Plasma Materials Interactions & Diagnostics Symposium

Tuesday 21 May 2024 - Thursday 23 May 2024

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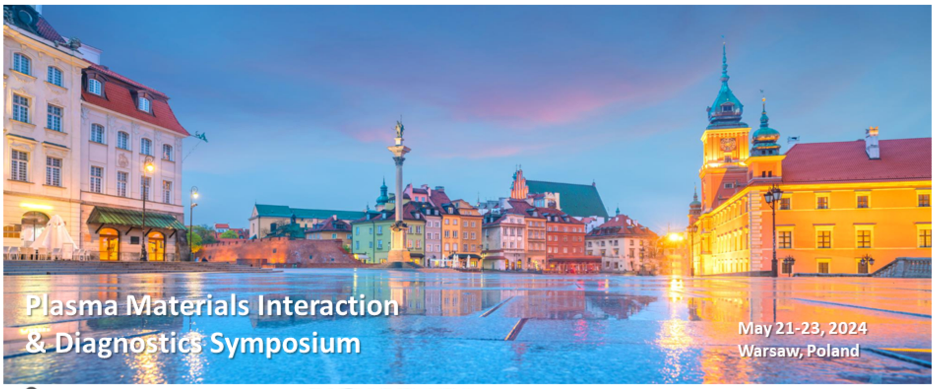

Narodowe Centrum Badań Jądrowych
National Centre for Nuclear Research
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NOMATEN
Centre of Excellence in Multifunctional Materials for Industrial and Medical Applications

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Book of Abstracts

Only accepted abstracts are presented in the book.

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Session 2: Plasma Diagnostics II / 4

Review of optical emission spectroscopy applications of the plasma and the PFC materials interaction study in Plasma-Focus and Rod Plasma Injector devices

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This overview presents a study of the plasma interaction with the plasma-facing components (PFC) materials in the Plasma-Focus (PF) and the Rod Plasma Injector (RPI) devices using optical emission spectroscopy (OES). The mentioned devices generate intense plasma streams, but they differ in operational parameters. The measurements were performed using PF-360 (NCBJ), PF-1000U (IFPiLM) and RPI-IBIS (NCBJ) facilities.
The OES study was separated into two parts. First, the time-resolved and time-integrated spectra of freely propagating plasma were recorded. Using those results it was possible to deduce the purity of plasma, plasma dynamics and, in some cases, plasma electron density. Next, on the basis of the spectroscopic investigation of plasma interaction with PFC materials, the impact of plasma on the chosen sample was determined. The explored samples were made of carbon fibre composite (CFC), tungsten and steel.

Session 2: Plasma Diagnostics II / 3

Cherenkov detectors as an auxiliary diagnostic for the studies of the runaway-electrons beams recorded in the tokamak's Scrape-Of-Layer

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The NCBJ team had proposed to use Cherenkov detectors with diamond radiators for measurements of fast electrons inside the Magnetic Confinement Facilities of the tokamak type many years ago. The main idea was the application of a Cherenkov Effect for measurements of electron-beams in the energy range of (50-300) keV. In MCF the studies were performed for runaway electrons that undergo acceleration up to relativistic energies, which can pose a threat to high energy plasma facilities and experiments.
The use of diamond crystals was dictated by its high refractive index and high thermal conductivity, which allowed to record Runaway Electrons with energies above 51 keV and, simultaneously, helped to keep radiators' temperatures sufficiently low.
The most interesting measurements of the fast runaway electrons by means of the presented detectors have been performed in the COMPASS, FTU and TCV tokamaks within their scrape-of-layers, but also a little bit behind the Last Closed Flux Surfaces. This presentation summarizes the most important results of fast electrons measurements performed in different tokamaks by means by the reported diagnostic

Session 2: Plasma Diagnostics II / 2

Numerical reconstruction of Langmuir probe measurements obtained from the negative ion source for ITER (SPIDER)

