-Planck Institute for Iron Research GMBH
June 1	Wade Karlsen	Transmission Electronic Microscopy of non-fissile radioactive materials	VTT
June 15	Pascal Aubry	Possible applications of Additive Manufacturing (AM, and, principally, Laser Additive Manufacturing, LAM) and the potentialities of High Entropy Alloys in the nuclear field	Commissariat à l'énergie atomique, CEA
FALL SESSION			
DATE	**SPEAKER**	**TOPIC**	**AFFILIATION**
September 14	Tomasz Dudziak	High temperature corrosion and materials coatings	Krakow Institute of Technology
September 28	Nick Jones	Characterization of high entropy alloys at elevated temperatures	University of Cambridge
October 12	Kristiina Iljin	Recombinant antibody technologies for diagnostic and therapeutic applications	VTT
October 26	Jérôme Weiss	Paradigms of wild plasticity	CNRS/University of Grenoble
November 9	Gabriela Kramer-Marek	Exploring changes in PD-L1 expression via immuno-PET	Institute of Cancer Research, London
November 23	Filip Tuomisto	Applications and theory of positron annihilation spectroscopy	University of Helsinki
December 7	Prof. Dierk Raabe	Materials science of the sustainable metallurgy	Max-Planck-Institut für Eisenforschung GmbH

POLISH NATIONAL AGENCY FOR ACADEMIC EXCHANGE

NAWA GRANT FOR THE 1ST NOMATEN INTERNATIONAL CONFERENCE ON MATERIALS INFORMATICS (JUNE 2022)

Through a generous contribution from Poland's NAWA fund (NAWA – Narodowa Agencja Wymiany Akademiskiej – National Agency for Academic Exchange), NOMATEN has been organizing a conference on June 1–3, 2022, with the title „Materials Informatics". The scientific importance of this workshop is the, widely defined, interplay of materials science with machine learning, and it will feature presentations from renowned experts in applied mathematics, drug design, material science, and renewable energy. Materials Informatics has become a rather fast-emerging novel paradigm in materials science, that requires non-trivial data processing methods in Large Data for the identification of novel scientific pathways. This conference plans to explore the latest developments in materials informatics, with particular focus being on the modeling, capture, prediction and classification of defects in materials at extreme conditions, such as high-T or/and irradiation. We expect that this event will be an excellent opportunity to share, develop and collaborate on new ideas in the very frontiers of this scientific field.

The conference program will be chaired by NOMATEN's Stefanos Papanikolaou, who is the Materials Structure, Informatics and Function Research Group Leader. The program committee includes NOMATEN's director Prof.Mikko Alava, and also, world leading figures in the field of Materials Informatics, such as Alexandra Goryaeva (CEA-Saclay), Cosmin Marinica (CEA-Saclay) and Michael Zaiser (FAU Erlangen). The Program Committee has been currently working on finalizing the list of speakers and the program of the conference that already includes world renowned figures in machine learning and materials informatics, such as: Wing-Kam Liu (Northwestern, USA), Surya Kalidindi (Georgia Tech, USA), James D. Kermode (U. Warwick, UK), Stefan Sandfeld (Julich, DE), Luca Messina (CEA-Cadarache, FR), and Duane Johnson (Ames National Lab, USA). The program will aim at exploring major themes in materials informatics that are also very important for NOMATEN's research goals, with more than 5 appropriate focus sessions organized, titled as:

1. Defects in Crystals, Large Data and Machine Learning For Extreme Conditions
2. Machine Learning Methods for Multiscale Materials Modeling
3. Physics From The Machine: Learning The Behavior of Materials in the (digital) Lab
4. Material Discovery and Materials by Design: From Simulations To The Lab
5. Mathematical Methods and Data Operability Approaches in a FAIR world

For the proceedings of the conference, a special issue has been organized in the open-access, peer-reviewed, journal Materials Theory of the Springer-Nature publisher, dedicated to this workshop, and the open-access fee will be partially covered by the conference funds, for all speakers, including contributed presentations, if they decide to submit a contribution by the time of the conference (either novel research results or topic review).

NOMATEN WINTER SCHOOL ORGANIZED BY CEA IN PARIS

In this conference, we expect to host more than 20 invited international researchers, and more than 30 Polish researchers, in an effort to lead and expand NOMATEN's efforts on performing high impact research in the Materials Informatics community. In the conference program and following NOMATEN CoE directives, we have a sincere goal to support gender and minority balance.

The European NOMATEN project, launched at the end of 2019, aims to support the structuring and scientific influence of the NOMATEN Center of Excellence (CoE) dedicated to multifunctional materials for industrial and medical applications, created in Poland at the end of 2018.

In order to support the training of new generations of young Polish researchers (education programme) and to boost the growth of the NOMATEN CoE and its capacity to implement and manage research programmes, the first Winter School has been scheduled. Organized by CEA, this first edition of a school was related to material sciences and took place in Paris from November 16 to November 19th, 2021. It's agenda focused on modeling and simulation of the behaviour of materials under irradiation – also confronted with experimental approaches. This NOMATEN Winter School was designed for PhD, post-doctoral students and researchers with a priority

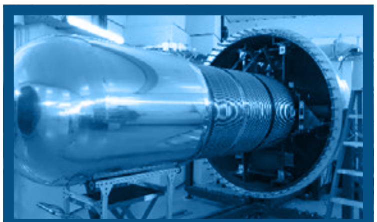
NOMATEN Winter School Participants (CEA, NCBJ and VTT staff)

for NOMATEN and NCBJ, VTT, CEA as well. Lasting four days, the school included two sessions (1st day) dedicated to reminders and/or upgrades in the form of courses given by experts from CEA and VTT but also from NOMATEN CoE.

Additionally, two poster sessions, during which about 20 students (PhD, post-docs from NOMATEN and CEA and VTT institutes) presented their research works, were organized. It should be underlined that one contribution was focused on challenges concerning industry partnerships and communica-

Remote manipulator in a hot cell in the LECI hot laboratory (CEA Saclay)

Frédéric Joliot Institute for Life Science (SCBM hot laboratories)



Epimethee accelerator of JANNuS-Saclay irradiation platform (CEA)

tion towards companies, science and public sector. The last day was devoted to visits at selected CEA Saclay facilities: i) the LECI hot laboratory and ii) the JANNuS-Saclay irradiation platform (both from the Division of Energies, DES) and the Molecular labeling and bio-organic chemistry unit (from the Division of Fondamental Research, DRF).

