Unveiling Surface Chemistry and Hardening Mechanisms in Fusion and Nuclear Materials

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ABSTRACT

- **Nuclear Hardening:** Combining experiments and simulations, this work unravels the mechanisms behind hardening in irradiated and pristine nuclear materials, paving the way for stronger materials.
- **Fusion Coatings:** Surface chemistry and chemical sputtering analysis of Lithium and boron coatings on amorphous carbon under D plasma.
- **Modeling Advancements:** The research highlights the advantages of combining advanced modeling tools with experimental data for a more comprehensive understanding of material properties.

COMPUTATIONAL AND EXPERIMENTAL METHODS

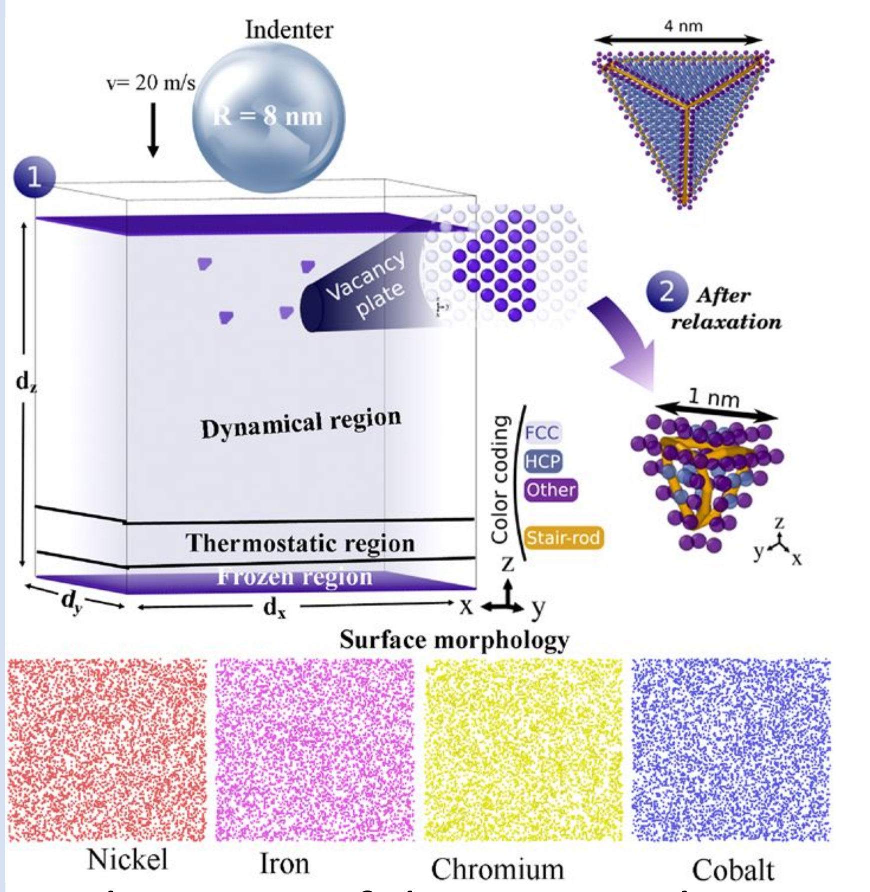
Nanoindentation modeling: Large scale MD simulations are performed with a spherical indenter tip at 25°C for FCC Ni-based alloys and BCC metals with modified interatomic potentials for open boundary simulations.

Experimental Nanoindentation Testing: NanoTest Vantage system was used. Synton-MDP diamond Berkovich indenter (tip radius 50-100 nm) was employed for 150 mN load on 100 indentations spaced 100 µm apart.

