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COMPUTATIONAL ATOMISTIC DISLOCATION PLASTICITY MODELLING OF PRISTINE AND IRRADIATED CRYSTALS

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F.J. DOMINGUEZ-GUTIERREZ[*,†], S. PAPANIKOLAOU[*], P. SOBKOWICZ[*] AND M. ALAVA[*,‡]

[*] NOMATEN Centre of Excellence, National Centre of Nuclear Research
A. Soltana 7, 05-400 Otwock, Swierk, Poland
javier.dominguez@ncbj.gov.pl and http://nomaten.ncbj.gov.pl/
† Institute for Advanced Computational Science, Stony Brook University, Stony Brook, NY 11749, USA
‡ Department of Applied Physics, Aalto University, P.O. Box 11000, 00076 Aalto, Espoo, Finland

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ABSTRACT

The development of new technologies for efficient energy production requires novel materials that have favorable thermo-mechanical properties and numerous industrial applications in extreme environments [1]. For example, in the nuclear fusion technology it is of utmost importance to study materials that can operate in high-radiation environments at high temperatures to find homogeneous and stable materials with improved radiation tolerance [1,2]. Therefore, a combination of experimental and modeling efforts can reveal the mechanisms of damage accumulation under prolonged irradiation in materials.

In this symposium, we discuss the study and characterization of mechanical properties of a BCC metal: Molybdenum (Mo), which is considered as an excellent candidate for designing next generation nuclear machines due to its outperform at high temperatures. Computational modelling of mechanical nanoindentation responses of pristine and irradiated single-crystalline Mo will be presented to analyze the related radiation induced microscopic dislocation defect behaviors. Atomistic simulations to prepare irradiated samples at dose range of 0.01 to 0.5 dpa (displacement per atom). Finally, we show that results point towards both qualitative and quantitative differences in the response of pristine and irradiated samples, that can be tracked by the material hardness, and dislocation nucleation images that can be compared to TEM and SEM observations of experimental nanoindentation tests.

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