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The experimental fusion reactor ITER will be heated by injection of a fast neutral beam generated by acceleration and neutralization of negative ions. The negative ion source used for this purpose (SPIDER), constructed at the Consorzium RFX (Italy) consists of 8 driver volumes where radio-frequency (RF) power is inductively coupled to the plasma electrons and an expansion chamber containing a magnetic filter (MF). The physical and numerical principles of a comprehensive fluid model of this source is presented. The model gives a self-consistent two-dimensional description of the source, including the neutral gas flow, plasma chemistry, RF coupling in the source driver and plasma transport through the magnetic filter. The different particle species (electrons, the three types of the positive ions: H+, H2+,H3+, negative ions H- and the neutral species: hydrogen atoms H and molecules H2) are described by separate continuity equations and the electron temperature is governed by the electron energy balance equation. The particle fluxes are found from momentum equations neglecting the inertia terms (drift-diffusion approximation). The model accounts for the losses of particles and electron energy in the third dimension. The electrostatic coupling between electrons and ions is described by the Poisson equation.
The inductive coupling between radio frequency (RF) waves and the plasma, which is decisive in determining the characteristics of the plasma conditions at the beginning of the expansion region forms an essential ingredient of the model. The details of the RF model and the necessary code developments to simulate the currents in the source induced by the radio-frequency (RF) currents flowing in the feeding coils are outlined. In our approach, the RF electrical field is split in a plasma part plus another one in vacuum, E = Ep + EV, which simplifies the boundary conditions for Ep while EV is obtained from a theoretical formulation for the field generated by a current loop, which results in a fast and flexible numerical algorithm providing converged solution for the RF field after a few iterations, even for the cases with high conductivity of the plasma.
The coupled system of model equations is solved numerically, by a FORTRAN code FSFS2D (Fluid Solver For SPIDER in 2D), taking into account both the time evolution and two spatial dimensions. The method is based on finite volume approximation and 9-point discretization on a non-uniform, staggered mesh is used to account for anisotropy due to magnetic field. Semi implicit numerical solver allows for large time steps (> 1000 x explicit time step) producing steady-state solution in a reasonable time (few hours for 100x100 mesh).
An important element in the development of the numerical framework is the validation of the code results against the experimental data. For that aim a series of numerical simulations have been performed to reproduce some of the experimental results from the SPIDER experimental campaigns. The existing data base of Langmuir probe measurements at different positions in the SPIDER device provides a complete set of profiles of plasma parameters along one spatial direction (axial profiles) as well as parametric scans at fixed probe positions.
Critical assessment of the validation results and outline of the necessary code/model enhancements required to improve the predictive capability of the FSFS2D code is discussed.

Session 6: Junior Talks / 1

Interplay of Alloying Elements in Concentrated Solid-Solution Alloys: A Computational Study on Irradiation-Induced Defect Evolution

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Concentrated solid-solution alloys (CSAs) have recently emerged as promising candidates for enhanced irradiation resistance. This computational study delves into the intricate interplay of alloying elements on the generation, recombination, and evolution of irradiation-induced defects in single-phase CSAs. Employing molecular dynamics simulations, we explore defects evolution in Ni-based CSAs, considering a spectrum of vacancy defects in face-centered cubic (FCC) structures. The study encompasses various shapes such as cubic, tetrahedral, octahedral, truncated octahedral, spherical, and stacking fault tetrahedral. Collision cascades are simulated over a temperature range of 10 to 900 K, with a primary knock-on atom (PKA) energy of 10 keV. This systematic exploration progresses through model crystals, starting from pure Ni, advancing to binary alloys like NiCr20, and culminating in the more complex NiCoCr20 alloy. Our findings unveil the pivotal role of chromium-rich materials in facilitating dislocation emissions and inducing the nucleation of stacking fault tetrahedra in the vicinity of nanovoids. This phenomenon is attributed to Shockley partial interactions, resulting in the nucleation of stacking fault tetrahedra primarily formed by Stair-Rod dislocations. Notably, among the alloys studied, NiCr20 and NiCoCr20 stand out as the sole materials capable of manifesting this unique mechanism.
This research provides valuable insights into the design principles governing irradiation resistance in CSAs, emphasising the significance of specific alloy compositions, particularly those incorporating chromium. The observed defect evolution mechanisms contribute to the fundamental understanding of material behaviour under irradiation, offering guidance for the development of advanced materials with improved performance in radiation-intensive environments.

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Advancing Fusion Materials: Case Studies in Characterization by NCBJ

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Developing materials for fusion technologies is a critical component in advancing fusion development and facilitating its commercial application. Among the key challenges in this process is the need to preselect and rigorously test materials that can withstand the extreme conditions within a fusion reactor. To address this challenge, advanced materials such as Oxide Dispersion Strengthened (ODS) and Reduced Activation Ferritic-Martensitic (RAFM) steels are being explored for their promising properties in fusion applications. The successful integration of these materials necessitates a multifaceted approach, encompassing material selection, optimization of production processes, and refinement of fabrication techniques.

The presentation looks at real examples from NCBJ, where we've tested fusion materials. Examples include the assessment of electron beam welded joints in EUROFER97 blocks (incorporating non-destructive testing methods) and the mechanical analysis of Fe-14%Cr-based ODS steel manufactured by Hot Isostatic Pressing (HIP). Both investigations aim to contribute to the overall goal of developing robust methodologies for material testing and optimizing the production of fusion reactor components.

