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Computational study of nanoindentation–induced incipient plasticity of lattice defected crystalline Molybdenum: An atomistic dislocation model

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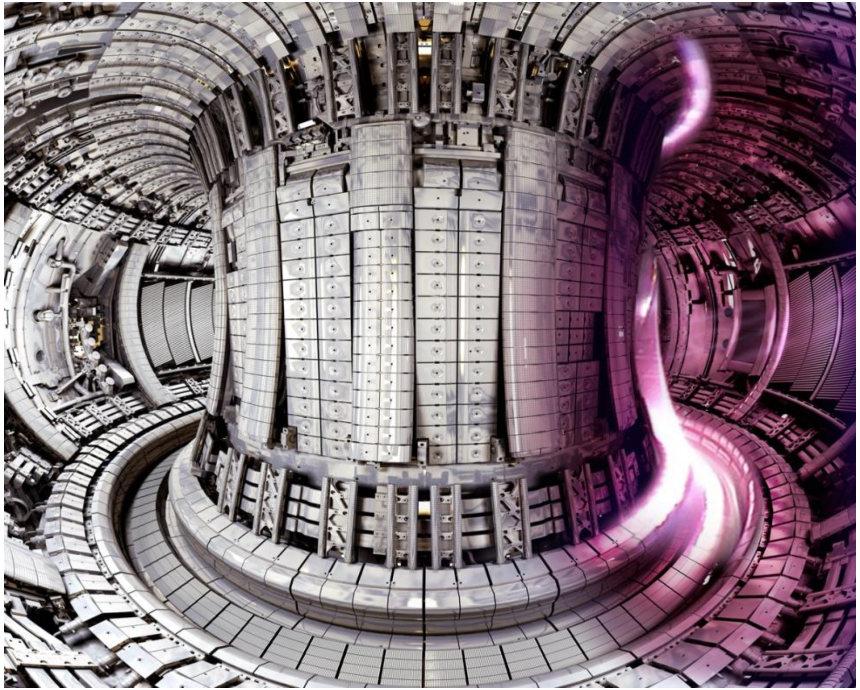
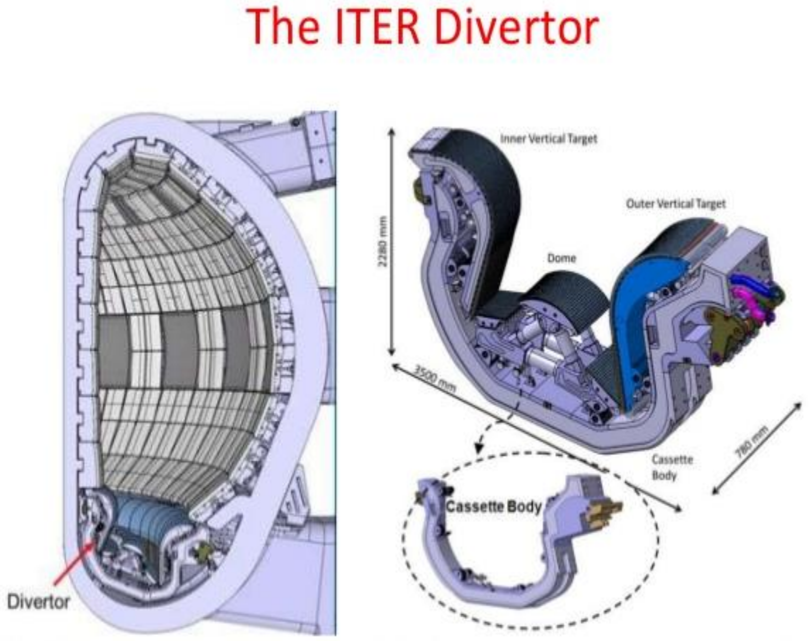
Motivation: Optimal materials for extreme operating conditions





