Hypervelocity impacts; W on W using Molecular Dynamics

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Abstract

In this work, the atomistic mechanisms of damage initiation during high velocity (v up to 9 km/s) impact of Tungsten (W) projectiles on W has been investigated using molecular-dynamics (MD) 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 materials undergo massive plastic 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 [1, 2].

Introduction

Plasma-material interactions are a key issue in the realization of practical fusion power reactors, which is recognized since the beginning of magnetic fusion research [3]. Controlling plasma-wall interactions is critical to achieving high performance in present day tokamaks. W is the main candidate as plasma facing components for a fusion reactor and will be exclusively used in the ITER divertor [3]. The presence of high velocity impacts has been reported in several studies, with velocities being around 500 m/s to a few km/s [4].

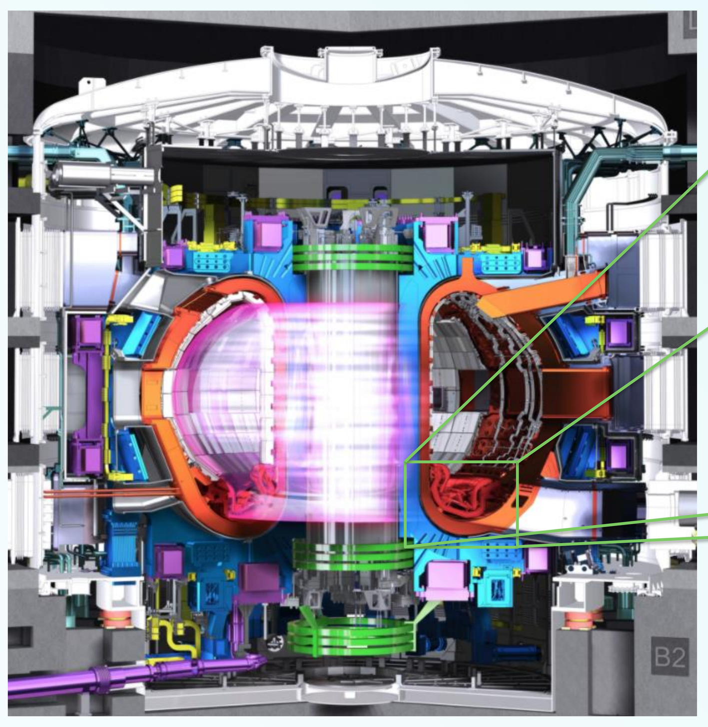

FIG. 1 A cutaway ITER tokamak

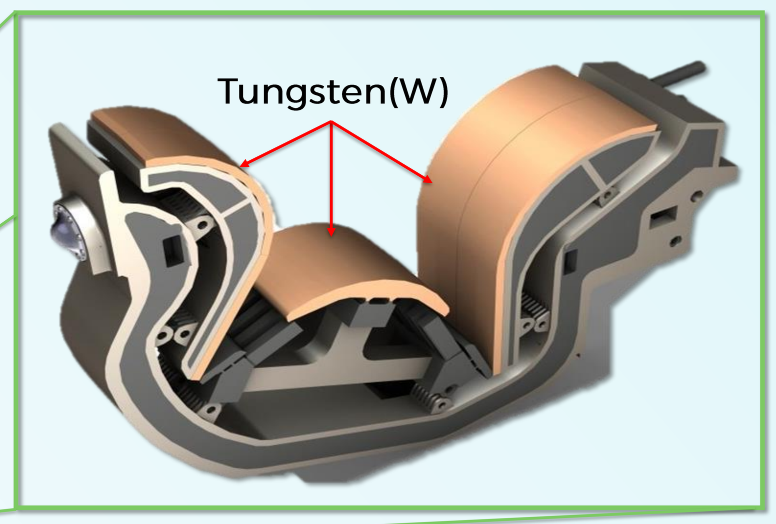

FIG. 2 ITER Divertor

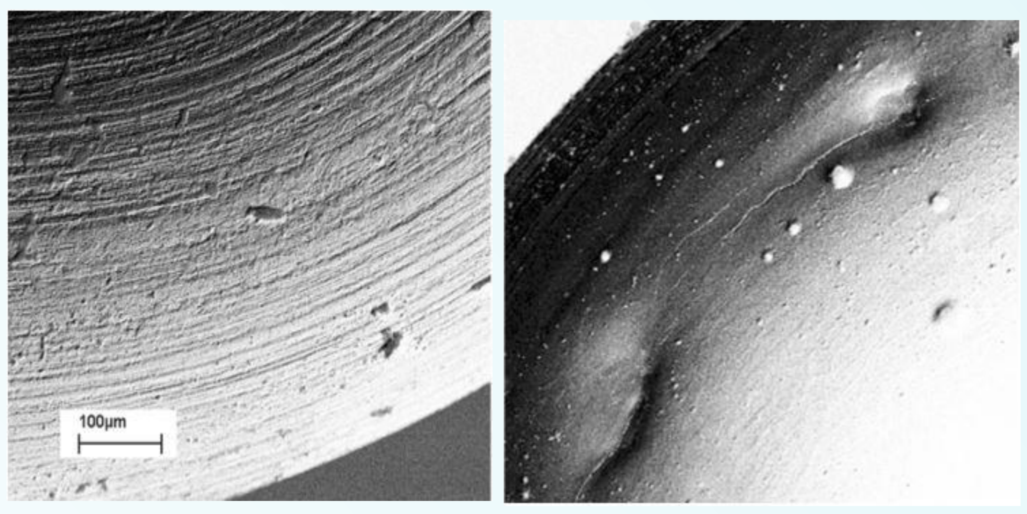

FIG. 3 Electron microscope analysis on the surface of probes. It revealed that surface of the probe exposed to plasma exhibits craters in the range from several to 100μm (right), while no craters were observed on 'unexposed probe (left) [5].

