European Funds

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FNP Foundation for Polish Science

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Nanoindentation and Defect Behavior in Irradiated FCC NiFe Alloys: Experimental Insights and Atomistic Modeling

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SCAN ME

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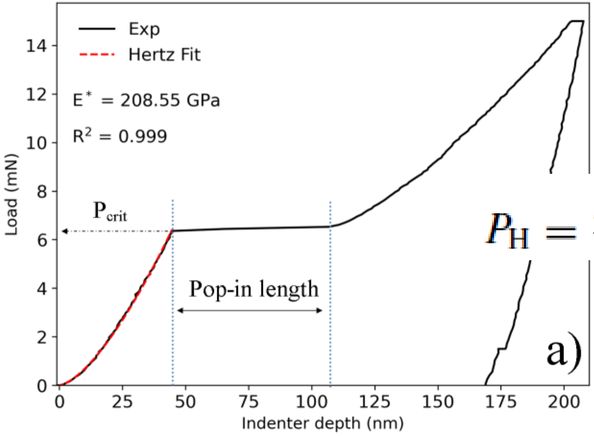
Basics of nanoindentation tests

To measure the elastic modulus and hardness of the material from load-displacement curves.

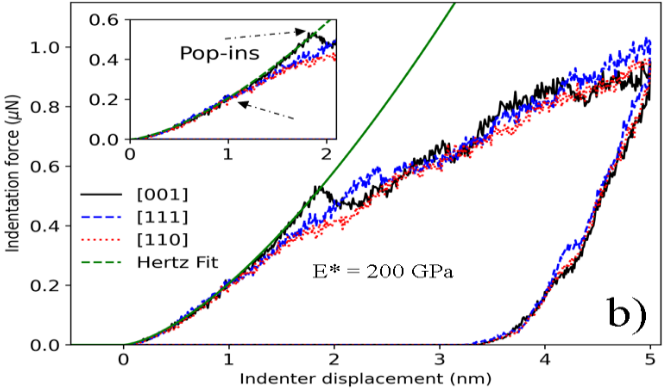
$$\frac{P_{max}}{A}$$

rr method

$$h - h_f)^m$$



$$P_H = \frac{4}{3} E_{eff} R^{1/2} h^{3/2}$$



W. C. Olvier and G. M. Pharr. J. Mater. Res. 19, 1 (2004).

K. Mulewska et al. NIM-B 539, 55 (2023)

K. Mulewska et al. J. Nuclear Materials 586, 154690 (2023)

L. Kurpaska et al. Materials & Design 217, 110639 (2022)

Basics of nanoindentation tests: MD Modeling

Large scale MD simulation for rT nanoindentation of pristine single-element Fe matrix.
Simulations cell are define by **~25 million atoms: 57x56x70nm^3 size.**