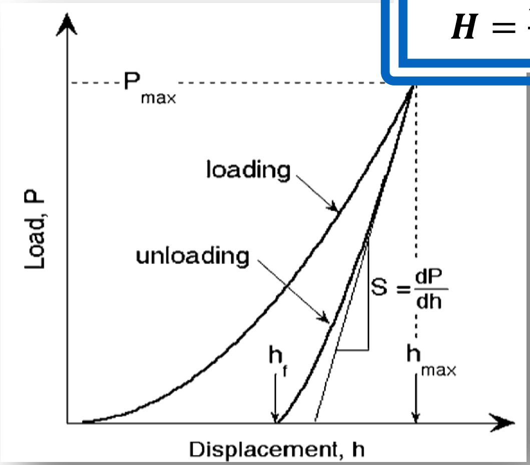
Mo and W

BCC materials for fusion applications

Basic theory of nanoindentation tests

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

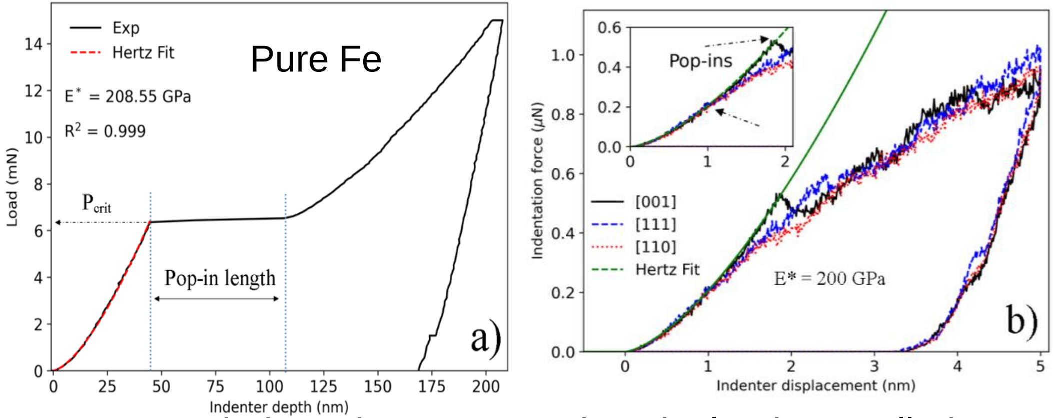
$$H = \frac{P_{max}}{A}$$



Oliver-Pharr method

$$P = P_0 \left(h - h_f\right)^m$$

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



Nanoindentation tests are done by load-controlled mode, with the pop-in occurs as a result of a plastic process taking place, the same load is maintained as the indenter penetrates suddenly into the material

- MD simulations of nanoindentation are performed by the displacement-controlled penetration of the indenter; here the displacement is controlled by the penetration rate.

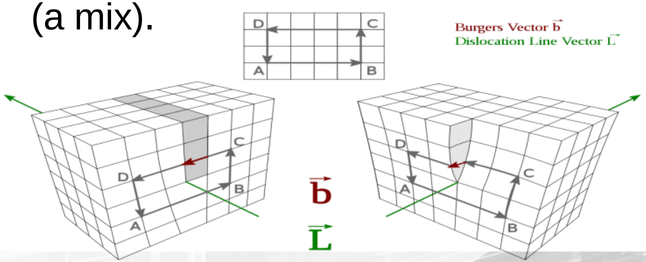
[1] *K. Mulewska, F. J. Dominguez-Gutierrez et al. Under review in J. Nucl. Materials (2020).*

Dislocation theory

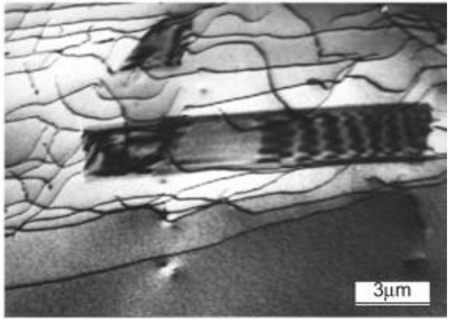
Dislocation introduce defects into the crystalline material which are related to modification of the mechanical properties of the material

Burgers vector is:

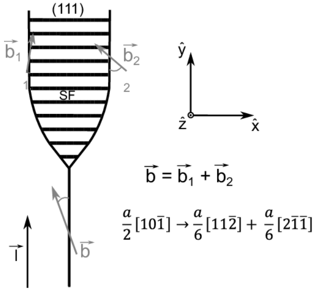
- A crystal vector, specified by Miller indices, that quantifies the difference between the distorted lattice around the dislocation and the perfect lattice.
- the representative characteristic feature of a dislocation, it defines the magnitude and the direction of slip: Edge and Screw (a mix).



Transmission electron microscope (TEM) is the most commonly technique used to visualize and analyze dislocations networks in the material where information of Burgers vectors and density of dislocation is provided.



Dislocation dissociation: it happens when the strength of dislocation is more than unity where the reaction is **b -> b_1+b_2**



Hull, D.; Bacon, D. J. (2001). Introduction to dislocations (4th ed.). Butterworth-Heinemann.

