NOMATEN

Centre of Excellence in Multifunctional Materials
for Industrial and Medical Applications

NOMATEN - novel materials

for extreme conditions

Mikko Alava

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NOMATEN: the team

Director Mikko Alava, RGLs Stefanos Papanikolaou, Lukas Kurpaska, MCSA Fellow Aleksandra Baron-Wiechec, Director for Scientific Operations Pawel Sobkowicz, RGL Iwona Jozwik (right), Marek Pruzynski






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NOMATEN: groups

Alava: **Materials' Complexity**, Papanikolaou: **Materials' Structure - Informatics and Function**, Kurpaska: **Functional Properties of Materials**, (Baron-Wiechec: **Corrosion and Electrochemistry**), Jozwik: **Materials' Characterization**, Pruzynski: **Radiopharmaceuticals**

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The mission of NOMATEN

The NOMATEN Centre of Excellence: **a new research organization** in which international world-class research teams design, develop and assess innovative multifunctional materials – combining advanced structural and functional properties – for industrial and medical applications.

NOMATEN develops **partnerships with the industry and research organizations** in order to perform and deploy go-to-market solutions in the field of innovative materials and radiopharmaceuticals. NOMATEN's scientists are supported by the team of experts with an extensive experience in the fields of marketing, communication, human resources and international cooperation.

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Modern research environment

High-Resolution Field Emission Transmission Electron Microscop
System **JEOL JEM–F200** has been installed in July 2023

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Centre for Design and Synthesis of Molecularly Targeted Radiopharmaceuticals (CERAD)

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Understanding behaviour of steels and alloys under irradiation – Combining experimental and multi-scale numerical approach

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Nanoindentation
➢ at rT and HT (up to 650°C)
➢ spherical nanoindentation

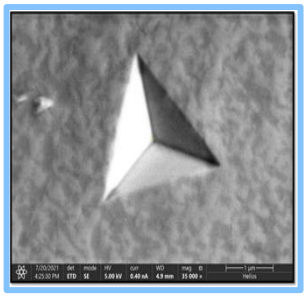
- Hardness and Young's modulus;
- Indentation stress-strain curves → yield stress, work hardening rate and ultimate tensile strength (UTS)
- Pop-ins

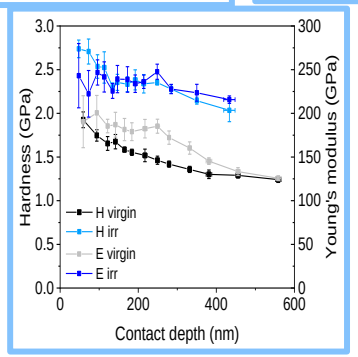
GND's from EBSD maps + simulation (MD,3D-DDD)

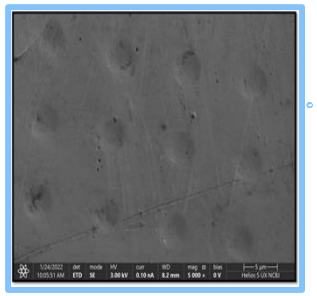
Fig. b and f shows an array of indents made on a grain with a preferential orientation of [101]. More GNDs are visible near the indenter tip and on one side, on the direction {110} slip plane. To better understand the mechanism of the loop formation, MD (fig. c) and DDD (fig. d) was carried out to simulate the indentation process.

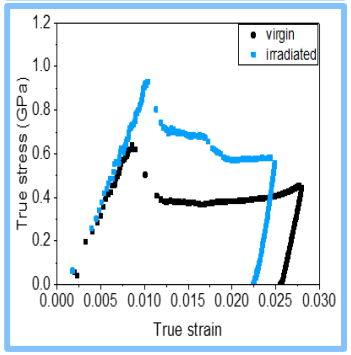
TEM imagines + simulations (MD, 3D-DDD)