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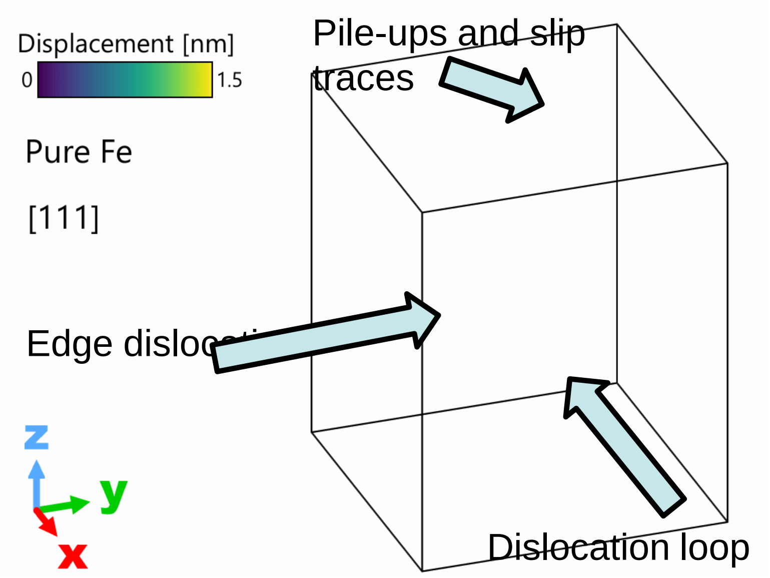
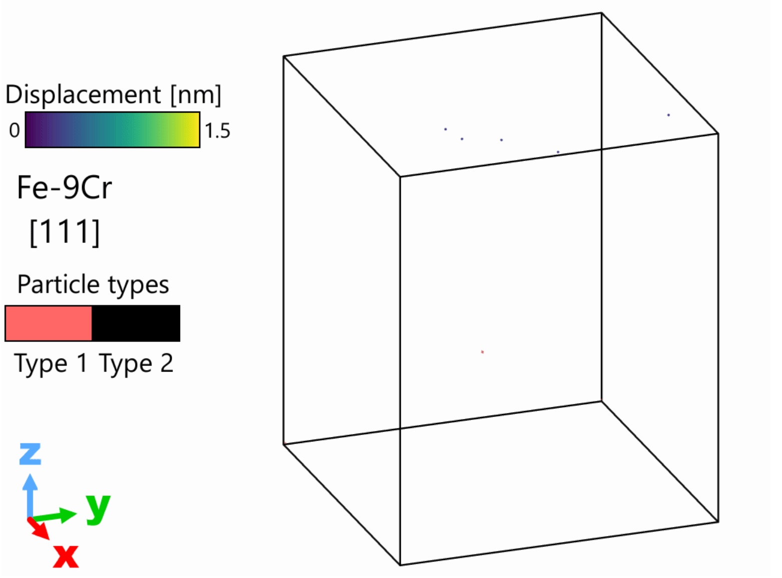
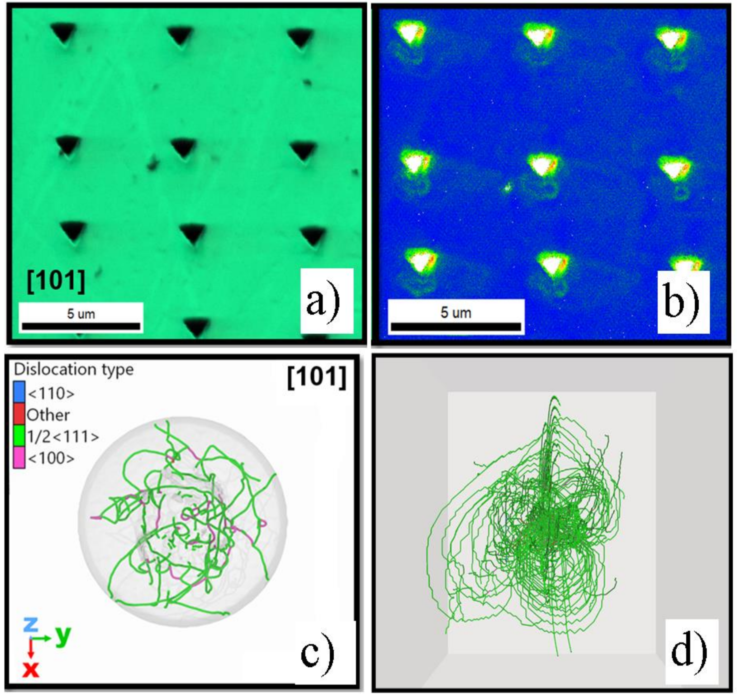
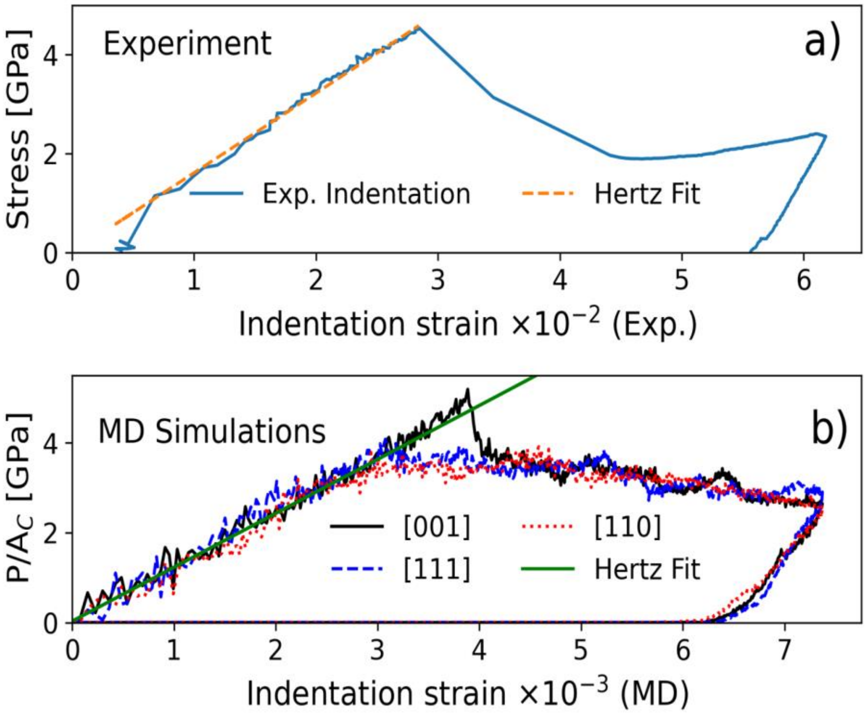




F. J. Dominguez-Gutierrez, S. Papanikolaou et al. *Materials Science & Engineering A 826 ,141912 (2021)*
L Kurpaska, F. J. Dominguez-Gutierrez,Y. Zhang et al. Materials & Design 217, 110639 (2022).
A. Naghdi, F. Pellegrini, F. J. Dominguez Gutierrez et al. Acta Materialia 277, 120200 (2024).

Nanoindentation test: Towards multiscale modeling





GNDs visualization by EBSD images, and MD, and DDD simulations

K. Mulewska et al. NIM-B 539, 55 (2023)
K. Mulewska et al. J. Nuclear Materials 586, 154690 (2023)

Nanoindentation test: Towards multiscale modeling

At this moment, the nanoindentation CPFEM model based on the tensile properties confirmed the realistic prediction of force-displacement curves, hardness, dislocation density evolution, stress & strain distribution patterns, and indentation pile-ups shapes in iron from RT to 500 °C[1].