During this first part, 3 lectures focused on basic and fundamental reminders related to material and irradiation issue, concerning specifically the primary damage, the point defects formation, migration and properties and the concept of cascade. The second topic was dedicated to thermodynamics, diffusion and phase stability under irradiation. The last subject covered the mechanical aspects by introducing the plasticity at atoms scale, the motion of dislocations and the interactions of irradiation defects. Then two more applicative subjects related to the characterization and mechanical behavior were discussed: the use of nano-indentation to characterize irradiated materials (technique, applicfations and results) and the evaluation of the embrittlement of reactor pressure vessel (RPV) materials from Barsebäck nuclear power plant.

Another two sessions (2nd & 3rd days) were dedicated to scientific communications (total = 20) from CEA, VTT and NOMATEN/NCBJ researchers. In this part, a wide spectrum of topics were discussed ranging from i) the modelling of irradiated materials from molecular dynamics to nanoidentation, ii) the Machine Learning for atomistic materials science, iii) the application of calphad method to the multiscale modeling of plasticity with discrete dislocation dynamics, and iv) the use of micromechanical modeling as part of the Integrated computational materials engineering strategy for irradiated materials and v) the study of tritium trapping in fusion relevant materials.

NEW LABORATORIES AND INFRASTRUCTURE

1.1. XRD DIFRACTOMETER

NOMATEN received a crucial device – the X-ray diffractometer, that helps Materials Characterization and Functional Properties of Materials groups.

Bruker AXS (Advanced X-Ray Solutions) D8 Advance diffractometer is equipped with a sealed Cu X-Ray tube, LYNXEYE XE-T strip detector and TWIN-TWIN optics. The incident and scattered beam optics includes Göbel mirror at the tube and 0.2° Soller slits at the detector useful for parallel beam geometry as well as a set of motorised divergent slits at both sides suitable for working with divergent beam in Bragg-Brentano parafocusing geometry. The detector has energy resolution better than 380 eV at 8 keV (i.e. Cu radiation) what makes $K\beta$ filter and secondary monochromators redundant, and specimen fluorescence an irrelevant phenomenon, while both Cu $K\alpha$ and $K\beta$ lines can be utilised in measurements.

The diffractometer has also attachments for grazing incidence diffraction (GID) and an in-situ high-temperature (1200°C) measurement chamber connected to vacuum-gas system. With this brilliant set of tools one can comprehensively characterise the inner structure of materials without damaging the specimen. The range of information covers crystal phase identification, description of the crystallinity or amorphousness, evaluation of stress and strain, texture analysis, investigation of layered structures with control of the penetration depth and conducting experiments in the working environment of the specimen.

"SEM allows the fast characterization of the sample with nanometer details

1.2. SCANNING ELECTRON MICROSCOPE (SEM)

The Helios 5 UX (ThermoFisher Scientific) is a fully digital, high-resolution Scanning Electron Microscope (SEM) equipped with Focused Ion Beam (FIB) technology, Energy Dispersive X-ray Spectroscopy (EDS), and Electron Backscatter Diffraction (EBSD) systems. This device is being used by the Materials Characterization and Functional Properties of Materials groups.

It allows the fast characterization of the sample with nanometer details, obtaining information about the topography, relative differences in composition, crystallographic orientation, or analysis of elemental composition of the material (both qualitative and quantitative). The use of FIB itself provides preparation of ultra-thin transparent samples for transmission electron microscopy (TEM and HRTEM) and cross-sectioning of the multiphase materials with in-situ imaging in SEM (the sectioning may be conducted in a strictly defined area, for example specific grain boundary, precipitate or crack in the material).

MAGNIFICOR LAB FUNDED BY MARIA CURIE GRANT

NOMATEN will be a host institution for ABW Marie Skłodowska-Curie Actions (MSCA fellowship) awarded by the European Commission Research Executive Agency within Horizon 2020 programme.

The MagniFiCor project proposal scored 94.8 out of 100, it is worth to mention that the number of applications broke all record in the Horizon 2020 framework program (2014–2020). It is second successful individual MSCA fellowship won by dr Aleksandra Baron-Wiecheć, the first was awarded in 2007, the host institution was the University of Manchester. The project name is “Magnetism for the functionalization of metallic materials surfaces and its effect on corrosion phenomena” (acronym MagniFiCor, 101026899 MSCA-IF-2020 — Individual Fellowships). The research project is dedicated to study magnetism for the functionalization of metallic materials and understanding its effect on corrosion phenomena in harsh environments, such as the fission and fusion industry. Fusion reactors experience many commonalities with advanced fission reactors and high-power accelerator spallation targets. Nevertheless, the operational requirements of the structural materials in future fusion power plants are beyond today’s experience. This includes elevated operating temperature, cyclic operation with long hold time, stress gradients, high neutron irradiation damage and a very high production rates of helium and hydrogen as well as an aqueous and non-aqueous corrosion. Databases supporting mathematical models and designs of future fusion power plant are mainly derived from relatively few tests facilities. The proposed research program will focus on characterisation of electrochemical behaviour of structural materials with particular emphasis on phenomena of aqueous corrosion in the presence of cyclic temperature changes, strong magnetic field and flowing electrolytes. The topic is of paramount importance for nuclear fusion where structural materials will be expose to changing magnetic fields as high as 10 T. I aim to exam in-situ the effect of varied intensities and shapes of magnetic fields on electrochemical behaviour of materials surface and phenomena occurring at the interface between electrolyte and the solid-state material. The effect of a magnetic field on the above-mentioned processes is an unusual variable with relatively limited data in the literature. The project is divided between institutions in France, Finland and Poland and combine experimental research and theoretical modelling of the observed processes using Materials Informatics. The project may open also opportunity for a new initiative, namely cooperation with Guangdong Technion – Israel Institute of Technology located in China, where ABW is currently employed. The scope of the cooperation would be focused initially mainly on students and staff exchange and short joint projects between the two institutions. The memorandum of understanding (MoU) is planned to be signed with next year. It is expected the start of the project to be in second half of 2022, the planned delay in the start of the MC project is a result of a current global unstable travel situation. Thus it is crucial for better exploiting the mobility potential of the project.