Methodology

- The crystal structures of both W projectile and W target are BCC and lattice constant 3.165 Å.
- The (0 0 1) plane is set parallel to cluster impacting direction.
- The simulations are performed in the microcanonical ensemble (NVE).
- Timestep is 0.1 fs.
- A uniform velocity perpendicular to the surface was given to all atoms belonging to the projectile in the beginning of each simulation.

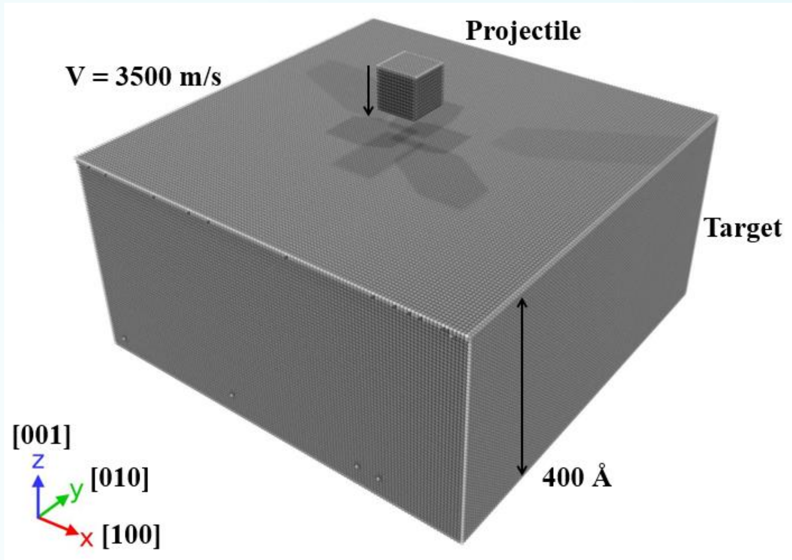

FIG. 4 Scheme of the initial configuration. Projectile and target are made of the same material, W. Number of atoms in target depends on the KE of the projectile.

- The total simulation times are 100 ps, sufficient to track the fast increase of dislocation density and ulterior recombination (See Fig 9)
- Temperature is set to 300 K. All MD simulations were performed with LAMMPS [6] and visualization of the atomic structures and analysis was done with the aid of OVITO [7].
- We selected two interatomic potentials (IP), referred as Bonny [8] and Olsson[9]. Both potentials are smoothly joined to the universal repulsive interatomic potential of Ziegler, Biersack and Littmark [10] at small interatomic separations.
- Depending on the total projectile KE (for higher values very big targets were simulated), total CPU times amounted up to 50,000 CPU hours per impact, which limited our study, in the high KE regime, to one or two simulations per impact.