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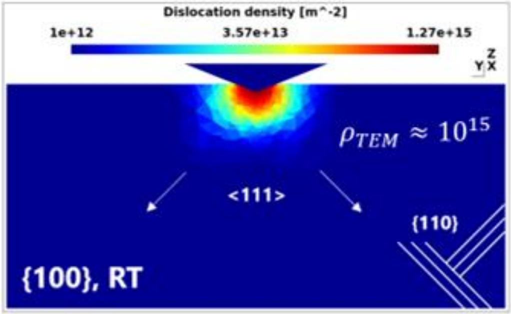
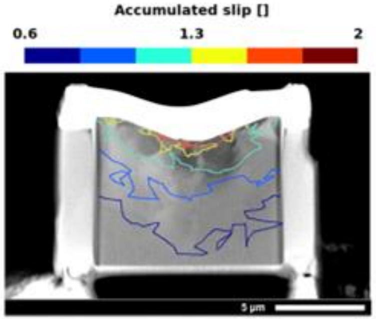
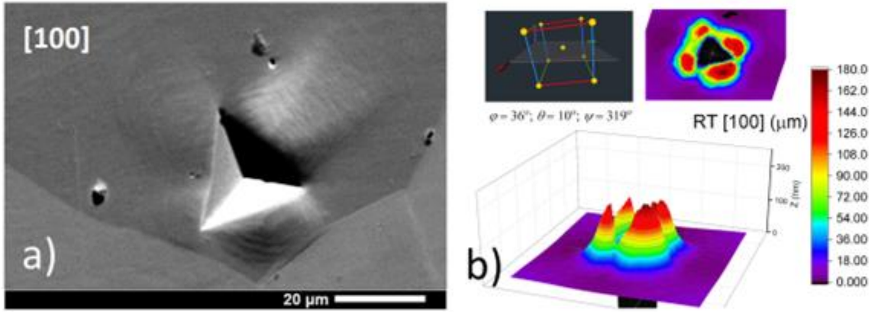


Dislocation density evolution from FEM and measured with TEM.



Acc. slip color map superimposed with sub-surface lamella of the indented zone inspected with SEM.



a) Indent inspected with SEM; b) Indent predicted by FEM.

[1]T. Khvan et al. JNM 567, 153815 (2022)

Dr Tymofii Khvan - NCBJ

Nanoindentation test of self-irradiated BCC Fe

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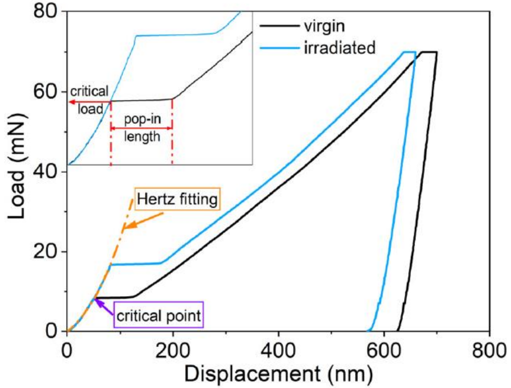