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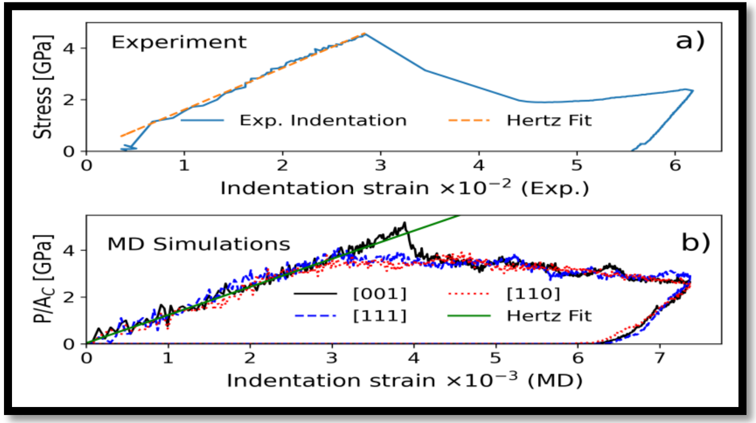
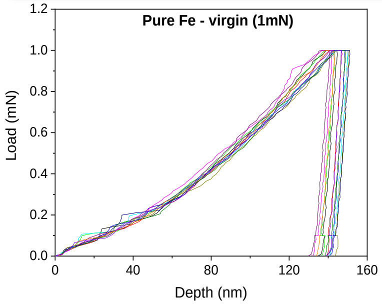
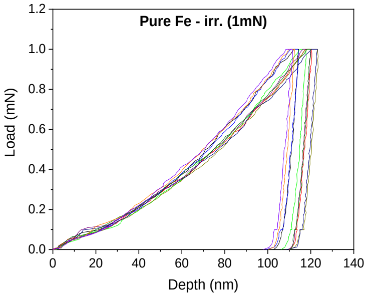
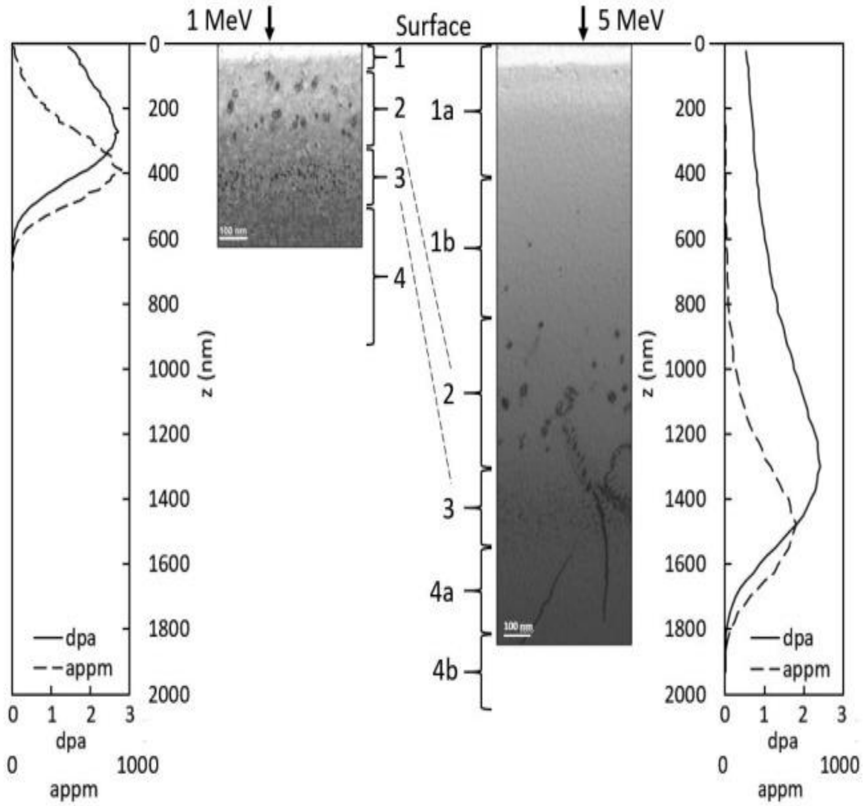
Basic theory of nanoindentation tests: irradiated case