Moreover, the adaptation of mechanical testing methods to the unique demands of fusion applications necessitates the development of specialized protocols and methodologies. The presentation underscores NCBJ's research capabilities, showcasing the exploration and understanding of material behaviours under diverse conditions, including high temperatures. A part of this presentation will focus on the launch of NCBJ's small-scale mechanical lab, which will serve as a crucial platform for advancing our understanding of fusion materials and their mechanical properties.

Acknowledgments
This work has been carried out within the framework of the EUROfusion Consortium, funded by the European Union via the Euratom Research and Training Programme (Grant Agreement No 101052200 — EUROfusion). Project co-financed by the Polish Ministry of Science and Higher Education under the program entitled International Projects Co-financed.

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Bridging the gap between atomistic defect evolution and continuum elasticity with an Object kinetic Monte Carlo approach

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Since the degradation of macroscopic properties of irradiated materials occurs over relatively long irradiation times, the Object kinetic Monte Carlo method, which only follows the evolution of off-lattice defects, seems to be appropriate as it allows reaching physical times close to those achieved experimentally. In the absence of external forces and in an ideal perfect crystal lattice,
defects can be considered as independent random walkers. However, in any realistic material, the host lattice is often locally distorted by the presence of external loads, dislocation lines, grain boundaries, small precipitates or other defects. This elastic distortion might bias the direction of the jumps depending on the elastic interaction energy of the defect when moving in different directions.
Here, we propose a general novel computational method to include elastic interactions in OkMC simulations considering anisotropic elastic behavior and any defect distribution, curved dislocations and phases with different elastic properties. The approach does not rely on the dipolar approximation but instead is based in obtaining numerically the elastic fields of the defect map using a micromechanical FFT approach combined with defect eigenstrains or static
field dislocation mechanics. The method developed will be used to analyze the evolution of <111> prismatic dislocation loops in Fe in the presence of other defects and immobile dislocations. The dislocation loops appear as consequence of the irradiation of steels under harsh environments such as those found in fission or in future fusion reactors and are responsible of the change of mechanical properties of steels.

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Development of a semi-empirical method to interconnect ion and neutron radiation-induced hardening in structural steels for nuclear applications using nanoindentation and crystal plasticity finite element method

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Reduced activation ferritic/martensitic (RAFM) steels are the main candidates for the construction of structural components in future nuclear reactors. To ensure safe reactor employment, RAFM-based materials require efficient methods for their characterization under constant neutron irradiation. However, neutron irradiation for research purposes is an expensive and long process, and therefore a limiting factor to steadily investigate its effect. Hence, a safer and cheaper solution of ion irradiation as a tool to surrogate the neutron damage is becoming more and more popular. The presented study demonstrates a semi-empirical approach to effectively interconnect the ion and neutron radiation-induced hardening in RAFM steels. The applied set of tools, based on nanoindentation and tensile tests, as well as their finite element method simulations, allows us to extract the irradiation effect on the material law, and accurately reproduce the experimental data. Ultimately, the analysis performed on an ion-irradiated specimen can provide the macroscale (neutron irradiated) yield stress values in a range of dpa doses, which correlate with the literature.

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Fast X-ray tomographic inversions for impurity transport analysis in tokamak plasmas

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In tokamak plasmas, estimating the local impurity concentration can be subject to many uncertainties. In particular, it requires accurate knowledge of plasma temperature, magnetic equilibrium, impurity cooling factor and the spectral response of the diagnostics used. When all other plasma parameters are well-known, the impurity density profile can be reconstructed in the core with the help of X-ray tomography. In this contribution, we introduce some tools aiming at validating and speeding up the X-ray tomographic inversions. The traditional approach based on Tikhonov regularization, including magnetic equilibrium constraint and parameter optimization, is presented. The advantages and drawbacks of substituting it with neural networks for fast inversions are investigated. Finally, the perspectives for plasma profiles reconstruction and validation are discussed.

