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

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Molybdenum is a promising material for designing future nuclear fusion experiments and power plants by considering that its activation can be diminished by isotopic adjustment, which makes it attractive as an alternative material to tungsten for manufacturing fusion devices [1].

However, experimental exploration can be aid by atomistic computational models revealing the mechanisms of damage accumulation in materials; which saves financial resources and exhausting laboratory trials. In this work, large scale Molecular Dynamics (MD) simulations are performed to investigate the crystallographic effects on the mechanisms of nanoindentation–induced plasticity of lattice defected crystalline Mo [2]. We analyze the dynamical deformation processes connected to dislocations nucleation (Fig. 1) and their evolution of a Mo matrix with a low density of lattice defects like interstitials and vacancies [3]; that are obtained by performing few collision cascades at room temperature with open boundaries. In addition, we report the corresponding surface morphology during spherical nanoindentation test and shear stress. Due to the nature of MD simulations considering 20 million atoms and huge computer memory, we utilize the CIŚ High Performance Computing facility in NCBJ, using 128 processors with an average wall time of 36 hours to complete.

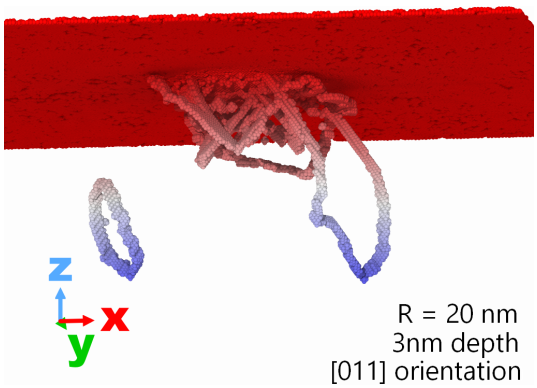

Figure 1: *Visualization of dislocation loop, 'lasso'–like process, and stacking fault planes in [011] Mo during loading at 3 nm depth by using an indenter tip radius of 20 nm.*

References

[1] M.R. Gilbert et al., Nucl. Fusion **60** 106022 (2020)

[2] F. J. Dominguez Gutierrez, S. Papanikolaou et al. Mat. Sci. Eng. A 826, 141912 (2021).

[3] F. J. Dominguez-Gutierrez, J. Byggmastar et al. Modelling Simul. Mater. Sci. Eng. **29** 055001 (2021).