Pristine pure Fe







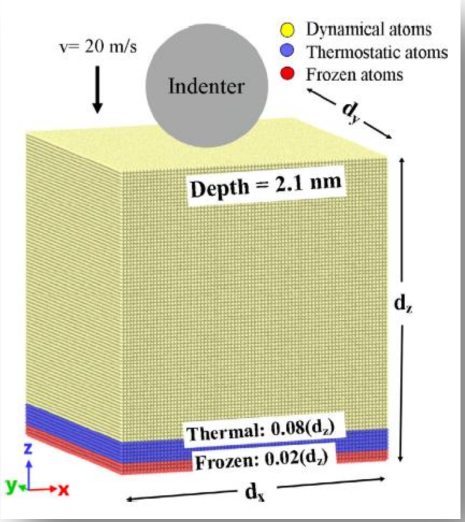


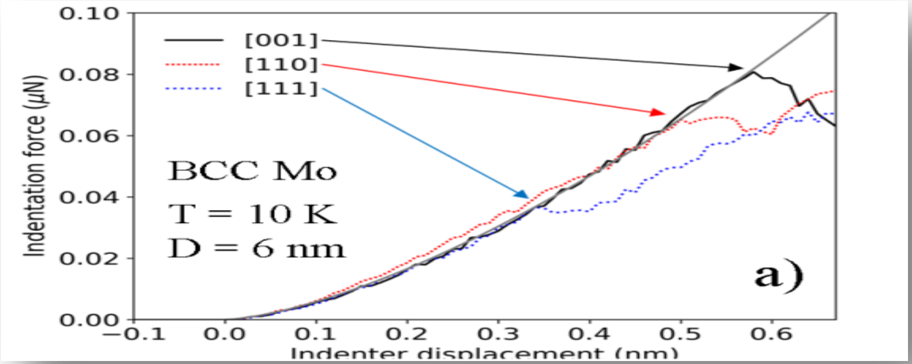
[1] S. Pathak and S. Kalidindi. Materials Science and Engineering R 91, 1-36 (2015)
[2] L. Malerba et al. Nucl. Materials and energy 29, 101051 (2021).
[3] **K. Mulewska et al. Under review to J. Nucl. Materials (2022)**

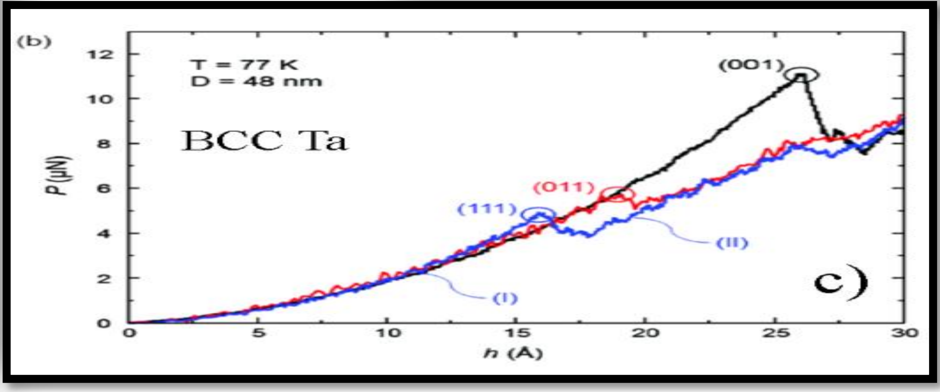
BCC metals: Molybdenum

Numerical simulation setup:

1. LAMMPS code with EAM+ZBL+FS potentials
2. Sample temperature: 10-1000K
3. NVE simulation for nanoindentation test
4. Spherical indenter and a time step = 1 fs







Hertz Fit

$$P = \frac{4}{3} E_{eff} R_{eff}^{1/2} h_e^{3/2}$$

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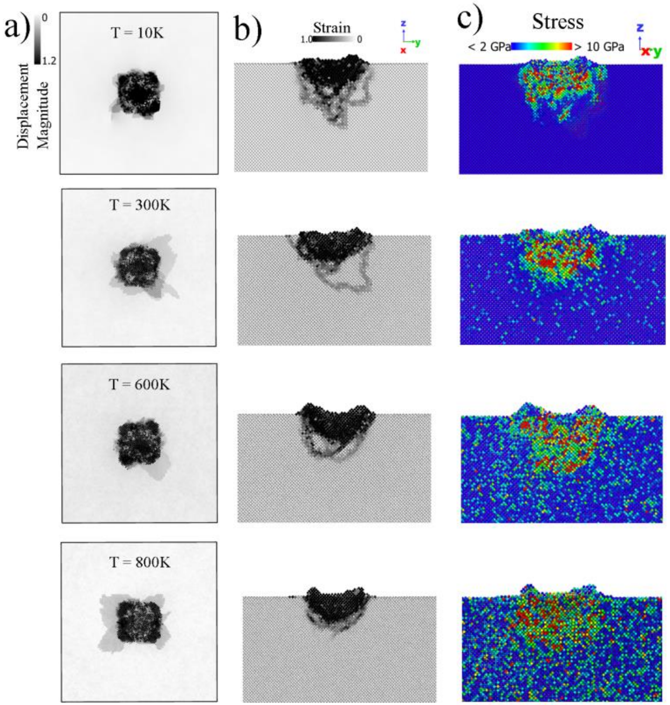
[1] **F. J. Dominguez-Gutierrez, S. Papanikolaou et al.** *Materials Science & Engineering A 826 ,141912 (2021)*