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High resolution neutron spectrometer for fusion plasma using a GEM detector

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The purpose of neutron diagnostics used in fusion plasma research is to provide information about the behavior of the plasma. One such neutron diagnostics is, for example, neutron energy spectrometry. By measuring the neutron energy spectrum, it is possible to determine not only the ionic temperature for a plasma in thermal equilibrium but also plasma parameters such as: plasma rotation, fuel ion ratio nT/nD [1] as well as the intensities of various neutron spectrum components because of plasma heating and the fuel ion distribution in the plasma [2].
Neutron spectrometers were used to measure both pure deuterium plasma and deuterium-tritium plasma. The most common type of neutron spectrometer uses the time-of-flight (ToF) or thin film proton recoil (TPR) technique. These spectrometric techniques have been used, for example, on the Joint European Torus (JET). Experiences from JET have been used in the design of the high-resolution neutron spectrometer (HRNS) proposed for ITER. The HRNS proposed for ITER will use four different spectrometric techniques, including a TPR spectrometer equipped with segmented silicon detectors. Recently, the state of the HRNS system dedicated to ITER has been shown in [3].
The disadvantage of this solution may be the poor radiation resistance of silicon detectors. Taking the above into account, it can be worth developing and testing a new, compact neutron spectrometer system, which, meeting the ITER measurement requirements, could be used in the HRNS. Such a

spectrometer can be designed based on a Gas Electron Multiplier (GEM) type detector.
The conceptual design and operational principle of a novel TPR neutron spectrometer based on GEM, intended for future spectrometry applications dedicated to fusion plasmas, is described.

[1] G. Ericsson et al. (2010) Rev. Sci. Instrum. 81, 10D324.
[2] C. Hellesen et al. (2010) Nucl. Fusion 50, 022001.
[3] M. Scholz et al. (2019) Nucl. Fusion 59, 065001

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Development of long pulse scenario at Wendelstein 7-X

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Stellarators offer a relatively straightforward route to steady state fusion power operation. Future reactors, such as DEMO, are expected to operate quasi-continuously with divertor heat fluxes as low as 5 MW/m2 [1]. Such a low level of acceptable incoming heat flux leads to the requirement that most of the power leaving the plasma has to be radiated away by the plasma impurities and to operate in the so-called detached regime, where the divertor target plates are protected from the hotter plasma by a dense layer of cold (Te < 5 eV) plasma. One of the objectives of the Wendelstein 7-X research is to achieve and optimise the long pulse scenarios. The recently installed high heat flux divertor, consisting of water-cooled CFC target elements, can handle power loads of up to 10 MW/m2 in continuous operation, which for W7-X plasmas means up to 30 minutes.
During the W7-X operational phase OP1.2, which took place in 2017-2018, 100 s of discharge were achieved with the divertor attached [2], while about 30 s were achieved with the divertor detached [3]. The experiments performed showed that a robust detachment scenario allows to reduce the peak heat flux by almost an order of magnitude, and no significant increase in impurity concentration was observed.
In the present campaign, we were able to significantly extend these scenarios with plasma durations of up to 8 min in the attached state and up to 2 min with almost completely detached divertor. These plasmas were heated by electron cyclotron resonance heating (ECRH) with an input power of 3.5 MW in the attached scenario and 5 MW in the detached scenario.
In the attached case, the line-integrated density was set to approximately 5⊠1019 m-2 and kept constant throughout the discharge with the feedback system. The diamagnetic energy was kept at a level of about 430 kJ, and the ion and electron temperatures were 1.5 keV and 2 keV, respectively. Such a scenario did not lead to any overloading of the surface of the components facing the plasma.
In the case of detached plasmas, a more sophisticated scenario had to be developed. Both intrinsic (mostly carbon) and seeded (neon) impurities were used to keep the plasma radiation level at the frad above 0.8, which is a prerequisite for detachment. The plasma density was set at a level of 1.31020 m-2, resulting in both ion and electron temperatures at the level of 1.5 keV and a diamagnetic energy of about 0.6 MJ. Reduced heat fluxes to the divertor during the entire detached phase resulted in low surface temperatures (150-160℃). As a consequence, no significant increase of impurity concentration occurs with the cooler plasma boundary, and the Zeff stayed below 1.5. In the PHA spectra, no significant increase of carbon or oxygen lines was observed during the discharge suggesting stable plasma during the entire discharge.

[1] N. Asakura et al., Nuclear Fusion 57, 126050 (2017).
[2] T. Klinger et al., Nuclear Fusion 59, 112004 (2019).
[3] M. Jakubowski et al., Nuclear Fusion 61, 106003 (2021).

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Measurements of Spontaneous Magnetic Fields in Laser-Produced Plasma using Complex Interferometry

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Spontaneous magnetic fields (SMF) are phenomena occurring in laser plasma that can affect the plasma density and temperature distributions, laser radiation absorption and ablation pressure. For this reason, knowledge about mechanisms of SMF generation is important in studies related to inertial confinement fusion as well as in astrophysical research.
The most reliable and efficient method for investigating the SMF is the method based on the magnetooptical Faraday effect, as it provides information on the SMF distribution in the entire area of investigated plasma, but requires simultaneous polarimetric and interferometric measurements. A particularly useful variant of this method is complex interferometry, which involves obtaining information about SMF directly from a phase–amplitude analysis of a complex interferogram.
During the lecture, the theoretical foundations of complex-interferometry will be discussed and the results of experiments using complex interferometry will be presented.