“ The MAGNIFICOR LAB project is dedicated to study magnetism for the functionalization of metallic materials and understanding its effect on corrosion phenomena in harsh environments, such as the fission and fusion industry

VTT ACTIVITIES

VTT has continued supporting the NOMATEN CoE in the TEAMING project during the second project year (M13-M24):

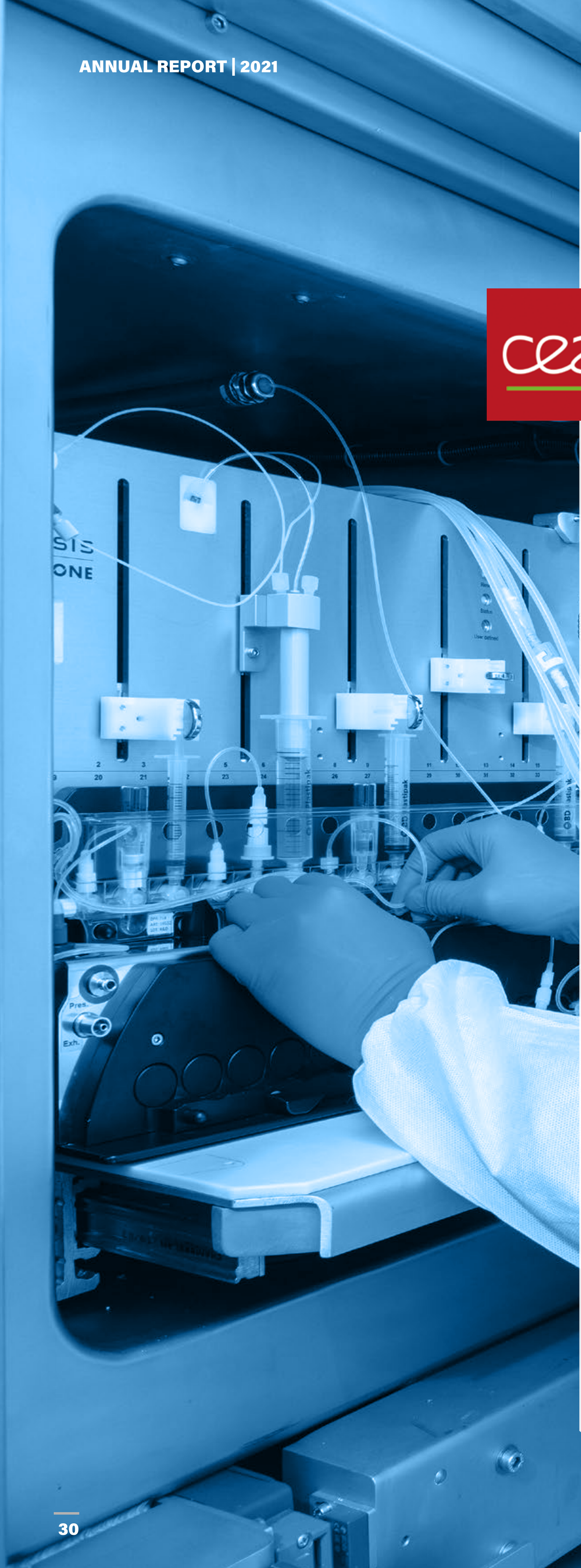
In general, VTT continued supporting the development of NOMATEN CoE by actively participating to the monthly Project Management Board meetings, and to the NOMATEN Steering Group and General Assembly meetings. VTT is currently the chair of the Steering Group. VTT participated and supported the recruitment of NOMATEN Research Group Leaders as part of the ISC. VTT's major contributions during the second year were related to the *WP7 Innovation-based sustainability*, which VTT leads. Two deliverables were formulated and published with the support from other partners: **D7.2 NOMATEN CoE IPR protection, commercialization and technology transfer strategies**, which defines the strategy and guidelines relating to immaterial property rights at NOMATEN CoE, and the first version of **D7.3 Report on business development, commercialization and technology transfer**, which describes the activities in WP7, including e.g. creation of the initial Market Strategy, activities related to international positioning and the activities supporting the marketing and business development towards industry. Work

"VTT participated and supported the recruitment of NOMATEN Research Group Leaders


Hot cells at VTT in Espoo

on the research infrastructure continued by publishing the first version of **D4.2 Report on research infrastructure use and build-up activities**. VTT also contributed the development of NOMATEN's *Capacity Building Programme (WP6)* with support to the first report on **D6.1 implementation of capacity building and education programmes**, and planning the training programmes on commercial operations to be arranged during autumn 2021 and onwards. For *WP8 Dissemination, Communication and Outreach*, VTT has contributed by sharing information of NOMATEN activities in social media (LinkedIn) and internally for VTTers, and also given a presentation at the NOMATEN seminar: Neutron-Irradiated Microstructure of Light Water Reactor Materials by Principal Scientist Wade Karlsen.

> **"VTT continued supporting the development of NOMATEN CoE by actively participating at the monthly Project Management Board meetings**



CEA ACTIVITIES

Within the framework of the NOMATEN project, CEA is, among various contributions, the workpackage leader of the WP6 dedicated to the Capacity Building Programme. In this context, CEA stimulates and encourages activities and initiatives between NOMATEN and its partners. During the year 2021, CEA has contributed to the writing of several reports, namely, the 6.1 implementation report, the 1st technical report and the 1st periodic report. On the other hand, the 14th of June, 2021, CEA participated to the 1st project review of NOMATEN project.

In 2021, due to the remaining restrictions and consequences induced by the COVID-19 pandemic, the holding of workshops initially identified were successfully replaced by the organization of scientific seminars (about 12) with invited speakers. CEA largely contributed to two of them, the 3rd of May and the 15th of June 2021. The first concerned the JANNuS-Saclay irradiation platform (Accelerator testing for nuclear materials – JANNuS irradidiation facility) and the second was focused to the additive manufacturing and high entropy alloys: new opportunities for nuclear applications. In 2021, in this context, it was also decided to organize specific webinars by CEA, NCBJ an VTT institutes. A first Webinar was remotely organized by the CEA the 10th of March and was dedicated to the multiscale approach to predict mechanical properties of nuclear materials. With about 50 participants from all the institutes, the webinar was very successful.

Within the framework of NOMATEN project, it was also decided, at the end of 2020, to plan the organization of a first scientific school, related to material sciences only, with the major concern to design it for PhD, post-doctoral students and researchers with a priority for NOMATEN. From March 2021, CEA has worked on the organization of this school held in Paris (16–19 November 2021). A specific working group has been implemented and teleconferences were regularly organize on this subject. As already mentioned (see above), the school consisted of several sessions: one dedicated to lectures by experts, to provide basic and fundamental reminders in the field of irradiated materials, a second session consisting of communications by researchers of the three institutes (CEA, NCBJ and VTT) with two additional poster sessions. The school ended by the visits of selected CEA Saclay facilities, two related to material sciences, and one related to radiopharmaceutical sciences.