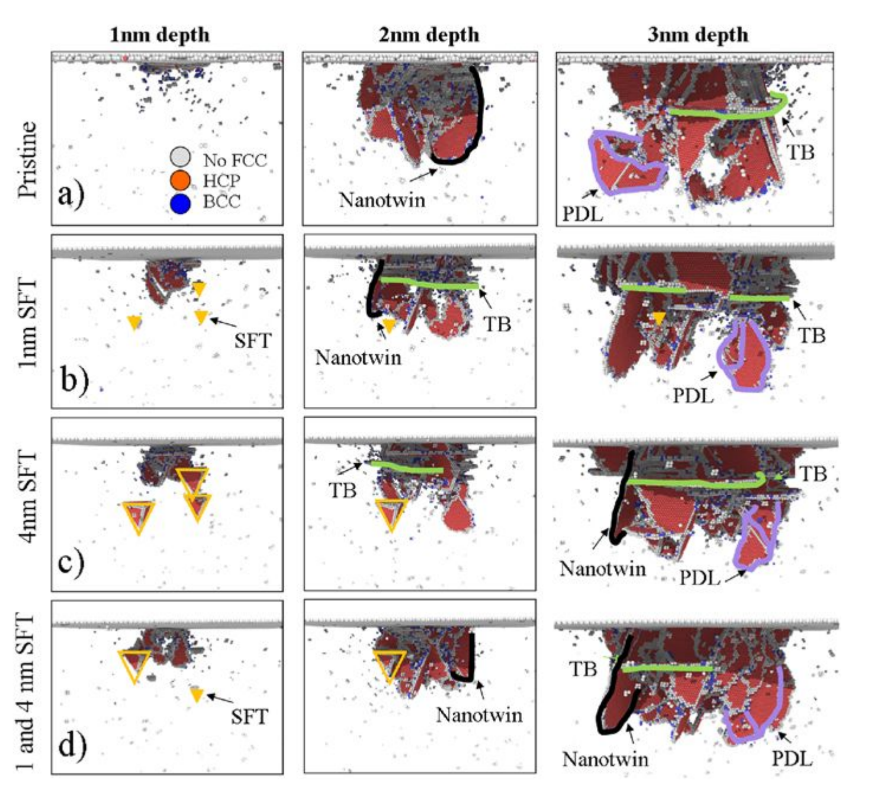
Plasma Surface Interaction: Chemical sputtering of boronized/lithiated and oxidized amorphous carbon surfaces by deuterium impact at 30 eV using CMD with the ReaxFF potentials [1] at 25°C; an initial atomic distributions of 20% O and B, and 60% of C, estimated from the experiments.

Nanoindentation of FCC Ni-based high entropy alloys

Nanoindentation MD simulations are perform to investigate plastic deformation mechanisms of defected NiFeCrM alloys at different crystal orientation. SFT are inserted artificially into the initial sample [1].