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From direct fuel removal monitoring to AI supported multipurpose technique. A brief history of LIBS for PWI

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Once upon a time, when carbon based materials were expected to be applied in the ITER divertor, laser-based techniques were proposed as a tool for co-deposit removal of the chemical erosion products. To monitor the removal progress, the observation of deuterium alpha line in the laser produced plasma was proposed. Then tungsten replaced carbon which mitigated chemical erosion and laser-based cleaning techniques became irrelevant.
Nevertheless, it was revealed that the simple observation of the deuterium line may be expanded to measurements of the broad optical spectrum by the means of LIBS (Laser Induced Breakdown Spectroscopy) technique, and thus become very useful not only for fuel retention quantification but for monitoring of the chemical composition of the wall.
With its potential of being contactless and non-interfering diagnostics, LIBS became an important element of the research in PWI (Plasma Wall Interactions) area, which was under intensive investigation of numerous teams from Europe and China. The advantages of this effort demonstrated successful analysis of the surface materials in EAST and WEST tokamaks and deployment of the remotely controlled LIBS head to conduct LIBS measurements at FTU. Scheduled on summer 2024 the experiment with remotely controlled LIBS head at JET will be the final prove that LIBS constitutes a technique utterly relevant for ITER.
Despite these achievements, applying LIBS to the next-step fusion device remains challenged by uncertainties. These uncertainties stem from the undetermined morphology of co-deposits in ITER and potential issues with controlling laser beam and plasma parameters. These control issues can lead to inaccuracies in estimating the chemical composition of plasmafacing components. Additionally, the vast amount of measurement data expected in ITER could further complicate the diagnostic performance.
On a positive note, recent years have seen the emergence of new tools that capitalize on large datasets. These tools are artificial intelligence (AI) methods, particularly Artificial Neural Networks (ANNs) and Convolutional Neural Networks (CNNs). These methods enable deep learning, a technique highly adept at identifying patterns in data. Models built using these methods have already demonstrated superior performance in various scientific, industrial, and information technology tasks. Recognizing this potential, the IPPLM team began work on adapting these methods to LIBS for PWI research in 2020.
After presentation of the crucial achievements of LIBS in fusion technology this contribution will focus on the achievements and plans for application of AI methods in this field.

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Ab initio determination of tungsten ions ionization energies for plasma diagnostic purpose

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For modelling calculations and for diagnostics of key tokamak plasma parameters, it is important to know highly accurate atomic data for all stages of ionization of tungsten, with ionization energies at the top of the list. Ionization energies data for tungsten ions collected in the NIST Atomic Spectra Database have varied accuracy, moreover, the reported accuracy of NIST data for some high-ionization states of tungsten may be doubtful. Fully relativistic Multi-Configuration Dirac-Hartree-Fock method with Configuration Interaction has been employed to provide the reference values of ionization energies of tungsten ions with uncertainties substantially reduced comparing to the previous reference values.

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Metastable Structure of Layers Shaped During Pulse Magnetron Sputtering

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The forming the properties of materials consists in fulfilling the sequence of different energy states. First, one should obtain the state of increased free energy, as the excited initial state for subsequent treatments and then conduct controlled relaxation of this energy excess in order to reach a lower level
of non-equilibrium energy state of material - defined as a new degree of structure metastability, both in phase and morphological terms. This grade determines the usable properties of the material as a synthesis product. Effectiveness in implementation the above sequence, which is crucial for obtaining
the desired properties of materials, is directly dependent on recognition of the synthesis environment.
In the case of plasma surface engineering methods, this effectiveness is conditioned by ensuring of high levels of the energy and the degree of non-equilibrity of plasma at the same time. The pulse processes that minimize the risk of uncontrolled arcing and electrode degradation at high power densities are the most advantageous from this point of view. Additionally these conditions create a unique chance for freezing of metastable states of synthesis products on cold substrates, difficult or impossible to achieve by other means. Plasma that meets above-mentioned features I defined as an "active" synthesis environment, because such plasma contains factors that directly determine the possibility of achieving high-energy excitations of primary synthesis products.
This talk will give an overview of research results concerning of use pulse magnetron sputtering method in case of synthesis of different metastable layers material.