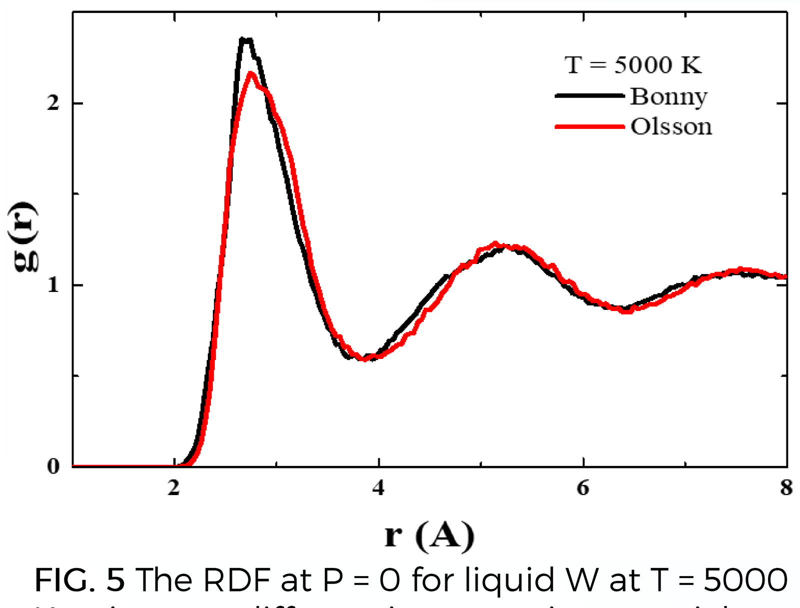

FIG. 5 The RDF at P = 0 for liquid W at T = 5000 K, using two different interatomic potentials as labeled.

	Olsson	Bonny	Exp
C_{11}	532	523	523
C_{12}	205	203	203
C_{44}	163	160.	160
T_m (K)	4102	3874	3695
ΔH (KJ/mol)	40.34	48.40	52.31
B (GPa)	313.8	320.0	310.8
ΔS (J/molK) as $\Delta H/T_m$	9.83	12.49	9.62
ΔV (cm^3/mol)	8.36	11.1	10.20

Table. 1 The melting temperatures, T_m, ΔV, ΔH, and ΔS, of W using two different potentials and the experimental values for comparison.

Results

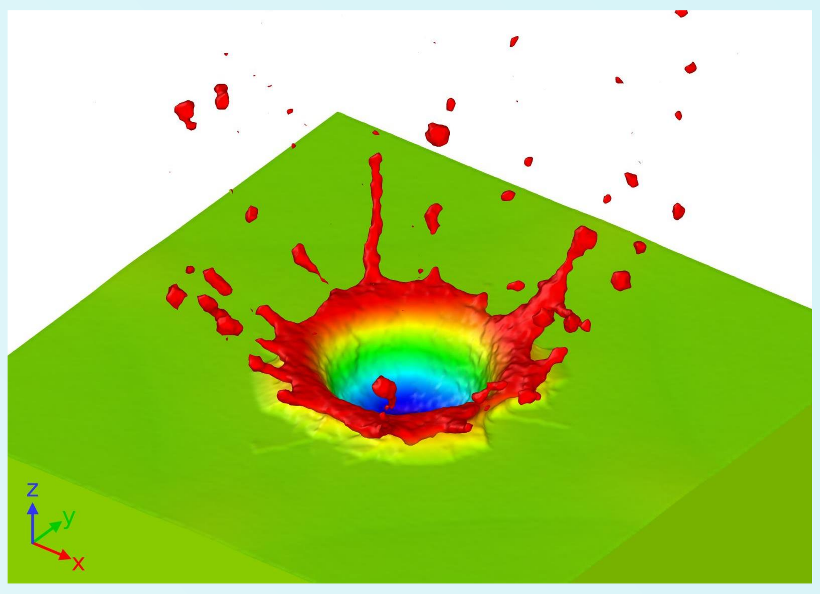

FIG. 6 **Crater view**, Potential: Olsson, v = 3500 m/s , at 20 ps, Color code: z value to target surface. Red: up; blue: down