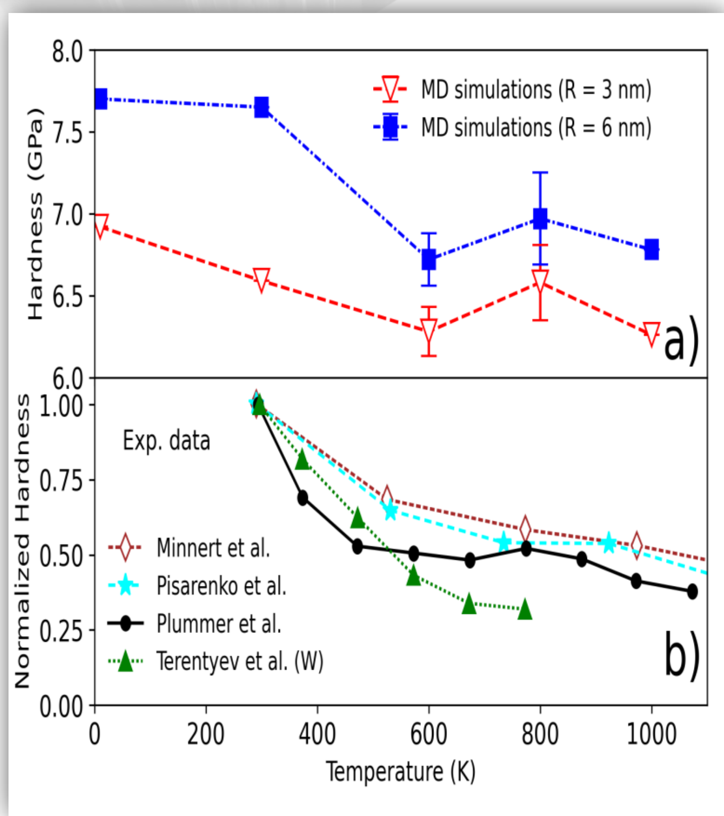
[2] J. Alcala et al Phys. Rev. Lett. 109, 075502 (2012)

BCC metals: Molybdenum



<100> dislocation junctions take responsibility

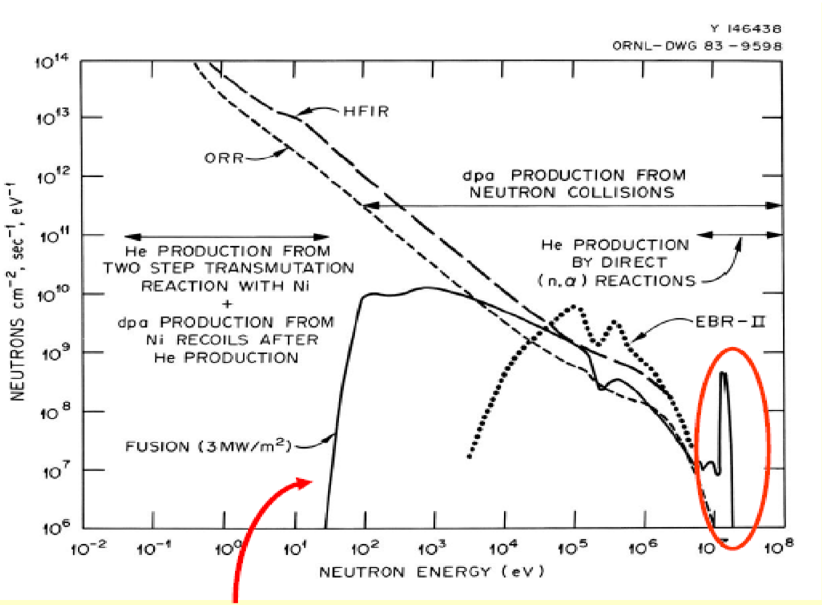
Slip occurs on {110}, {112}, and {123} planes in the <111> directions and a Burgers vector
b = a/2 [111]



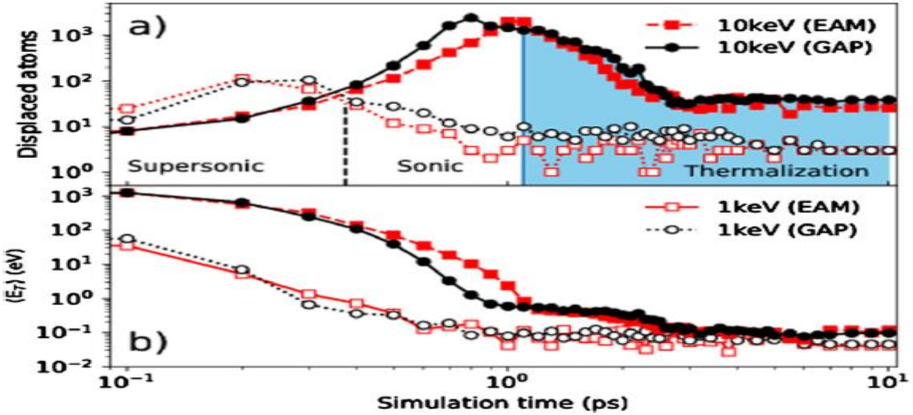
[1] **F. J. Dominguez-Gutierrez, S. Papanikolaou et al.** ***Materials Science & Engineering A 826 ,141912 (2021)***
[2] F. Dominguez-Gutierrez, J. Byggmästar, K. Nordlund et al. Modelling Simul. Mater. Sci. Eng. 29, 055001 (2021)