During the fourth trimester of 2021, given the significant improvement in exchange and travel conditions, CEA and NOMATEN team started to plane short stays in relationship with trainings and/or the initiation of collaborative works. During November 2021, the visit of two members belonging to the NOMATEN / RG « Functional materials » was planed and hosted at the CEA / Laboratory for the Study of Mechanical Behavior of Materials of the Nuclear Materials Department (DMN). On NOMATEN side, the major interest for the researchers was to be able to freely discuss technical details with CEA researchers, in particular mechanical equipment and devices for materials studies, especially those related to creep, fatigue and tensile (dynamical) systems.

In addition, following various proposals made by CEA in July 2021, two training sessions were also planed in November 2021: the first one was related to the JANNuS Irradiation platform (facility presentation, beam production, radioprotections rules, irradiation parameters and experiment achievement); the second one was dedicated to the multi-scale simulation of the mechanical behavior of heterogeneous materials through the use of the AMITEX_FFTP code, an efficient and massively parallel tool allowing the exploration of the limits of conventional crystal plasticity in the context of polycrystalline materials and the achievement of 3D numerical simulations of polycrystals to estimate the macroscopic behavior as well as local stress heterogeneities.

Finally, with a view to develop scientific exchanges and education programmes, the RGL of the NOMATEN RG « Materials Structure, Informatics & Functions » and one PhD student have benefit of a short stay at the CEA Saclay (4 weeks, October 18 – November 15, 2021) to work with the SRMP team (Physical Metallurgy Research Section) of CEA / DMN Department, on the identification of defects in HEA for multiscale modeling in connection with a Machine learning approach. In addition, preliminary discussions took place between the CEA / SRMP team and the NOMATEN RG « Functional Properties » about a possible collaboration on the understanding of the radiation damage mechanism in high Entropy Alloys (HEA).

On the radiopharmaceutical sciences side, the main achievement is the involvement of the CEA / JOLIOT in the recruitment of the future members of the radiopharmaceutical group (leader = Marek Pruszynski). One first PD candidate together with one first PhD candidate have been selected by the organizing committee, which included a member of the CEA / JOLIOT. A first face-to-face scientific meeting with CEA / JOLIOT researchers and the radiopharmaceutical GL has also been organized at the CEA / SHFJ (Orsay), in parallel to the first Winter School mentioned above.

COOPERATION WITH THE INDUSTRY

One of NOMATEN CoE goals is the delivery of solutions and expertise for industrial customers and governmental entities, according to PL, EU, and US standards spanning its competency, as well as the development of a network of links with industrial customers.

Depending on the customer's preferences, NOMATEN CoE is flexible to deliver its products and services using channels and instruments, which can have forms of collaborative research projects, direct contracts, consultations, etc.

In addition to open, competitive research grants, NOMATEN develops and grows research services oriented at the industrial sector and designed to influence and improve its international positioning directly.

We expect NOMATEN to engage in a wide variety of activities with industrial partners. These activities can be generally divided into three main streams, distinguished

A partner of NOMATEN: Mercedes Benz Manufacturing Poland factory in Jawor, Poland by the nature of the activity, the end-user expectations and the role of the international partners. These would include joint research projects funded by public bodies in competitive programs (national and international), where either NOMATEN/NCBJ or an industrial partner could play the leading role. The second possibility are research and R&D activities conducted within specific individual contracts with an industrial customer. The third direction are accredited services related to NOMATENs expertise and infrastructure. The last direction, least known at this time, is the potential for joint commercialization of NOMATEN IPR, in the form of licensing or creation of spin-off companies.

The NOMATEN CoE offers the customers the wide range of products and services:

- New knowledge,
- New solutions,
- Product/services prototypes,
- Technological services,
- Access to research infrastructure,
- Advanced training programmes,
- Expert opinion.

The COVID-19 pandemic has slowed down the development of the direct contacts with the industry, but we have used the summer and autumn of 2021 to establish contacts and develop common projects. NOMATEN specialists met with potential customers (including both large ompanies and SME sector) and presented our offer in industry fairs, such as 15th International Railway Fair TRAKO (devoted to industries serving railroad transport) or 23rd International Fair of Technologies for Foundry METAL. NOMATEN ILG and communication specialists are also part of the team organizing a conference of Polish nuclear industry to be held in November 2021, chaired by the Ministry of Climate.

1.1. NETWORK OF ADVISORS

One of the crucial aspects of creating a successful cooperation between research and industry is the development of a common understanding. To achieve this goal, NOMATEN has invited representatives of industry to create a Network of Advisors.

The establishment of the Network of Advisors was envisaged in the assumptions of the International Research Agenda NOMATEN. The new research unit would remain in constant contact with the industry, respond to its real needs and facilitate two-way communication between companies and the science sector. Currently, the Network includes:

- Jolanta Ziaja – Project Director in the Bloki 200+ Program, Polimex Energetyka;
- Thomas Kaiser, Senior Manager – production, maintenance, facility management; head of the Mercedes-Benz Manufacturing Poland factory in Jawor;
- Krzysztof Krajewski – Operations Manager, Development and Innovation Department, PGE SA;
- Zbigniew Wiegner – Site Director at OSBL Włocławek ANWIL / ORLEN, PROCHEM.

During the first meeting of the Network, which took place in early October 2021, the members of the Network of Advisors strongly supported its expansion, including by representatives of the SME sector. The fact that the improvement of cooperation between scientific communities and enterprises is important, also for the latter, is demonstrated by the participation of representatives of various industries in the Network. More importantly, our first meeting was not only formal: from the very beginning, we talked about specific activities, such as developing a model process for analyzing research opportunities, translated into indicators relevant to the economy (e.g. benefits expressed in ROI language or risk analysis), which can be a communication tool between researchers and entrepreneurs. The inaugural meeting was the first step to strengthen NOMATEN's offer for industrial customers.

1.2. RESEARCH COOPERATION WITH MERCEDES BENZ MANUFACTURING POLAND

Mercedes Benz Manufacturing Poland has chosen the National Centre for Nuclear Research as a partner in materials research concerning the lifecycle of the tools for engine's mechanical processing. The expertise will be run by the NOMATEN Centre of Excellence team based at the National Centre for Nuclear Research Warsaw capital city. The technological challenge that Mercedes Benz plant in Jawor faces is the heterogeneity of the ceramic tools used in the cylinder honing process, i.e. too fast wear of the tools and the deposition of undesirable residues inside them. Therefore Mercedes Benz Manufacturing Poland asked NOMATEN Centre of Excellence to perform research and expertise on this topic.