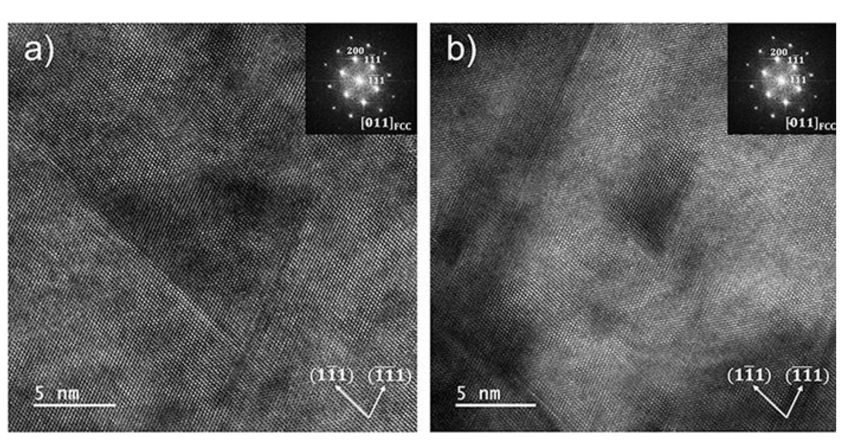


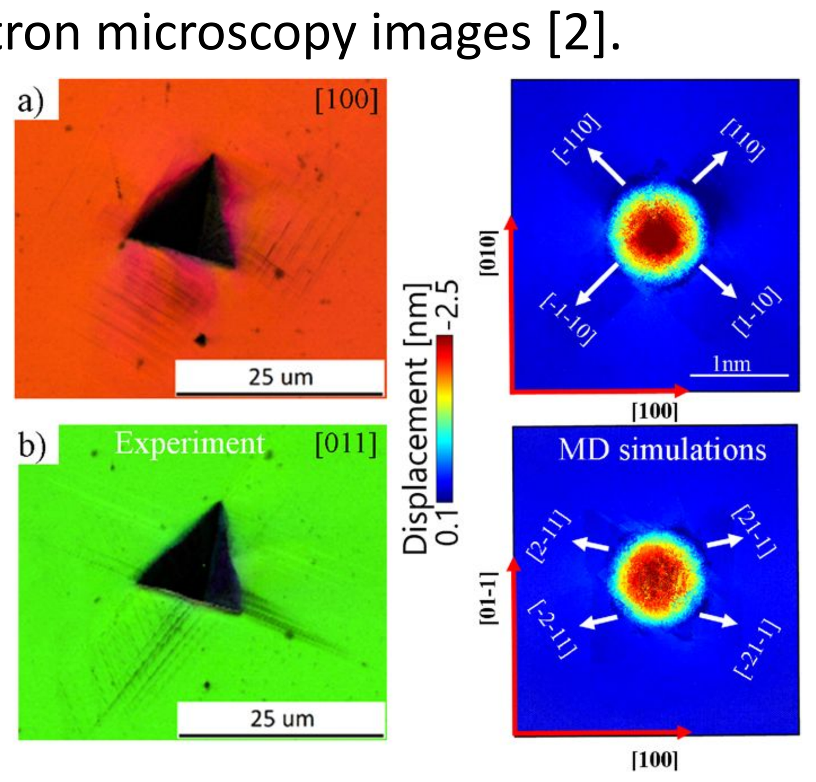
Schematics of the MD simulation



Plastic deformation evolution during loading of [111] NiFeCrM alloy

In the experimental realm, the production and characterization of NiFeCrMn alloy leverage an arc melting technique. Subsequently, nanoindentation tests are conducted, allowing for the acquisition of material characterization through electron microscopy images [2].

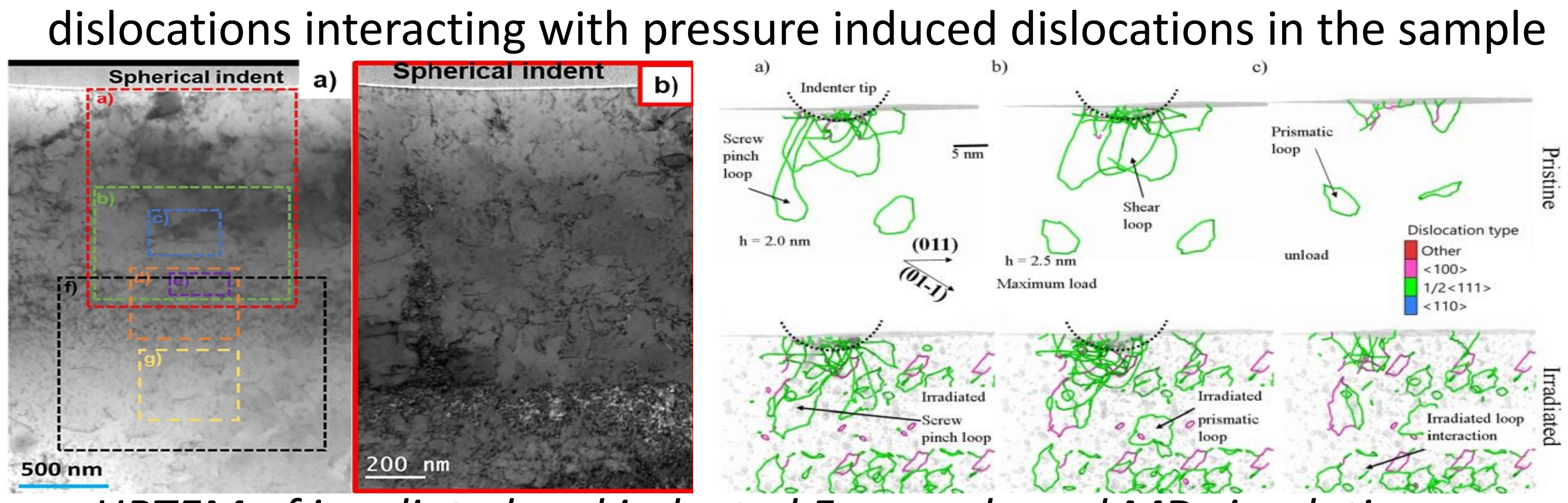




HRTEM of SFT in indented alloy and SEM and MD results comparison of pileups formation.