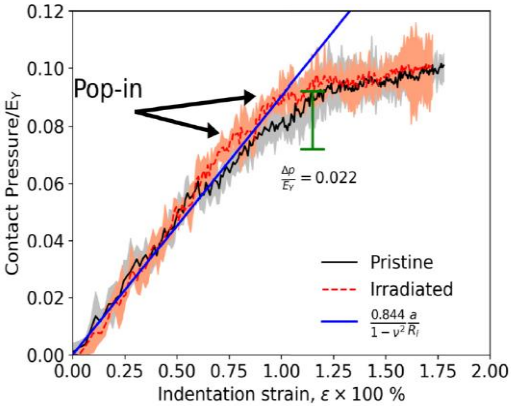

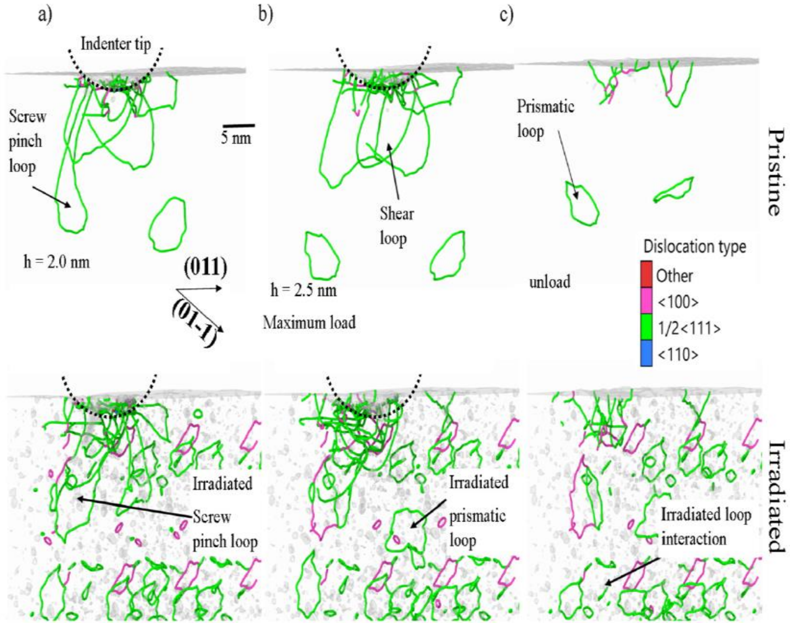

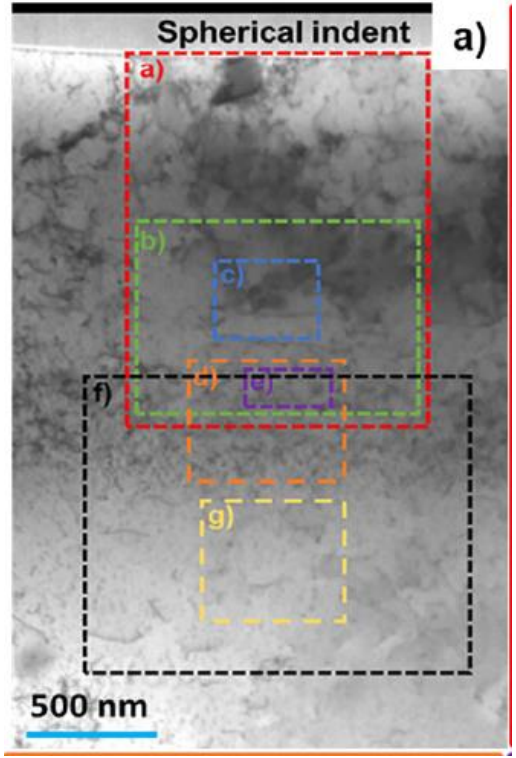

K. Mulewska, F. J. Dominguez-Gutierrez et al. J. Nucl. Materials 586, 154690 (2023)

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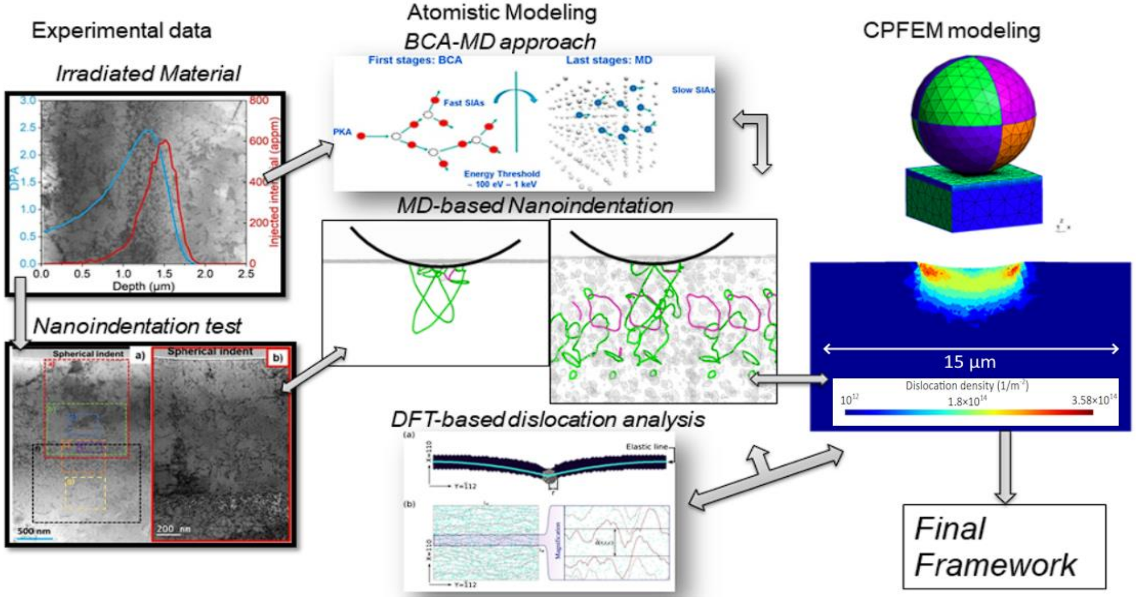
EMIIDNA

CONNECT NM

Coordination of the European Research Community on Nuclear Materials for Energy Innovation

Summary:



An experimentally guided multiscale modeling approach is developed to study irradiation-induced defect formation and its impact on FeCr alloys' mechanical behavior under ion implantation. It integrates BCA-MD, MD, CPFEM, and DFT with nanoindentation, SEM/TEM imaging, and ML-based defect characterization.

RL 2: Advanced materials developing and manufacturing

RL 5: Advanced materials modeling and characterisation

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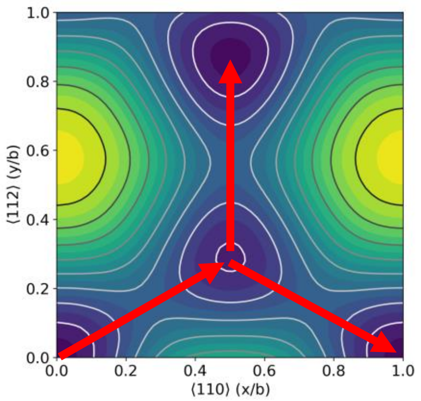
Technical Aspects: What do we need to perform Large scale MD simulation for nanoindentation?



Atomistic modelling, as close as possible to experiments

1. **Interatomic potentials:**
   - Surface information for pile-ups formation
   - Enough information for Stacking fault energies
   - Excellent modeling of elastic to plastic deformation transition
2. **HPC facilities**
   - due to the size of the cell with a minimum of 5 Million atoms (contact area)
   - interatomic potentials are now sophisticated and need long wall time
   - a minimum of 120 processors to run a MD simulation for EAM potentials
3. **Advanced tools to analyze the MD results**
   - Ovito with DXA sometimes miscount defects in the samples
   - Need of several frames to track the formation of defects
   - Quantification of dislocation densities and defects
   - Extracting images of the indented surface for comparison with SEM images

Single phase concentrated solid solution alloys: Ni and NiFe alloys

In collaboration with:
NCBJ

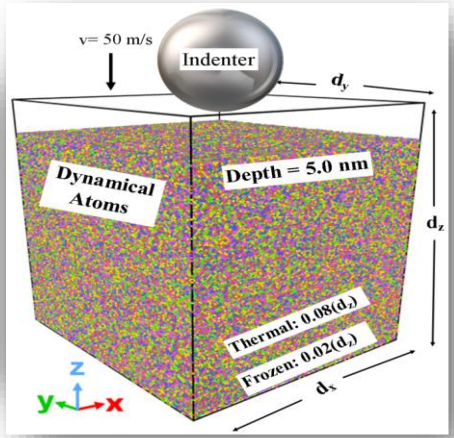
1. **L. Kurpaska**
2. **K. Mulewska**
3. A. Kosinska (SEM)
4. *R. Alvarez-Donado*
5. I. Jozwik
6. W. Chrominski
7. J. Jagielski