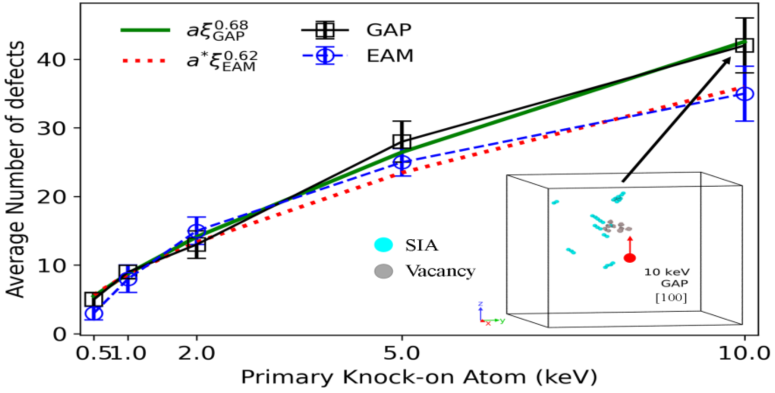
Collision cascades MD simulations

Molybdenum



note: many lower energy neutrons as well

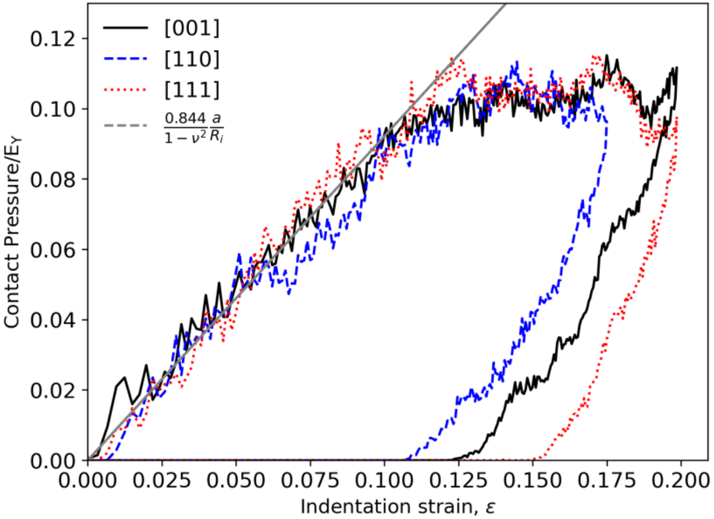


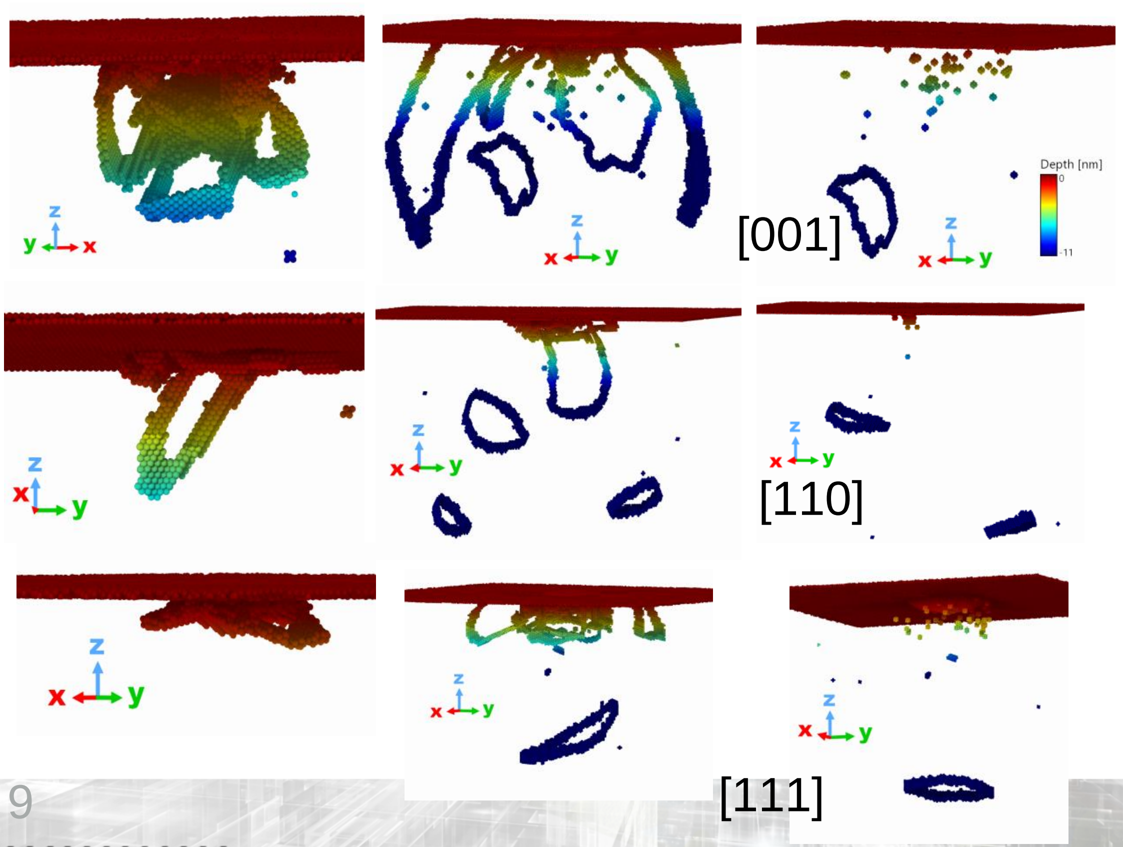


K. Nordlund et al. Nature Comm. 9, 1084 (2018)
W. Eckstein A. Mutzke et al., SDTrimSP: Version 5.00. IPP, Report, (12/8), 2011.
U. Von Toussaint et al. Computer Physics Communications 262, 107816 (2021)