Bio: Katarzyna Nowakowska-Langier works as a professor at the National Centre for Nuclear Research in the Department of Materials Physics. Currently she is the head of the Plasma and Ion Technologies division. She graduated of the Faculty of Metallurgy and Materials Science, Częstochowa University of Technology (M.Sc degree) and the Faculty of Materials Science and Engineering of the Warsaw University of Technology (Ph.D and D.Sc. degrees).
The scope of scientific activity of Katarzyny Nowakowskiej-Langier covers research related to materials engineering, the plasma surface engineering in particular. These are issues related to pulsed plasma in the context of its use in the synthesis of materials and coatings, as well as research, including the effects of interaction with the surface of materials, by actively participating in shaping their structure and properties.

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Digital image correlation and machine learning methods for the accurate development of multi-scale models of crystal plasticity

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Any material used for the ITER fusion reactor requires large resistance to extreme irradiation of fast neutrons. Fusion reactions in the tokamak are expected to send up to 1014 neutrons at every square centimetre of the device's walls, every second. Those impacts can cause all kinds of changes in the material compared to the original state, ultimately changing the materials' properties, such as reduction of strength and toughness, development of micro cracks or even rupture. In the very basics of such materials, the key problems that need to be addressed are mainly: i) the "invisibility" of irradiation defects, and ii) the non-destructive, continuous ability to develop structure-property relationships that can be used in multi-scale models that may be used in the future as digital twins. In this presentation, I will show how the combination of machine learning and physics intuition can be used on video imaging sequences of micromechanical testing (tension/bending), in a way that can provide information for multi-scale models of crystal plasticity, addressing the two key problems.

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Ab initio study of cementite – α-Fe interfaces under irradiation

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One of the materials that will be investigated in the IFMIF-DONES facility is EUROFER97, the European reference steel for the First Wall and the Breeding Blanket of DEMO, which is a reduced activation ferritic/martensitic (RAFM) steel. This steel is a Fe alloy containing mainly Cr, C, W, Ta, Mn, and V.
It is well-known that C impurities strongly affect point-defect properties in Fe-based alloys. However, many aspects of the mechanisms through which the C atoms arrange in bcc-Fe lattices are not yet clear. We aim at exploring the configuration adopted by C in the presence of cementite, a common carbide that precipitates in steels. For this, we employ Density Functional Theory (DFT) calculations.
Our current focus lies on the bcc-Fe – Cementite (α/θ) interface. It is crucial to understand the behavior and properties of cementite, since carbides can emit C atoms, interact with radiation defects, or even influence the thermal conductivity of steels, whose stability can be affected by irradiation.

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Detecting Plasticity in Material Mechanical Deformations through Digital Image Correlation and Unsupervised Machine Learning

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Digital image correlation (DIC) stands out as a powerful technique, providing a visual representation of strain maps during mechanical deformation while generating extensive data at every pixel, revealing surface strain components [1]. The true potential within this dataset is unveiled through materials informatics, seamlessly incorporating advanced statistical and machine learning methodologies. However, challenges arise when a comprehensive understanding is lacking, potentially leading to overfitting artifacts and unsuccessful machine learning training. To address this concern, the utilization of unsupervised machine learning techniques, exemplified by principal component analysis (PCA), proves to be insightful in navigating these complexities and can be used extracting valuable information from DIC strain data [2, 3].
In our study, we investigate inferring the mechanical properties of materials solely using local strain information produced by DIC with the use of our developed techniques based on unsupervised ML. As an example, we demonstrate the detection of the transition to the plastic deformation stage and prediction of plasticity localization using experimental DIC data from "creep" and "uniaxial tension" mechanical tests, as well as synthetic data from nano-indentation simulations.

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Sputtering yields by slow light ions with molecular dynamics

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In this talk, I will present results of molecular dynamics simulations of sputtering from W, Fe and Be surfaces by low-energy light ions including hydrogen isotopes, helium and nitrogen. Sputtering by low energy ions, especially at glancing incidence, is poorly modeled by the more efficient binary collision approximation (BCA) methods, yet is of paramount importance in the operation of a tokamak fusion device. At low energies, swift chemical sputtering processes lead to molecular species being sputtered, which results in non-zero sputtering yields below the theoretical threshold for physical sputtering, and also affects how the sputtered species interact with the plasma, hence correctly predicting these processes is crucial. I will discuss the effects of ion impact energy and angle, as well as surface structure and orientation, to highlight the conditions where the more accurate MD methods are preferrable over BCA model predictions.

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Silicon oxycarbide: a novel perspective material for nuclear applications

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Next-generation energy systems require novel materials with enhanced thermal stability, oxidation resistance, and radiation tolerance, specifically in case of nuclear applications. Silicon oxycarbide (SiOC) offers promise as a protective coating for metal components or TRISO-coated particles. SiOC, a two-phase material, consists of an amorphous silica-based matrix with carbon partially substituting oxygen ions and a dispersed graphite-like free carbon phase. This study focuses on developing and characterising SiOC-based coatings for nuclear reactor construction components. SiOC, derived from pyrolysis of silsesquioxanes, is deposited onto AISI 316L austenitic stainless steel. These coatings, with favourable mechanical properties and excellent adhesion, will enhance radiation tolerance

and oxidation resistance. Anticipated results will bridge the gap between fundamental research and industrial implementation in nuclear reactors.