Prof. Łukasz Kurpaska (Functional Properties Research Group Leader) and dr Iwona Jóźwik (Materials Characterization Research Group Leader) will manage the research activities at NOMATEN in orderd to develop the expertise for Mercedes Benz Manufacturing Poland. Moreover, NOMATEN will take advantage on lot of high performance scientific infrastructure like x-ray diffractometer (XRD) and the scanning electron microscope (SEM).

NOMATEN will conduct a series of research activities for Mercedes Benz Manufacturing Poland: among others macroscopic tests of the surface of ceramic elements before and after operation, microstructure tests, chemical and phase composition in selected areas of the tool surface, phase analysis by x-ray diffraction, tests of the surface topography of ceramic elements and mechanical tests of these elements – enumerates prof. Paweł Sobkowicz, director for scientific operations at NOMATEN.

Director Thomas Kaiser, production, maintenance and facility manager at Mercedes Benz Manufacturing Poland, joined the NOMATEN Network of Industrial Advisors. Its' task is to develop good practices related to the cooperation of companies with research units. Moreover, this team also includes representatives of, among others, chemical, construction and energy industries.

> **Mercedes Benz Manufacturing Poland asked NOMATEN Centre of Excellence to perform research and expertise on heterogeneity of the ceramic tools used in the cylinder honing process**

COMMUNICATION

Session of the NOMATEN Winter School in Paris

Poster session

NOMATEN is a valuable and unique research partner with highly skilled professionals and advanced research infrastructure. 2021 gave us a chance to reach out with out communication activities using a wide variety of tools. Our webpage and social media channels have been developed and extended to new topics and sections: scientific papers and conferences, events and special issues as NOMATEN WINTER SCHOOL. We released over 40 news releases and reached over 4500 unique users via webpage. Moreover, our LinkedIn profile (600 followers) reached over 40 000 people with NOMATEN's content.

Both for Polish government entities as well as international companies are nowadays able to notice NOMATEN's innovation and scientific potentials is drown from its three partners: highly equipped, A+ category National Centre for Nuclear Research of Poland (NCBJ) and two internationally-leading institutions with established reputations and outstanding scientific and innovation expertise: the French Alternative Energies and Atomic Energy Commission (CEA) and VTT Technical Research Centre of Finland Ltd. (VTT). At the event by Poland's National Centre for Research and Development during HORIZON2020 and WIDENING Days, NOMATEN has been a special guest and an example of EU funded success story.

Thus, NOMATEN can be trusted with solving industrial problems in research deployment of nuclear energy or development new materials for industry and radio-pharmaceutics for medicine. We use targeted actions like vocation of Industry Liaison Group, specially trained linkers between industry and science because we understand the problems with the dialog between the two. NOMATEN appeared at number of government, industrial and research related events: Intelligent Development Forum in Toruń, HORIZON2020 and WIDENING Days, Cybersec Forum 2021 and many others.

Moreover, we take advantage on some "door opener" facts for industry: NCBJ produces more than 10% percent of worlds demand on Mo99 isotope for radiopharmaceutics, exports to over 80 countries and has over 130 advanced radiopharmaceutical products to sell. In addition, NCBJ operates the only nuclear reactor in Poland and one of the few such research devices in Europe.

> **"**
> **NOMATEN performed 25 public events**

Last but not least, we undertake also the actions towards science and scientists. Together with Poland's National Centre for Research and Development we developed a video about NOMATEN, our team members and research goals. In addition, the series of seminars as well as brand new format – junior seminars – helped us gain NOMATEN's recognition among scientific community thanks to over 25 events mentioned above.

NOMATEN 2021 COMMUNICATION IN NUMBERS:

- OVER 4500 UNIQUE WEBPAGE USERS
- OVER 40 NEWS RELEASES AND COMMUNICATES
- ALMOST 600 FOLLOWERS AT LINKEDIN PROFILE
- 40 000 USERS REACH AT LINKEDIN
- 25 ONLINE PUBLIC EVENTS: SEMINARS, WEBINARS ETC.
- PRESENCE AT 10 INDUSTRIAL EVENTS

NOMATEN

9.2020–11.2021 PAPERS ABSTRACTS

T. MÄKINEN, J. KOIVISTO, L. LAURSON, M. ALAVA

SCALE-FREE FEATURES OF TEMPORAL LOCALIZATION OF DEFORMATION IN LATE STAGES OF CREEP FAILURE

Physical Review Materials 4, 18 September 2020, 093606
https://doi.org/10.1103/PhysRevMaterials.4.093606

Abstract

The last stage of material failure often shows a regime with power-law acceleration as the material lifetime is approached. We study this experimentally in tensile creep with paper samples using digital image correlation. The last, tertiary creep stage exhibits scale-free features in the sample response (strain rate) and its fluctuations. It is accompanied by an increasing localization of strain at the location of final failure. The main features are reproduced by a material model built on a viscoelastic fiber bundle model.

L. KURPASKA, M. FRELEK-KOZAK, M. WILCZOPOLSKA, W. BONICKI, R. DIDUSZKO, A. ZABOROWSKA, E. WYSZKOWSKA, M. CLOZEL, A. KOSINSKA, I. CIESLIK, M. DUCHNA, I. JOZWIK, W. CHMURZYNSKI, G. OLSZEWSKI, B. ZAJĄC,

STRUCTURAL AND MECHANICAL PROPERTIES OF DIFFERENT TYPES OF GRAPHITE USED IN NUCLEAR APPLICATIONS

Journal of Molecular Structure, Volume 1217, 5 October 2020, 128370 https://doi.org/10.1016/j.molstruc.2020.128370

Abstract

Graphite is known as a material with excellent thermo-mechanical, structural and neutron moderation properties. It is currently used as a core structural component for High Temperature Gas Cooled Reactor (HTGR). It is due to the fact that

graphite has been extensively tested and proved to satisfy most of HTGR operating requirements. However, one question still remain unclear. Graphite, depending from the manufacture method, type and purity shows different mechanical and structural properties. In addition to that, literature data is poor in comparative studies of current and used in the past materials. For this reason, series of tests involving Scanning Electron Microscopy, Raman Spectroscopy, X-ray diffraction and nanoindentation have been performed on the virgin samples of two types of nuclear graphite's: IG-110 and nuclear graphite used in decommissioned EWA reactor. Obtained results clearly shows differences in microstructural and mechanical properties of both types of graphite's. Reported changes have been discusses and attributed to the density of the material and its origin.