In collaboration with US

1. **Y. Zhang**
2. H. Bei
3. W. J. Weber

Samples:
Pure Ni, $Ni_{80}Fe_{20}$, and $Ni_{50}Fe_{50}$
[100] crystal orientation
300 K temperature

$$F(t) = K\left(\vec{r}(t) - R\right)^2$$



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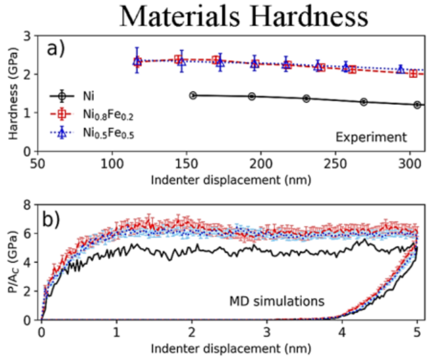
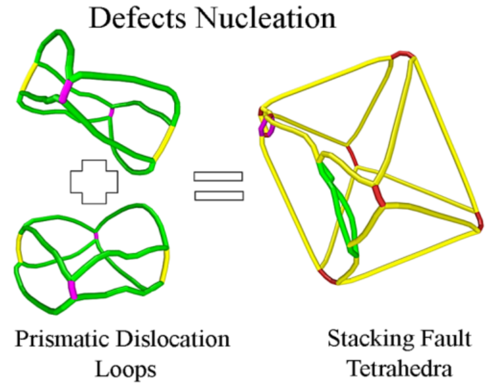
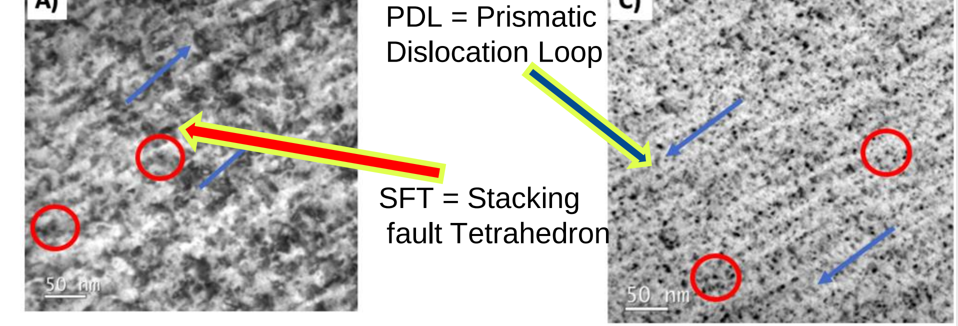




The agreement between experiments and modeling reveals that the nucleation of stacking fault tetrahedra (SFT) is a key factor contributing to the hardening of materials.



L. Kurpaska, F. J. Dominguez-Gutierrez, Y. Zhang et al. Materials & Design 217, 110639 (2022).

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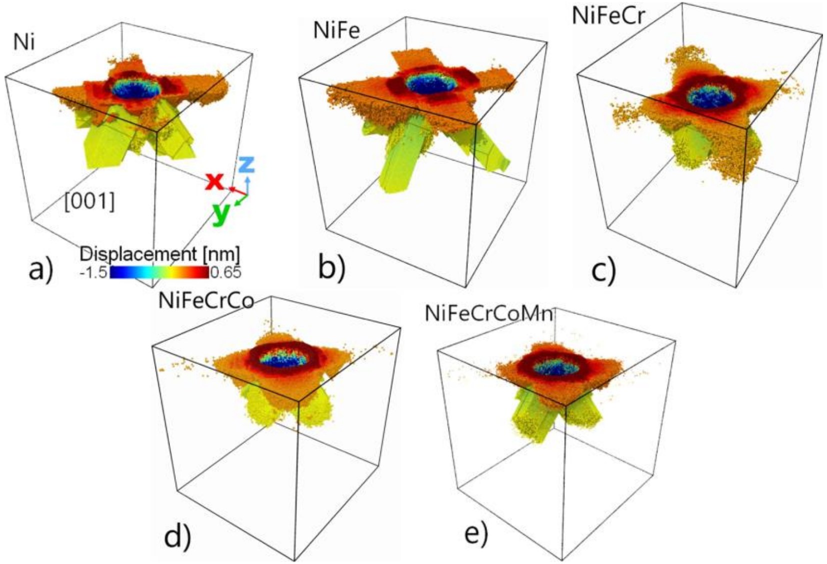
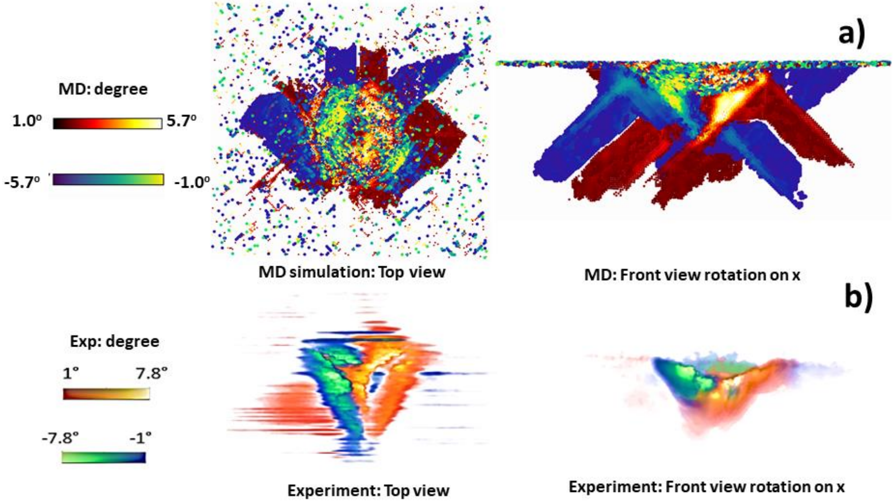
Problem-Solving and Decision-Making: room temperature Nanoindentation

Single phase concentrated solid solution alloys: FCC cantor alloy



Formation of pile-ups and slip traces observed in indented samples varies across different alloys, often accompanied by halo formation attributed to their intricate chemical compositions.