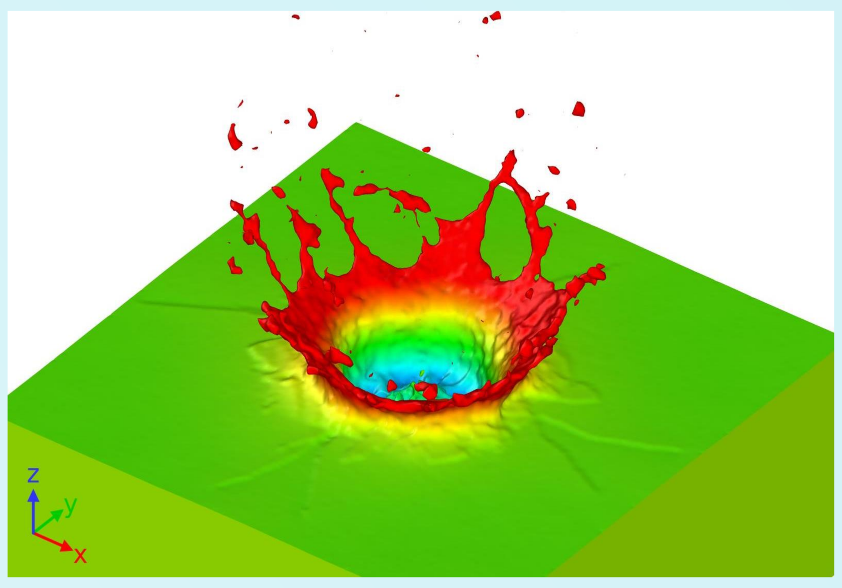

FIG. 7 **Crater view**, Potential: Bonny, v = 3500 m/s , at 20 ps, Color code: z value to target surface. Red: up; blue: down

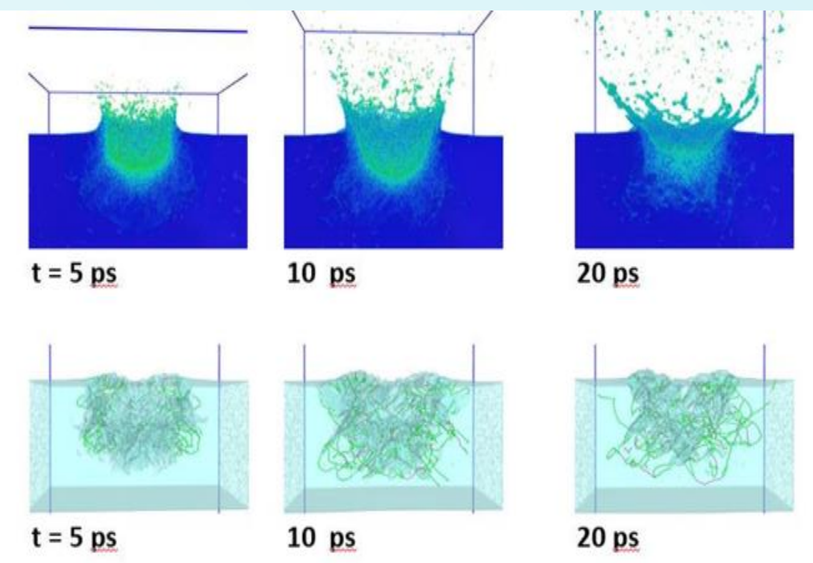

FIG. 8 MD simulation of a 40 nm size W cube (N = 17,500 atoms) impacting a W single crystal target with 5 km/s, at times 5, 10 and 20 ps after impact.

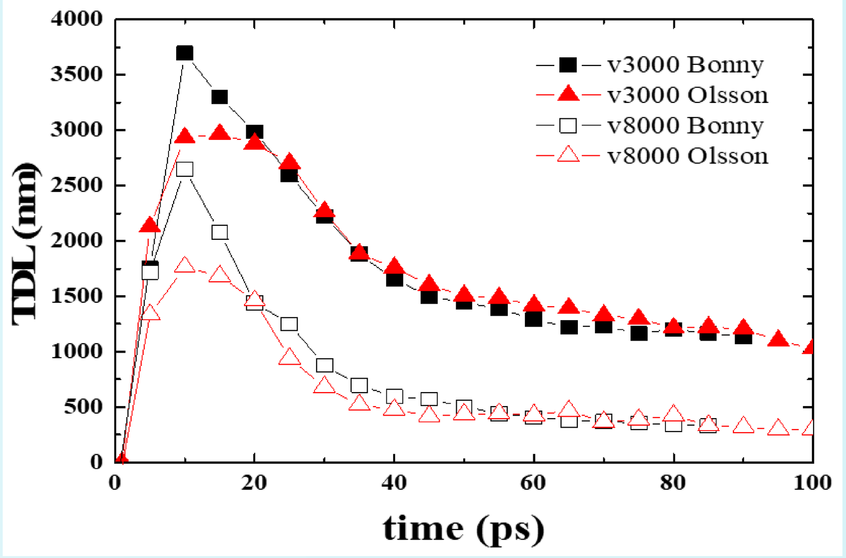

FIG. 9 Total dislocations length, in nm, after impact in the sample, vs time, in ps, for two different initial velocities, 3 km/s (full symbols) and 8 km/s (open symbols),