T. MÄKINEN, P. KARPPINEN, M. OVASKA, L. LAURSON, M.J. ALAVA

PROPAGATING BANDS OF PLASTIC DEFORMATION IN A METAL ALLOY AS CRITICAL AVALANCHES

Science Advances Volume 6, no. 41, 07 October 2020, eabc 7350 https://doi.org/10.1126/sciadv.abc7350

Abstract

The plastic deformation of metal alloys localizes in the Portevin–Le Chatelier effect in bands of different types, including propagating, or type "A" bands, usually characterized by their width and a typical propagation velocity. This plastic instability arises from collective dynamics of dislocations interacting with mobile solute atoms, but the resulting sensitivity to the strain rate lacks fundamental understanding. Here, we show, by using high-resolution imaging in tensile deformation experiments of an aluminum alloy, that the band velocities exhibit large fluctuations. Each band produces a velocity signal reminiscent of crackling noise bursts observed in numerous driven avalanching systems from propagating cracks in fracture to the Barkhausen effect in ferromagnets. The statistical features of these velocity bursts including their average shapes and size distributions obey predictions of a simple mean-field model of critical avalanche dynamics. Our results thus reveal a previously unknown paradigm of criticality in the localization of deformation.

H. SALMENJOKI, L. LAURSON, M. ALAVA

PROBING THE TRANSITION FROM DISLOCATION JAMMING TO PINNING BY MACHINE LEARNING

Materials Theory Volume 4, Article number: 5, 09 October 2020 https://doi.org/10.1186/s41313-020-00022-0

Abstract

Collective motion of dislocations is governed by the obstacles they encounter. In pure crystals, dislocations form complex structures as they become jammed by their anisotropic shear stress fields. On the other hand, introducing disorder to the crystal causes dislocations to pin to these impeding elements and, thus, leads to a competition between dislocation-dislocation and dislocation-disorder interactions. Previous studies have shown that, depending on the dominating interaction, the mechanical response and the way the crystal yields change.Here we employ three-dimensional discrete dislocation dynamics simulations with varying density of fully coherent precipitates to study this phase transition − from jamming to pinning − using unsupervised machine learning. By constructing descriptors characterizing the evolving dislocation configurations during constant loading, a confusion algorithm is shown to be able to distinguish the systems into two separate phases. These phases agree well with the observed changes in the relaxation rate during the loading. Our results also give insights on the structure of the dislocation networks in the two phases.

L. NOWICKI, J. JAGIELSKI, C. MIESZCZYŃSKI, K. SKROBAS, P. JÓŹWIK, O. DOROSHA

MCCHASY2: NEW MONTE CARLO RBS/C SIMULATION CODE DESIGNED FOR USE WITH LARGE CRYSTALLINE STRUCTU

Nuclear Instruments and Methods in Physics Research Section B vol 498, pp 9–14 https://doi.org/10.1016/j.nimb.2021.04.004

Abstract

A new tool for Monte Carlo simulation of ion channeling in crystals is described. The recently developed McChasy2 code follows the algorithm used previously in the McChasy program, but is well suited for simulations in large crystalline samples. The state of works on the validation of the code, and the possibilities of the new code for supplementing molecular dynamics with a tool supporting the experimental analysis of crystalline structures are presented and discussed.

F. J. DOMINGUEZ-GUTIERREZ, J. BYGGMÄSTAR, K. NORDLUND, F. DJURABEKOVA, U. VON TOUSSAINT

COMPUTATIONAL STUDY OF CRYSTAL DEFECTS FORMATION IN MO BY MACHINE LEARNED MOLECULAR DYNAMICS SIMULATIONS

Modelling and Simulation in Materials Science and Engineering, 202 https://doi.org/10.1088/1361-651X/abf152

Abstract

In this work, we study the damage in crystalline molybdenum material samples due to neutron bombardment in a primary knock-on atom (PKA) range of 0.5–10 keV at room temperature. We perform classical molecular dynamics (MD) simulations using a previously derived machine learning (ML) interatomic potential based on the Gaussian approximation potential (GAP) framework. We utilize a recently developed software workflow for fingerprinting and visualizing defects in damaged crystal structures to analyze the Mo samples with respect to the formation of point defects during and after a collision cascade. As a benchmark, we report results for the total number of Frenkel pairs (a self-interstitial atom and a single vacancy) formed and atom displacements as a function of the PKA energy. A comparison to results obtained using an embedded atom method (EAM) potential is presented to discuss the advantages and limits of the MD simulations utilizing ML-based potentials. The formation of Frenkel pairs follows a sublinear scaling law as ξb where b is a fitting parameter and ξ = EPKA/E0 with E0 as a scaling factor. We found that the b = 0.54 for the GAP MD results and b = 0.667 for the EAM simulations. Although the average number of total defects is similar for both methods, the MD results show different atomic geometries for complex point defects, where the formation of crowdions by the GAP potential is closer to the DFT-based expectation. Finally, ion beam mixing results for GAP MD simulations are in a good agreement with experimental mixing efficiency data. This indicates that the modeling of atom relocation in cascades by machine learned potentials is suited to interpret the corresponding experimental findings.

M. KALINOWSKA, E. GOŁĘBIEWSKA, L. MAZUR, H. LEWANDOWSKA, M. PRUSZYŃSKI, G. ŚWIDERSKI, M. WYRWAS, N. PAWLUCZUK, W. LEWANDOWSKI

CRYSTAL STRUCTURE, SPECTROSCOPIC CHARACTERIZATION, ANTIOXIDANT AND CYTOTOXIC ACTIVITY OF NEW MG(II) AND MN(II)/NA(I) COMPLEXES OF ISOFERULIC ACID

Materials 2021, 14, 3236 https://doi.org/10.3390/ma14123236

Abstract

The Mg(II) and heterometallic Mn(II)/Na(I) complexes of isoferulic acid (3-hydroxy-4-methoxycinnamic acid, IFA) were synthesized and characterized by infrared spectroscopy FT-IR, FT-Raman, electronic absorption spectroscopy UV/VIS, and single-crystal X-ray diffraction. The reaction of $MgCl_2$ with isoferulic acid in the aqueous solutions of NaOH resulted in synthesis of the complex salt of the general formula of $[Mg(H_2O)_6]$□$(C_{10}H_9O_4)_2$□$6H_2O$.