3D-EBSD reconstruction of Cantor Alloy for the grain reference orientation deviation (GROD) angles and MD simulations

M. A. Stróżyk, F. J. Dominguez-Gutierrez et al. under review in Ultramicroscopy (2025)

K. Frydrych, F. J. Dominguez-Gutierrez et al. Mechanics of Materials 181, 104644 (2023).

Nanoindentation simulations of Ni single crystal

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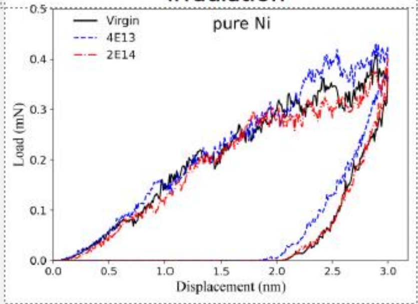
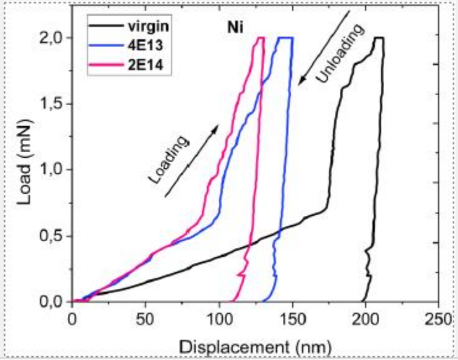
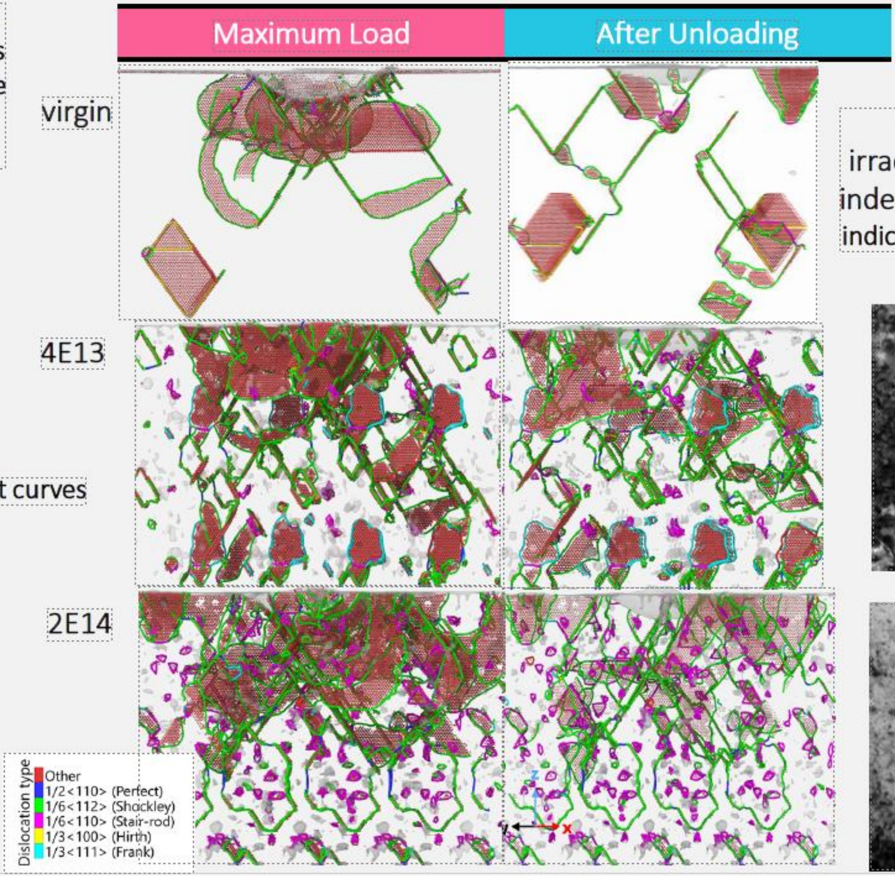
Load-displacement curves obtained by simulations showing that critical load is higher for irradiated material due to the presence of defects nucleated during irradiation



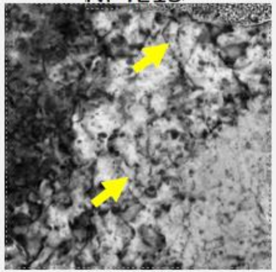
Experimentally-obtained Load-displacement curves



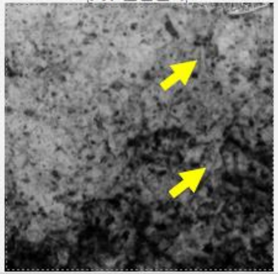


TEM images of irradiated Ni below the indenter tip (yellow arrow indicates dislocation loops)