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Fuel Retention Analysis using Laser-Induced Desorption: ex situ and in situ results from JET

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Monitoring the tritium retention of the walls of fusion devices is important due to radiation safety, the fuel cycle and material degradation. Laser-induced desorption (LID) allows to measure the gas inventory of plasma facing components (PFCs) by desorbing the retained gases using a ms long laser pulse to heat a 3 mm diameter spot on the PFC and quantifying them by quadrupole mass spectrometry (QMS). This method was applied ex situ to JET PFCs in the FREDIS device in Jülich where also thermal desorption spectrometry (TDS) was used on samples of the same PFC. A very good quantitative agreement between LID-QMS and TDS was found. Thus, LID-QMS was installed in 2023 on JET as a test run for ITER. The ex situ and in situ setups, working procedures and results are presented here. The in situ diagnostic came into operation during the D plasma campaign before the DT campaign. The detection limit of most of the QMS at JET was sufficiently low to detect the long-term D retention released from a single laser spot along the whole poloidal scan of the upper inner divertor of JET. Then, in the DT campaign, the successful detection of tritium retention at JET has been demonstrated and the tritium reduction after the DT campaign has been monitored. As DT plasmas were only used for 6 weeks this short-term retention was measured by fast repetition of up to 512 laser pulses every 20 ms every 3 mm. This raster mode was thus able to increase the desorbed area and the released gas amount by more than two orders of magnitude and allowed to study short-term retention on a daily basis.

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Analysis of W soft x-ray spectra gathered through the PHA system on the W7-X stellarator

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Soft X-ray Pulse Height Analysis (PHA) system [1,2] is routinely used in various fusion devices, including tokamaks and stellarators such as Wendelstein 7-X, during the experiments [3-6]. The PHA system serves the vital function of providing information regarding the impurity content and core electron temperature (Te) within the plasma environment. Additionally, it enables the estimation of the average effective charge (Zeff) by comparing experimental spectra with theoretical ones [4,5]. However, the interpretation of experimental X-ray spectra in terms of plasma parameters of interest necessitates prior identification and consideration of all relevant factors affecting the spectrum within theoretical radiation models. Therefore, for this purpose, two theoretical models have been applied. RayX code [7], which allows performance simulations for different plasma scenarios characterized by varying the temperature and density profiles as well as the electron cyclotron resonance heating power over a wide range, and Flexible Atomic Code [8], which allows to calculate various

atomic properties such as energy levels, cross sections for excitation and ionization by electron impact, transition probabilities for radiative transitions and autoionization, and any others as needed in the Collisional–Radiative approximation. The spectra recorded during experimental sessions OP1.2b and OP2.1 have been analyzed, striving to achieve agreement between the registered and simulated spectra. This comparison enabled us to ascertain both the effective charge (Zeff) and the level of impurities present in the plasma.

References

[1] M. Kubkowska et al., J. Instrum, 10, P10016, 2015.
[2] N. Krawczyk et al., Fusion Eng. Des, 123, 1006–1010, 2017.
[3] Z. Y. Chen et al., Nucl. Instrum. Methods Phys. Res, A 527, 604–608, 2004.
[4] A. Weller et al., 38th EPS Conference on Plasma Physics, P5.054, 2011.
[5] D. Pasini et al., Rev. Sci. Instrum, 59, 693–699, 1988.
[6] S. Muto et al., Rev. Sci. Instrum, 72, 1206, 2001.
[7] S. Jabłoński et al., J. Instrum, 10, P10021, 2015.
[8] M. F. Gu, Can. J. Phys, 86, 675-689, 2008.

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Study of the Interaction between hydrogen and screw dislocations in alpha-Fe by multiscale simulations

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The ubiquitous hydrogen atom is known to lead to the embrittlement of many metallic materials when present. In bcc Fe, hydrogen atoms penetrate easily and diffuse quickly through the crystal lattice [1], while the lattice solubility is relatively low. Hydrogen atoms interact with most of the other crystalline defects, modifying microstructures, mechanical properties and ultimately leading to embrittlement. In this work, we focus on the interaction between hydrogen and a screw dislocation, that are known to control plastic deformation in bcc Fe in low temperatures regime. The hydrogen effect on the dislocation mobility is still poorly understood and is influenced by many factors like strain rate, stress state, temperature, chemical environment and solutes mobility. Most of existing studies have focused on the interaction of a single straight dislocation with one or few H atoms. Antagonist effects have been observed such as a hardening effect due to hydrogen trapping in the dislocation core. The pinning of the dislocation line hinders the glide [2]. In contrast, a H softening effect may also be observed with a reduction of kink pair formation enthalpy [3,4], that could be due to a reduction of local electronic density promoting double kink nucleation [3,4].