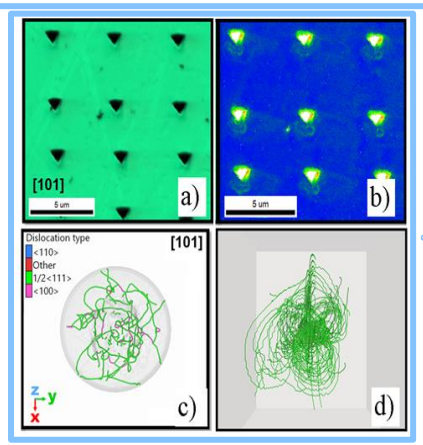
TEM image show the dislocation evolution at different depths. Dislocation lines recorded in the plastically deformed region are pinned on the small dislocation loops created during ion irradiation. These may hinder their movement, which contributes to the hardening effect. Simulation will help us to understand how dislocation are formed during the nanoindentation and how they interact with irradiation defects.

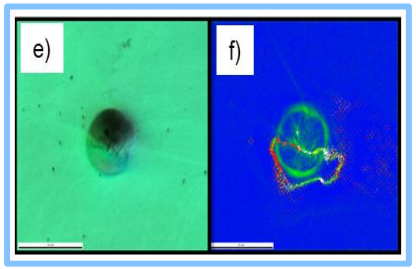


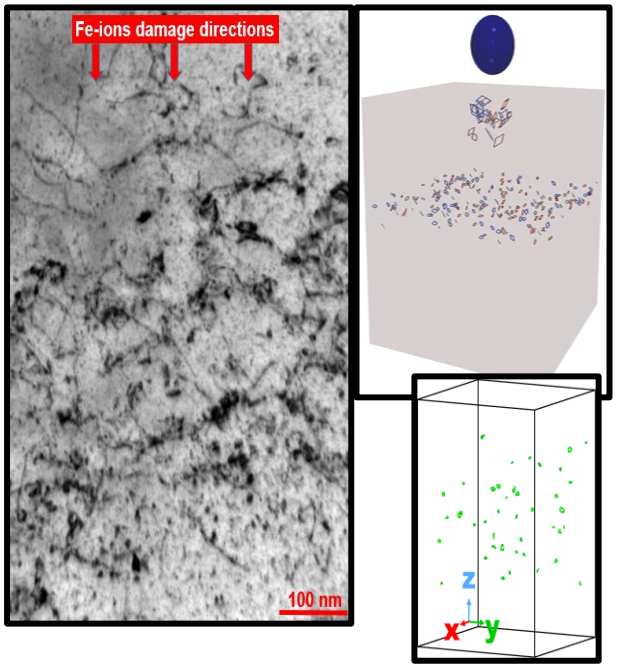












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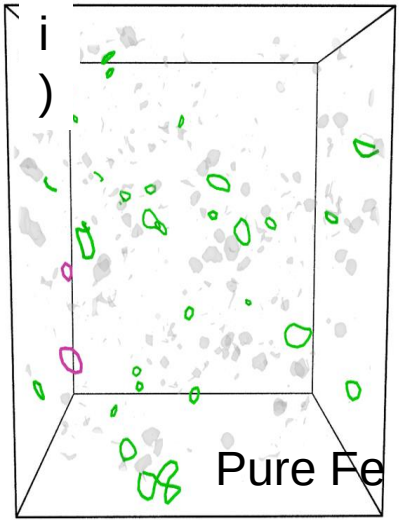
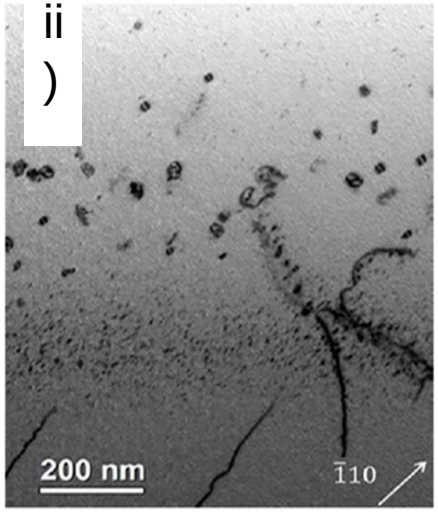
Irradiated Sample preparation