Ni 4E13



Ni 2E14



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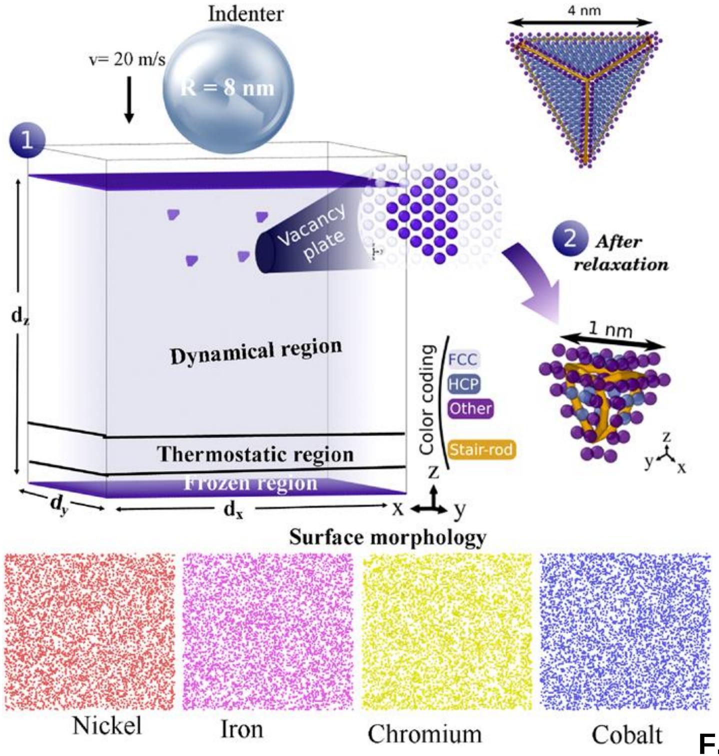
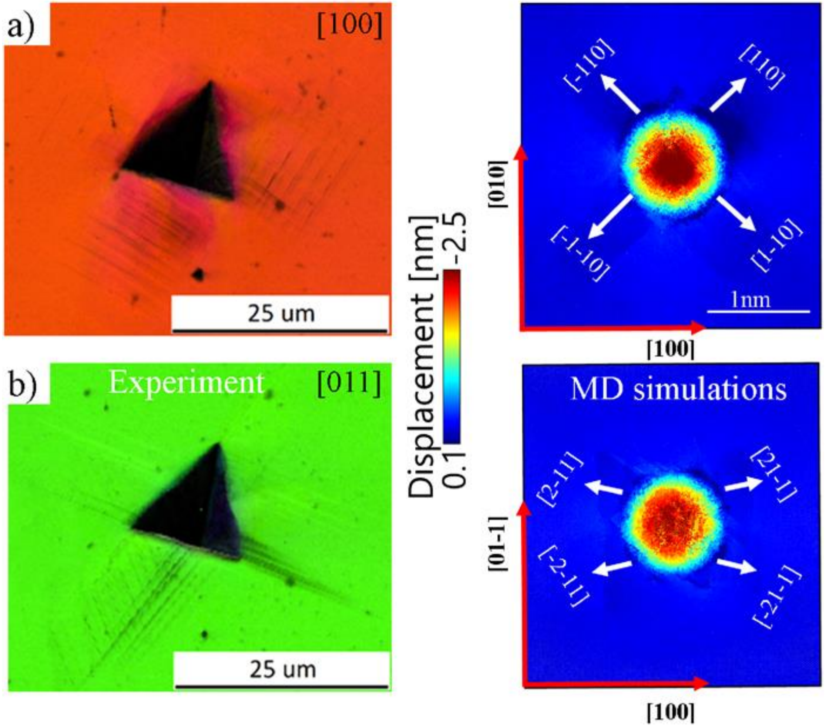
E. Wyszkowska et al. Under review in Nanoscale (2025)
A Aligayev, ML Dos Reis, A Chartier et al.Plasma Physics and Controlled Fusion 67, 055020 (2025).

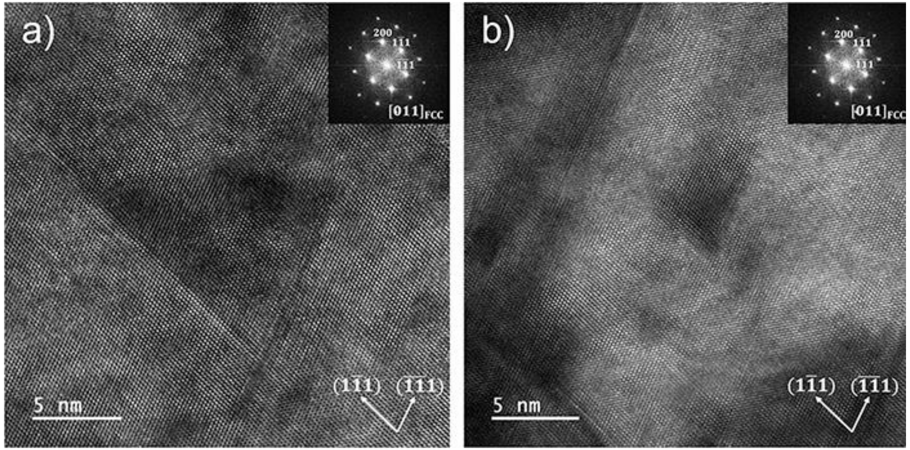
Stacking faults effects on nanomechanical response of NiFeCrCo alloy