Nanoindentation of self-irradiated pure Fe

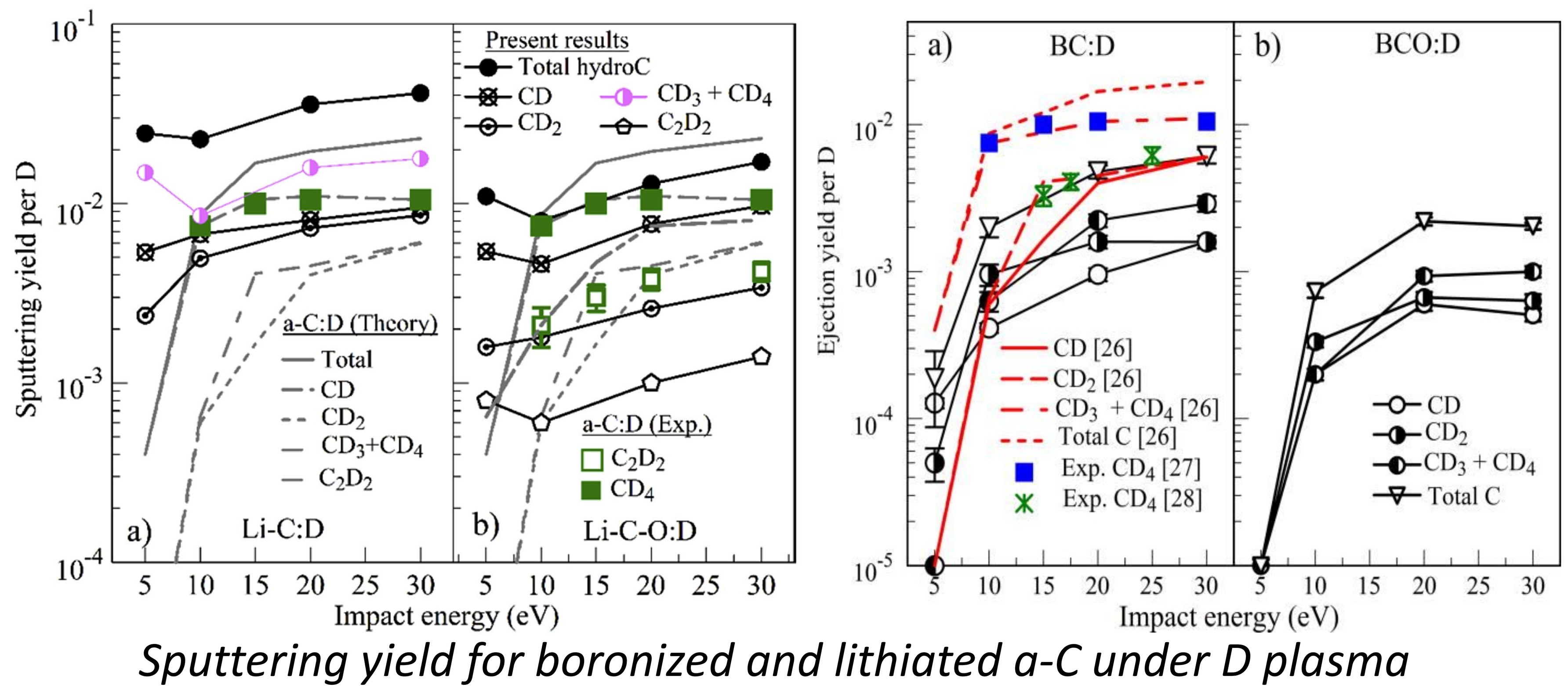
- The self-irradiated samples were prepared through experimental irradiation using Fe^{2+} ions at 5 MeV and 300 ◦C, as well as through MD simulations simulating overlapping collision cascades resulting in a dose of 0.15. displacements per atom (dpa) [3].
- The critical loads and shear stress values required for the transition from elastic to plastic deformation were higher, on average, for the irradiated material compared to the pristine material.
- Dislocation density of irradiated Fe samples decreases after nanoindentation test due to interaction the presence of pre existing dislocations interacting with pressure induced dislocations in the sample



HRTEM of irradiated and indented Fe sample and MD simulations.

Chemical sputtering of coated amorphous carbon surfaces

- Li (of which 60% is in atomic form) contributes almost equally to carbon to the total sputtering at 30 eV, while its contribution at lower energies dominates due to the weak bond of Li to C [4].
- Carbon erosion is suppressed by the boronization of the carbon surface. This effect is further enhanced by the presence of oxygen, with total carbon yields per D, made mainly of CD_3 and CD_2, staying in the range below 0.2%. Ejected oxygen is the dominant physical sputtered.



Sputtering yield for boronized and lithiated a-C under D plasma

CONCLUSION

- A synergistic study, combining experimental and numerical data, has been conducted to characterize nuclear materials for application at extreme operating conditions, where hardening mechanisms can be investigated at nanoscale for further materials design.
- The coupling between fusion material surfaces and the plasmas that interact with them has challenged our understanding of these extreme environments. The interaction of energetic particles drives materials far from equilibrium, resulting in dynamic changes to surface chemistry and physics at the plasma-material interface..

ACKNOWLEDGEMENTS / REFERENCES

[1] F. J. Dominguez-Gutierrez et al. J. Appl. Phys. 135, 185101 (2024); [2] L. Kurpaska et al. Materials & Design 217, 110639 (2022); [3] K. Mulewska et al. J. Nucl. Materials 586, 154690 (2023); [4] F. Javier Domínguez-Gutiérrez et al. Nucl. Fusion 57 086050 (2017).

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