We employed Molecular Dynamic simulations to compute segregation and migration energies of hydrogen solute in the vicinity to the dislocation. H-Fe interaction is described with a recent NNIP potential [5], which reproduces well existing DFT data. We mapped the interaction energy between one or several hydrogens and the dislocation core for various solute concentrations and configurations. When H is inserted inside the dislocation core, a strong binding energy is found and the hard core configuration becomes favored leading to partial or complete core change from the easy core observed when H is distant. The interaction energy rapidly decreases when H is placed away from the dislocation. To characterize the diffusion process close to the dislocation, we calculated migration barrier [6] between the different sites available. These results are compared to predictions from theory of anisotropic elasticity. Next, we assessed the stress driven mobility of a kinked screw dislocation immersed in a hydrogen concentration. For this, we developed a Kinetic Monte Carlo relying on the energety database obtained from MD. The dislocation velocity model and the KMC simulation results will constitute the cornerstone of DDD simulations.

[1] Ferrin, Peter, et al. Surface Science 606.7-8 (2012): 679-689.. [2] Blaschke, Daniel N., and Darby J. Luscher. International Journal of Plasticity 144 (2021): 103030., [3] Itakura, M., et al. Acta Materialia 61.18 (2013): 6857-6867., [4] Wen, M., S. Fukuyama, and K. Yokogawa. Acta Materialia 51.6 (2003): 1767-1773., [5] Meng, Fan-Shun, et al. Physical Review Materials 5.11 (2021): 113606., [6] Henkelman, Graeme, Blas P. Uberuaga, and Hannes Jónsson. The Journal of Chemical Physics 113.22 (2000): 9901-9904.

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Multi-scale simulation of crack propagation in FeNiCr alloy by using T-S law

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In this research, we examine the mechanical properties of FeNiCr alloy, a commonly used stainless steel in nuclear industries, to improve our understanding of its crack propagation under sharp crack conditions. The significance of this investigation is evident in its relevance to nuclear applications [1], highlighting the necessity for a thorough comprehension of its performance. Our analysis commences with molecular dynamics (MD) simulations to explore the alloy's response to uniaxial tensile loading using ternary interatomic potential properties [2]. Subsequent investigations focus on the physical mechanisms that impact crack propagation, aiming to elucidate the complex processes involved. By utilizing the Traction-Separation law as a framework, we assess the elastic, plastic, and damage characteristics of the material during crack propagation, allowing us to approximate its mechanical response at the crack tip.
Furthermore, we employ finite element analysis using the extended finite element method (XFEM) in Abaqus software to assess the material behavior in polycrystalline conditions, thus expanding our investigation to a broader scale. Experimental Electron Backscatter Diffraction (EBSD) results are incorporated to estimate the polycrystalline region in 2D standard compact tension (CT) specimen conditions concerning Voronoi tessellation distribution [3], allowing us to consider real-world conditions in our analysis. Throughout our study, we aim to focus on the influence of grain structure and mechanical properties on crack growth modes, recognizing their significance in shaping material behavior. By integrating these analyses, our goal is to obtain a comprehensive understanding of crack growth behavior in FeNiCr alloy, thereby contributing to the advancement of material design and optimization strategies in nuclear applications especially in irradiated materials. Ultimately, our efforts seek to enhance the safety and reliability of nuclear infrastructure, aligning with broader goals of ensuring the sustainability and resilience of nuclear technologies.

ACKNOWLEDGEMENT: This work is supported by the National Science Centre, Poland through the Grant No. UMO-2020/38/E/ST8/00453

REFERENCES
[1] Nordlund, Kai, et al. "Primary radiation damage: A review of current understanding and models." Journal of Nuclear Materials 512 (2018): 450-479.
[2] Bonny, Giovanni, N. Castin, and D. Terentyev. "Interatomic potential for studying ageing under irradiation in stainless steels: the FeNiCr model alloy." Modelling and Simulation in Materials Science and Engineering 21.8 (2013): 085004.
[3] Xie, Guiqiu, et al. "Grain size dependence of cracking performance in polycrystalline NiTi alloys." Journal of Alloys and Compounds 884 (2021): 161132.