F. J. Dominguez-Gutierrez et al. Modelling Simul. Mater. Sci. Eng. 29, 055001 (2021)

Nanoindentation: pristine sample

~16 million Mo atoms





R=10nm
Depth=3nm

$$\sigma_{IT} = \frac{P}{\pi a^2} \quad \text{and} \quad \epsilon = \frac{4h}{3\pi a}$$

[1] S. Pathak and S. Kalidindi. Materials Sci. and Eng. R 91, 1-36 (2015)

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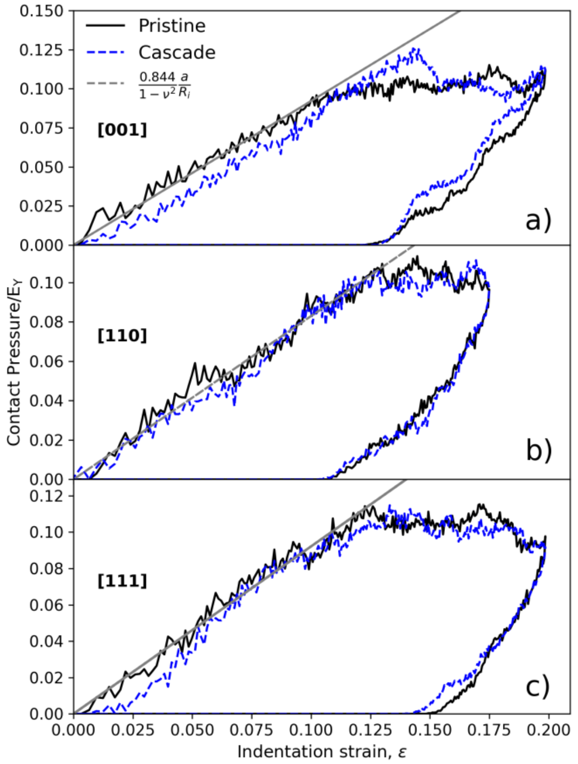
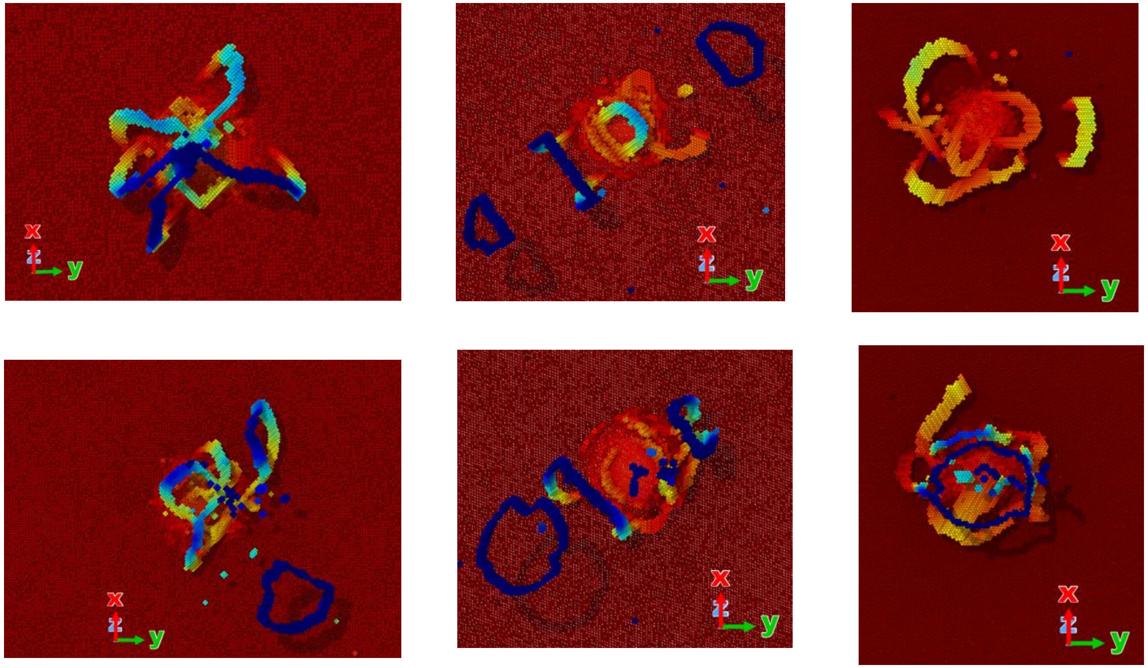
Nanoindentation: distorted sample