Pristine sample
5 keV PKA
575 K; 5 ps

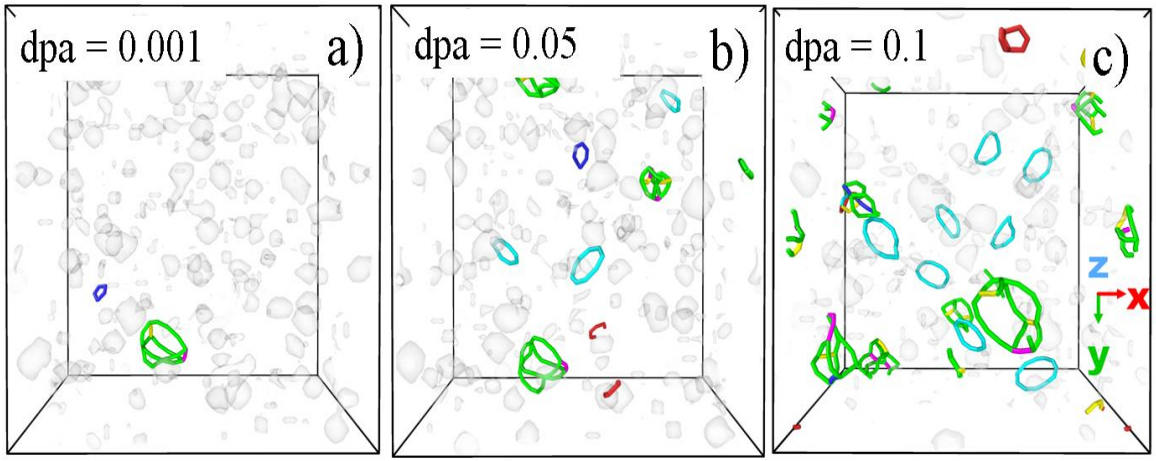
Run cascade simulations

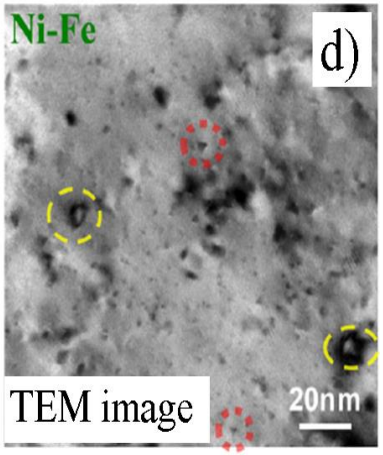
Experimental guidance



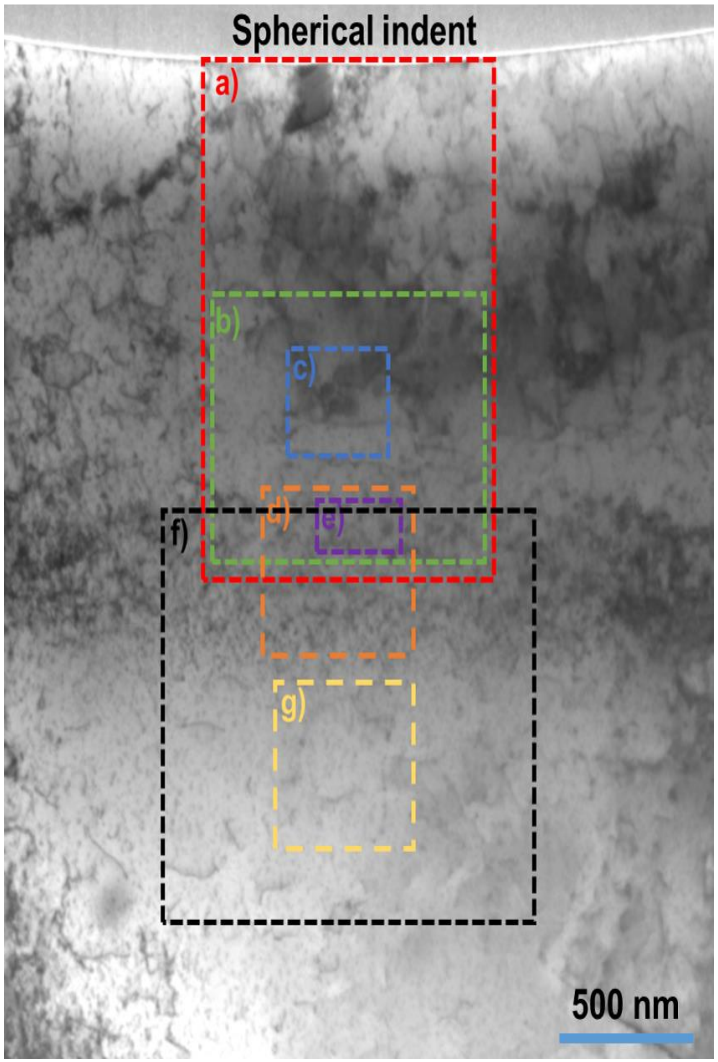


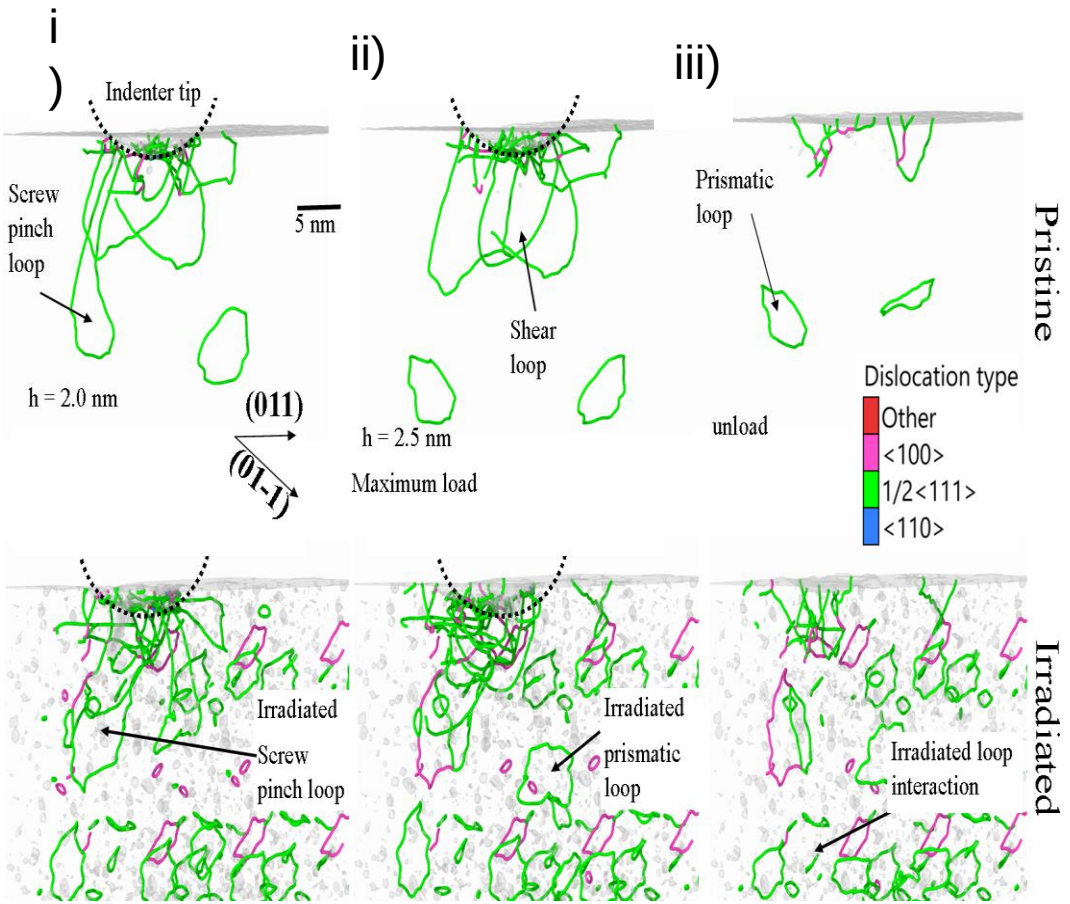
Fluence: 1.5 x 10^{15} ion/cm^2





Nanoindentation of irradiated Fe