The crystal structure of this compound consists of discrete octahedral [Mg(H2O)6]2+ cations, isoferulic acid anions and solvent water molecules. The hydrated metal cations are arranged among the organic layers. The multiple hydrogen-bonding interactions established between the coordinated and lattice water molecules and the functional groups of the ligand stabilize the 3D architecture of the crystal. The use of MnCl2 instead of MgCl2 led to the formation of the Mn(II)/Na(I) complex of the general formula [Mn3Na2(C10H7O4)8(H2O)8]. The compound is a 3D coordination polymer composed of centrosymmetric pentanuclear subunits. The antioxidant activity of these compounds was evaluated by assays based on different antioxidant mechanisms of action, i.e., with •OH, DPPH• and ABTS•+ radicals as well as CUPRAC (cupric ions reducing power) and lipid peroxidation inhibition assays. The pro-oxidant property of compounds was measured as the rate of oxidation of Trolox. The Mg(II) and Mn(II)/Na(I) complexes with isoferulic acid showed higher antioxidant activity than ligand alone in DPPH (IFA, IC50 = 365.27 μM, Mg(II) IFA IC50 = 153.50 μM, Mn(II)/Na(I) IFA IC50 = 149.00 μM) and CUPRAC assays (IFA 40.92 μM of Trolox, Mg(II) IFA 87.93 μM and Mn(II)/Na(I) IFA 105.85 μM of Trolox; for compounds' concentration 10 μM). Mg(II) IFA is a better scavenger of •OH than IFA and Mn(II)/Na(I) IFA complex. There was no distinct difference in ABTS•+ and lipid peroxidation assays between isoferulic acid and its Mg(II) complex, while Mn(II)/Na(I) complex showed lower activity than these compounds. The tested complexes displayed only slight antiproliferative activity tested in HaCaT human immortalized keratinocyte cell line within the solubility range. The Mn(II)/Na(I) IFA (16 μM in medium) caused an 87% (±5%) decrease in cell viability, the Mg salt caused a comparable, i.e., 87% (±4%) viability decrease in a concentration of 45 μM, while IFA caused this level of cell activity attenuation (87% ± 5%) at the concentration of 1582 μM (significant at $\alpha = 0.05$).

M. ALAVA

CROSSOVER OF FAILURE TIME DISTRIBUTIONS IN A MODEL OF TIME-DEPENDENT FRACTURE

Frontiers in Physics, Volume 9, 2021 https://doi.org/10.3389/fphy.2021.686195

Abstract

An important question in the theory of fracture is what kind of life-time distributions may exist for materials under load. Here, this is studied in the context of a one-dimensional fracture model with local load sharing under a constant external load, „creep". Simulations of the system with Weibull distributed initial life-times for the elements show that the limiting distribution follows from extreme statistics and takes the Gumbel form eventually, with longer and longer cross-overs in the system size from a Weibull-like distribution, depending on the initial Weibull-exponent.

F. J. DOMINGUEZ, S. PAPANIKOLAOU, A. ESFANDIARPOUR, P. SOBKOWICZ, M. ALAVA

NANOINDENTATION OF SINGLE CRYSTALINE MO: ATOMISTIC DEFECT NUCLEATION AND HERMOMECHANICAL STABILITY

Materials Science & Engineering A, 826 (2021) https://doi.org/10.1016/j.msea.2021.141912

Abstract

The mechanical responses of single crystalline Body-Centered Cubic (BCC) metals, such as molybdenum (Mo), outperform other metals at high temperatures, so much so that they are considered as excellent candidates for applications under extreme conditions, such as the divertor of fusion reactors. The excellent thermomechanical stability of molybdenum at high temperatures (400–1000 oC) has also been detected through nanoindentation, pointing toward connections to emera gent local dislocation mechanisms related to defect nucleation. In this work, we carry out a computational study of the effects of high temperature on the mechanical deformation properties of single crystalline Mo under nanoindentation. Molecular dynamics (MD) simulations of spherical nanoindentation are performed at two indenter tip diameters and crystalline sample orientations [100], [110], and [111], for the temperature range of 10–1000 K. We investigate how the increase of

temperature influences the nanoindentation process, modifying dislocation densities, mechanisms, atomic displacements and also, hardness, in agreement with reported experimental measurements. Our results suggest that the characteristic formation and high-temperature stability of [001] dislocation junctions in Mo during nanoindentation, in contrast to other BCC metals, may be the cause of the persistent thermomechanical stability of Mo.

RONG-GUANG XU, HENGXU SONG, YONGSHENG LENG, STEFANOS PAPANIKOLAOU

A MOLECULAR DYNAMICS SIMULATIONS STUDY OF THE INFLUENCE OF PRESTRAIN ON THE POP-IN BEHAVIOR AND INDENTATION SIZE EFFECT IN CU SINGLE CRYSTALS

Materials 2021, 14, 5220 https://doi.org/10.3390/ma14185220

Abstract

The pop-in effect in nanoindentation of metals represents a major collective dislocation phenomenon that displays sensitivity in the local surface microstructure and residual stresses. To understand the deformation mechanisms behind pop-ins in metals, large scale molecular dynamics simulations are performed to investigate the pop-in behavior and indentation size effect in undeformed and deformed Cu single crystals. Tensile loading, unloading, and reloading simulations are performed to create a series of samples subjected to a broad range of tensile strains with/without pre-existing dislocations. The subsequent nanoindentation simulations are conducted to investigate the coupled effects of prestrain and the presence of resulting dislocations and surface morphology, as well as indenter size effects on the mechanical response in indentation processes. Our work provides detailed insights into the deformation mechanisms and microstructure-property relationships of nanoindentation in the presence of residual stresses and strains.

KAROL FRYDRYCH, KAMRAN KARIMI, MICHAŁ PECELEROWICZ, RENE ALVAREZ, F. J. DOMINGUEZ – GUTIERREZ, FABRIZIO ROVARIS, STEFANOS PAPANIKOLAOU

MATERIALS INFORMATICS FOR MECHANICAL DEFORMATION: A REVIEW OF APPLICATIONS AND CHALLENGES

Materials 2021, 14, 5764 https://doi.org/10.3390/ma14195764

Abstract

In the design and development of novel materials that have excellent mechanical properties, classification and regression methods have been diversely used across mechanical deformation simulations or experiments. The use of materials informatics methods on large data that originate in experiments or/and multiscale modeling simulations may accelerate materials' discovery or develop new understanding of materials' behavior. In this fast-growing field, we focus on reviewing advances at the intersection of data science with mechanical deformation simulations and experiments, with a particular focus on studies of metals and alloys. We discuss examples of applications, as well as identify challenges and prospects

S. PAPANIKOLAOU, M. ALAVA

DIRECT DETECTION OF PLASTICITY ONSET THROUGH TOTAL-STRAIN PROFILE EVOLUTION

Physical Review Materials, 5, 083602 https://doi.org/10.1103/PhysRevMaterials.5.083602

MODELING OF THE PRIMARY DAMAGE AND THE PROPERTIES OF POINT DEFECTS

AUTHORS:JEAN-PAUL CROCOMBETTE

AFFILIATION:CEA SACLAY

Abstract

In this lecture, we want in a first part to address the various aspects of the modelling of the primary damage of irradiation and, in a brief second part to describe how one can calculate the basic formation and migration properties of the defects created by irradiation. The methodologies of each modelling step will be briefly recalled, the tools and codes used in CEA will be presented and the results will illustrated with examples from CEA's studies.