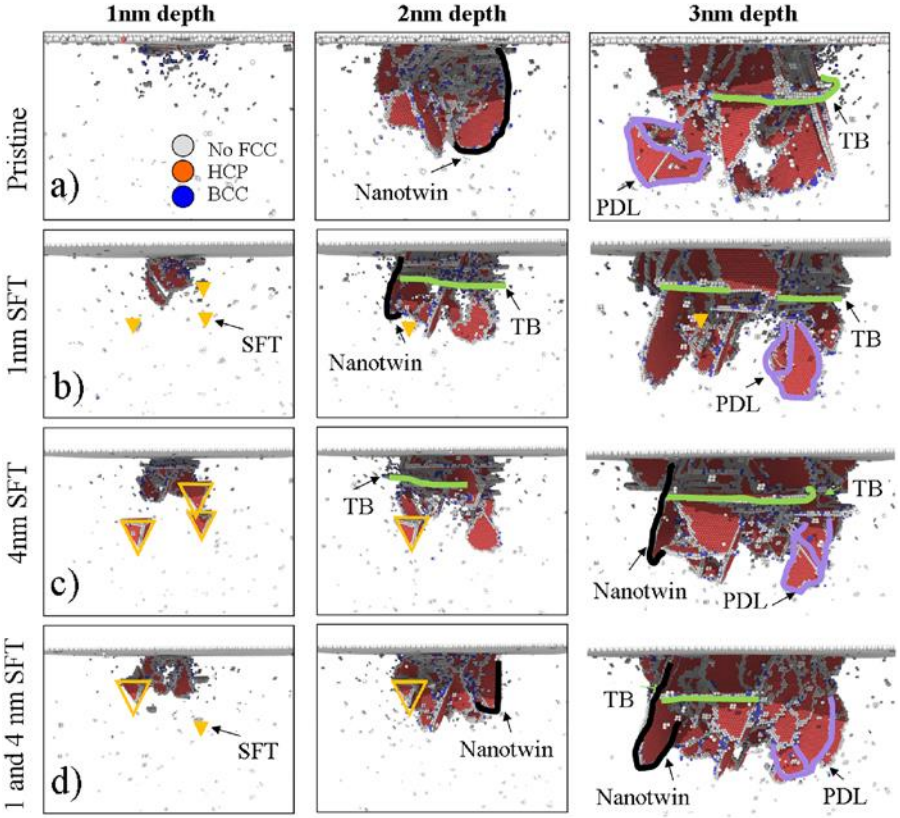




F. J. Dominguez-Gutierrez et al. J. Appl. Phys. 135, 185101 (2024)
A.Naghdi, F. J. Dominguez-Gutierrez et al. Phys. Rev. Lett 132, 116101 (2024).

Stacking faults effects on nanomechanical response of NiFeCrCo alloy



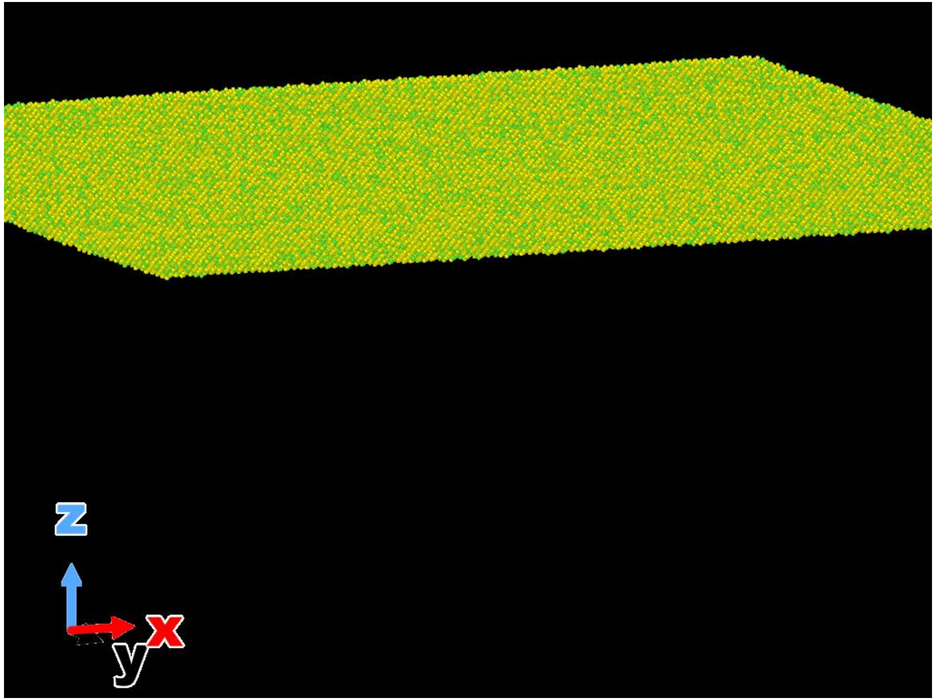


F. J. Dominguez-Gutierrez et al. J. Appl. Phys. 135, 185101 (2024)
A. Ustrzycka, F.J. Dominguez-Gutierrez et al. Int. J. of Plasticity 182, 104118 (2024)

Concluding Remarks

- Nanomechanical tests can be modeled by several interatomic potentials, but dislocation dynamics depends on the approach used showing the need of MD simulations to be as close as possible to experiments.
- Increasing the number of elements in the FCC Ni-based alloy slows down the evolution of dislocations
- **Team work makes the dream work!**

Collaborations:
javier.dominguez@ncbj.gov.pl



55 million atoms for WTa alloy with tailored MLIP, rT nanoindentation. (4-J team)
J. Očenášek, J. Byggmastar, J. Alcala, J. Dominguez. Submitted to Acta Materialia (2025)