[001] [110] [111]

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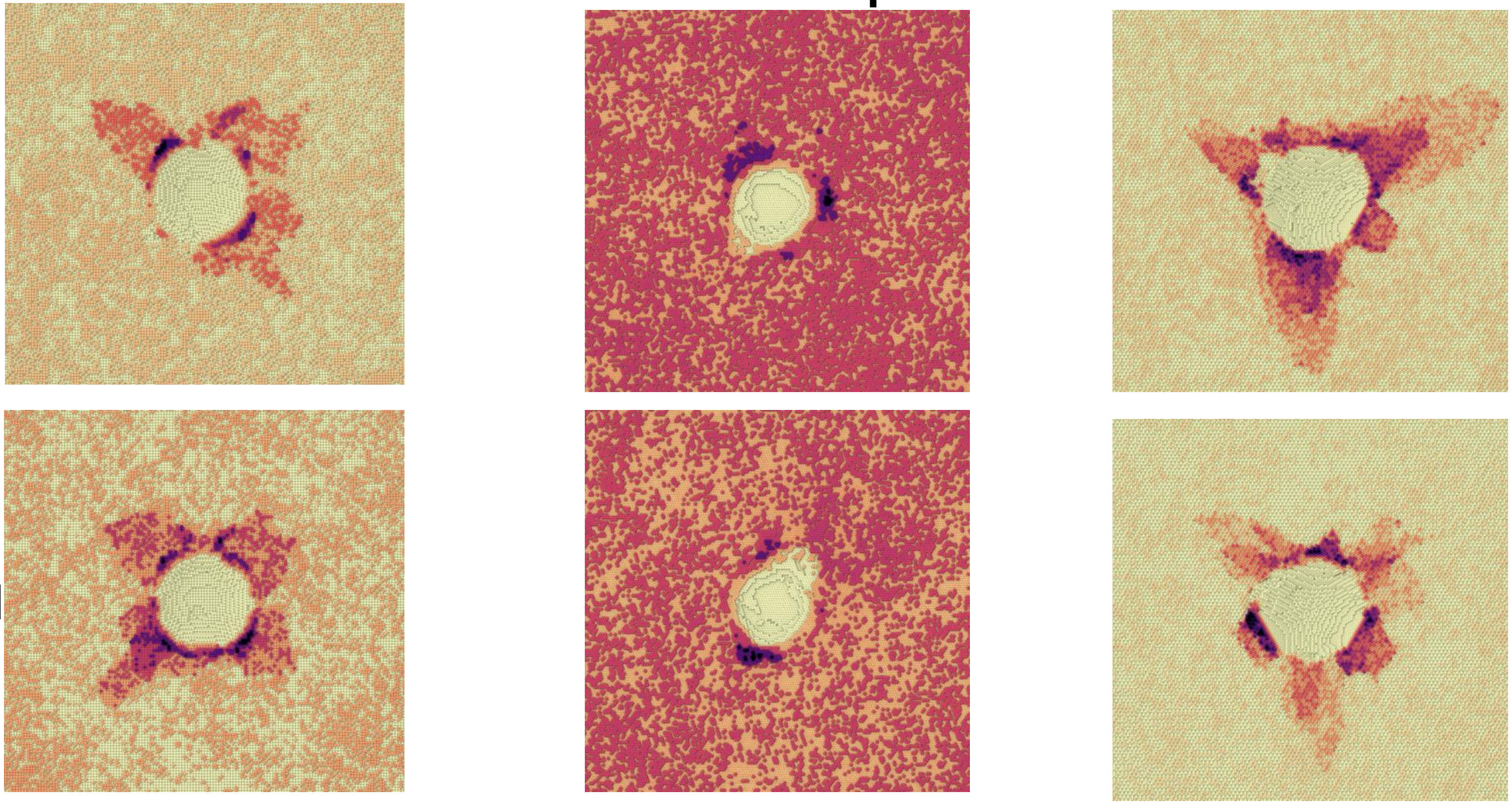
Nanoindentation: distorted sample

Pristine

Irradiated



[001] [110] [111]

Concluding Remarks

- For BCC molybdenum: Dislocation junctions are responsible of the thermo mechanical response of Mo at high temperatures..
- Distorted sample: Further analysis of nanoindentation test data can show changes of dislocation nucleation and dynamics.
- Crystallographic effects are observed in all cases.

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Thank you!

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