The simulation of primary damage starts with the determination of Primary Knocked-on Atom (PKA) spectrum for a given neutron flux. We use the DART code (Luneville et al. 2006), which also enables to study which ion beam could be contemplated to reproduce approximately a given neutron flux. Once the PKA spectrum (or ion energy) is determined, the primary damage modelling aims to describe the collision cascades created by the PKAs, and to obtain the amount and nature of created defects. In the case of ion irradiation, one is also interested in the spatial distribution of damage and ion implantation. There are two complementary simulation framework:

-The Binary Collision Approximation (BCA) which is specifically devoted to the modelling of irradiation damage. Some details will be given about these simulations. In particular, we will discuss the differences between and respective advantages of the so-called Full cascade and Quick-Calculations of damage in connection with NRT standard of damage creation. For ion irradiations, this modelling relies heavily on the famous SRIM code. We shall present the IRADINA code (Crocombette et al. 2019) which has been developed by the university of Jena and adapted by CEA to a nuclear context. We believe Iradina can be a nice alternative to the ageing SRIM.

-The Molecular Dynamics with empirical potential is the complementary tool. MD allows for a much more detailed description of the collision cascades. MD simulation provide a detailed description of the structure of cascade created defects as well as a much more precise evaluation of the number of these defects. The well – known overestimation of the number of defects by BCA simulations and NRT standard has recently led to a proposition of new standard, the so-called arc-dpa (Nordlund et al. 2018), which we shall present and briefly discuss.

Both simulation methodologies rely on the distinction between electronic and ballistic loses for the fast moving atoms. The electronic stopping power is usually tabulated. However in the recent years, Time Dependent Density Functional Theory (TD-DFT) has been used to calculate it ab initio. We shall mention the MolGW code (Maliyov et al. 2018), which implements TD-DFT to calculate electronic stopping power in an atomic basis.

The properties of defects we are interested in in the context of irradiation damage are their structure, and their formation and migration energies. DFT is the method of choice to study these properties. It usually proceeds through super-cell calculations. We shall introduce the ANETO code (Varvenne et al. 2013), which improves the convergence of the calculations with respect the supercell size considering the elastic dipole of the defects. With the same tool, noticeable stress effects on the migration barriers can be obtained which can be important for later microstructural evolution. DFT calculations are usually performed at 0K. Finite temperature can naturally affect the properties of defects. This will be illustrated with the PAFI code (Swinburne et al. 2018) for the calculation of finite temperature energy barriers.

We shall end-up with an introduction to a method that bridges the atomic-description of defects and the modelling of microstructure evolution while bypassing the detailed description of primary damage. Indeed the accumulation of Frenkel pairs within empirical potential MD has proven a valuable methodology to evaluate the possible microstructure evolution of a crystal under irradiation. This methodology will be presented in details I latter talk, but we shall introduce it with the case of the variation, with temperature and composition, of the amorphization dose of oxides (Chartier et al. 2009).

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[C. Varvenne, F. Bruneval, M. C. Marinica et E. Clouet2013] C. Varvenne, F. Bruneval, M. C. Marinica et E. Clouet, *Point defect modeling in materials: Coupling ab initio and elasticity approaches,* Physical Review B **88**: 134102 (2013)

Plasticity in solids is dependent on microstructural history, temperature, and loading rate, and sample-dependent knowledge of yield points in structural materials adds reliability to mechanical behavior. Yielding is commonly measured through controlled mechanical testing, in ways that either distinguish elastic (stress) from total deformation measurements or identify plastic slip contributions. In this paper, we show that yielding can be unraveled through statistical analysis of total-strain fluctuations during the evolution sequence of profiles, measured in situ, through digital image correlation. We demonstrate two distinct ways of quantifying yield locations in widely applicable crystal plasticity models for polycrystalline solids, using either principal component analysis or discrete wavelet transforms. We test and compare these approaches for synthetic data of polycrystals and a variety of yielding responses through changes in applied loading rates and strain-rate sensitivity exponents.

MONIKA KALINOWSKA, HANNA LEWANDOWSKA, MAREK PRUSZYŃSKI, GRZEGORZ ŚWIDERSKI, EWELINA GOŁĘBIEWSKA, KAMILA GRYKO, JULIA BRAUN, MONIKA BORKOWSKA, MAGDA KONIECZNA, WŁODZIMIERZ LEWANDOWSKI

CO(II) COMPLEX OF QUERCETIN-SPECTRAL, ANTI-/PRO-OXIDANT AND CYTOTOXIC ACTIVITY IN HACAT CELL LINES

Applied Sciences 2021,11(19) https://doi.org/10.3390/app 11199244

Abstract

In this study a cobalt(II) complex of quercetin was synthetized in the solid state with the general formula Co(C15H9O7)2·2H2O. The FT-IR, elemental analysis, and UV/Vis methods were used to study the composition of the complex in a solid state and in a water solution. The anti-/pro-oxidant activity of quercetin and the Co(II) complex was studied by means of spectrophotometric DPPH (2,2-diphenyl-1-picrylhydrazyl), FRAP (ferric reducing antioxidant activity) and Trolox oxidation assays. The cytotoxicity of quercetin and Co(II)-quercetin complex in HaCat cell lines was then established.

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PRODUCTION AND SUPPLY OF A-PARTICLE–EMITTING RADIONUCLIDES ½AQ1 FOR TARGETED A-THERAPY

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Abstract

Encouraging results of Targeted Alpha Therapy (TAT) have created significant attention from academia and industry. However, the limited availability of suitable radionuclides has hampered widespread translation and application. In the present review, we discuss the most promising candidates for clinical application and the state of the art of their production and supply. Along with forthcoming another two reviews on chelation and clinical application of alpha-emitting radionuclides, JNM will provide a comprehensive assessment of the field.

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