Classical molecular dynamics simulations of hypervelocity nanoparticle impacts on tungsten

P. Dwivedi¹, A. Fraile², G. Bonny³, T. Polcar¹

 ¹Department of Control Engineering, Faculty of Electrical Engineering, Czech Technical University in Prague, Karlovo náměstí 13, 121 35, Czech Republic
²Nuclear Futures Institute, Bangor University, Gwynedd, LL57 2DG, United Kingdom
³Nuclear Materials Science Institute, SCK CEN, Boeretang 200, B-2400 Mol, Belgium

The presence of dust in the scrape-off layer (SOL) close to the chamber walls is an important issue for the development of fusion reactors [1,2]. Hypervelocity dust particles can be particularly harmful if they collide with tokamak material surfaces. Therefore, controlling plasma-wall interactions is critical to achieve high performance in present day tokamaks. Tungsten (W) is the main candidate as plasma facing components for fusion reactor and will be exclusively used in the ITER divertor [1]. The presence of high velocity impacts has been reported in several studies, with velocities being around 500 m/s to a few km/s [3,4].



Fig. 1 High velocity impact (5 km/s) of a 40 nm-size W cluster on a W single crystal target, at times 5, 20 and 100 ps. Top row: Color code: Structural analysis. Bottom row: Same system, Blue surface indicate the sputtered atoms and Green curves corresponds to dislocations forest in the target.

In this work, the atomistic mechanisms of damage initiation during high velocity (v up to 9 km/s) impact of W projectiles on W has been investigated using moleculardynamics simulations involving very large samples (up to 40 million atoms). Various aspects of the impact at high velocities where the projectile and part of the target undergo plastic materials massive deformation. breakup, melting. or vaporization are analyzed. Different stages of the penetration process are identified. Whether the damage occurring in the subsurface of the target is described by collision cascades or as the effect of shock waves will be discussed.

References:

- [1] Federici G. et al 2001 Nucl. Fusion 41 1967.
- [2] Tsytovich V.N. and Winter J. 1998 Phys.-Usp. 41 815.
- [3] Castaldo C, et al. 2007 Nucl. Fusion 47 L5-L9.
- [4] Ratynskaia S, , et al. 2008 Nucl. Fusion 48 015006.