K. Mulewska, F. J. Dominguez-Gutierrez et al. Journal of Nuclear Materials (2023)

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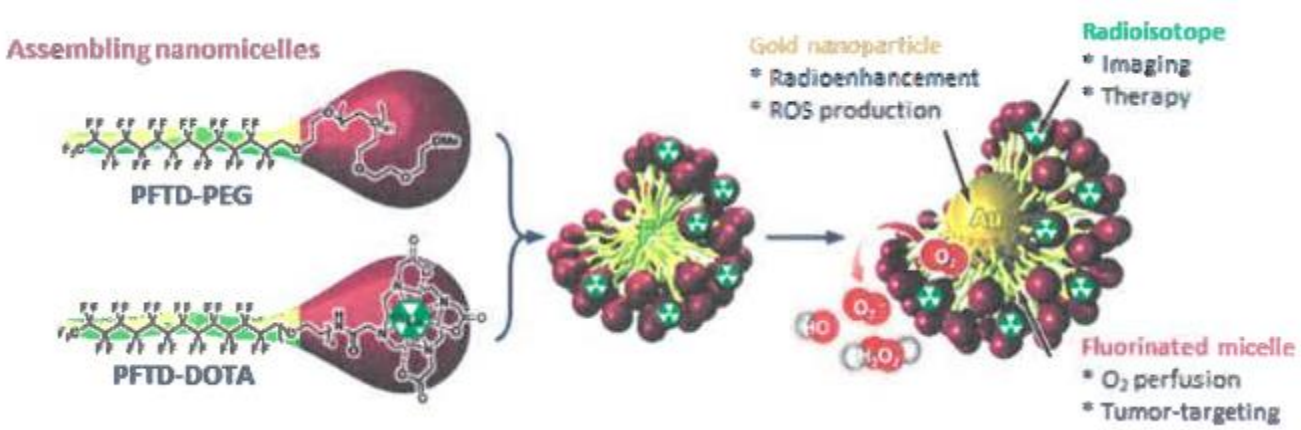
Nanomicelles and theranostics

Nanometric platforms from fluorinated nanomicelles + encapsulated Au nanoparticles + a radioisotope (^{177}Lu here as the target).

NOMATEN – CEA/U. Paris/Saclay co-tutelle collaboration (Ms. Mathilde Poncelle)



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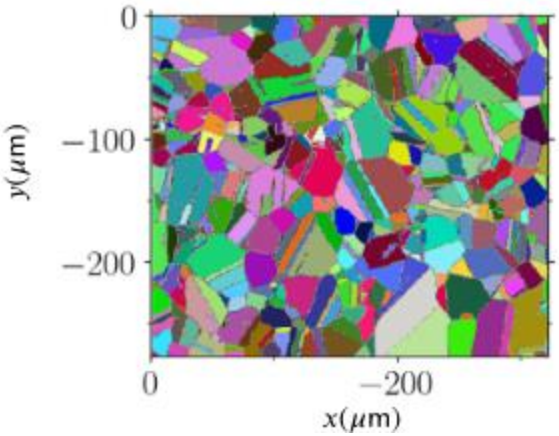
Materials research with Machine Learning

Prediction of steel nanohardness by using graph neural networks on surface polycrystallinity maps

Kamran Karimi [a,*], Henri Salmenjoki [b], Katarzyna Mulewska [a], Lukasz Kurpaska [a], Anna Kosińska [a], Mikko J. Alava [a,b], Stefanos Papanikolaou [a,*]



"Enabler" effect – combine different approaches to tackle a

Scripta Materialia 234 (2023) 115559

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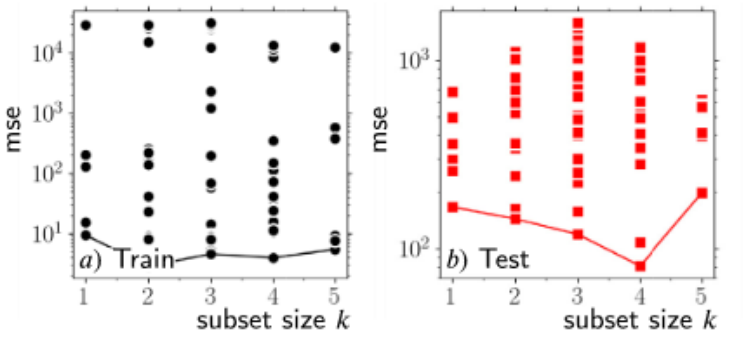
Graph Neural Networks

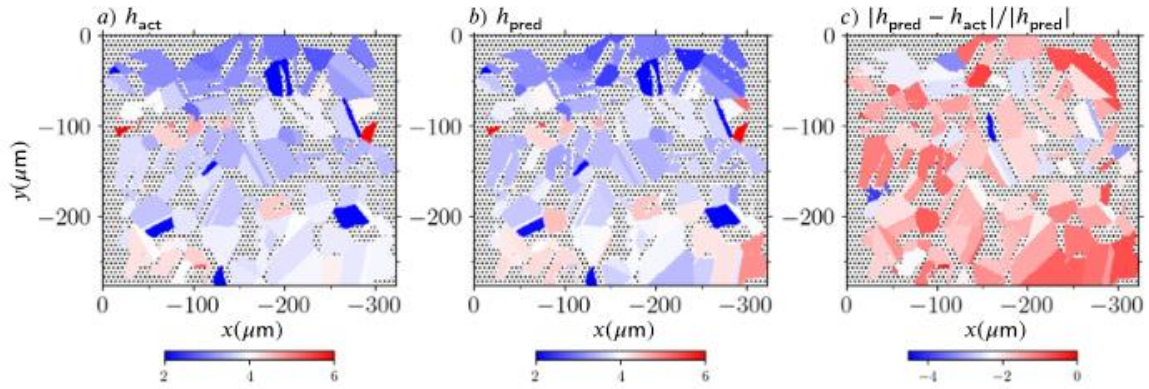


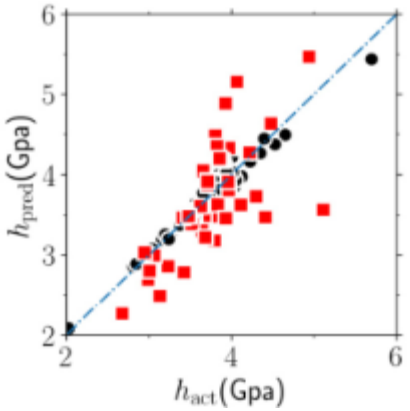
subset size k	1	2	3	4	5
area			†		†
perimeter			†	†	†
diameter	†		†	†	†
equivalentPerimeter		†		†	†
shapeFactor					†
numNeighbors		†		†	

Machine Learning, materials: what is important?

Descriptors!

ML and predictions





Local polycrystalline neighborhood + GNN:

Quantitative predictions – stepping stone to the future!

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Future outlook

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The CoE is now in an active research phase, with close to 50 research staff.

We expect in 2024 to expand this activity with new financial resources, and research openings.

Tight collaboration within the center, with external partners, and with our international contact network.

Exploitation of results (IPR) and industrial collaboration speeding up greatly.

National nuclear programme a huge opening, with strong Euratom participation.

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