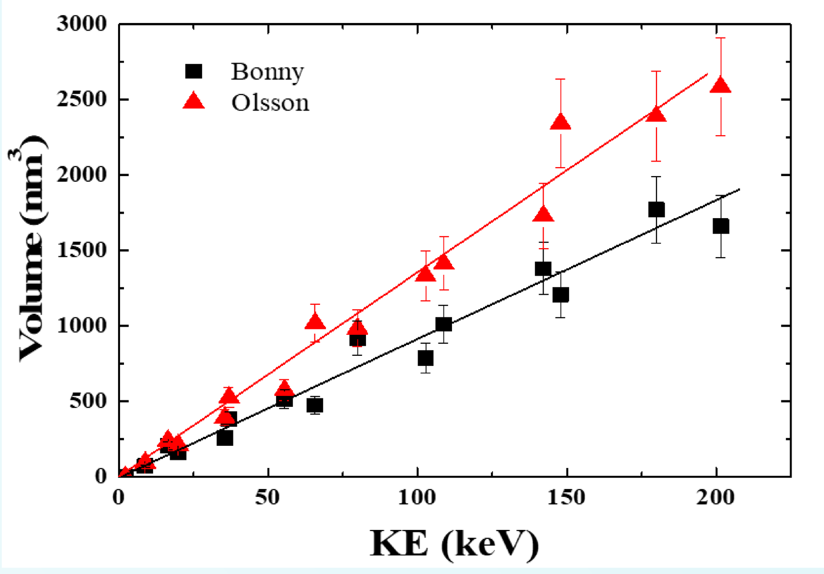

FIG. 10 Crater volume (in nm³) calculated from the number of atoms missing below the surface for different projectile kinetic energies.

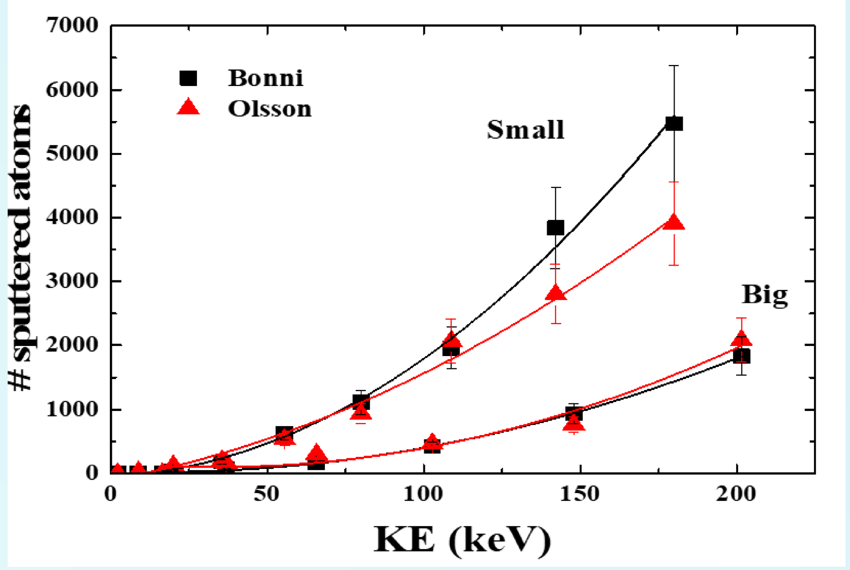

FIG. 11 Number of sputtered atoms (ejecta) in the sample vs kinetic energy, in keV,

Conclusion

- We have intensively used MD simulations to investigate the response of W to high velocity impacts. Our simulations describe the atomistic mechanisms of damage developed during impacts up to 9 km/s (KE up to 200 keV).
- The results highlight the vital role of large-scale simulations in elucidating the W response to high velocity impacts.
- We presented hypervelocity impact simulations which, despite its size, allows us to extract quantitative and qualitative information that sheds light on this complex phenomenon. For example:
  - Crater volume increases linearly with KE and results depend on the IP.
  - On the other side, the number of sputtered atoms seems independent on the IP employed but depends on the projectile size.
- **Work in progress:** a model is being developed to understand the damage produce by hyper velocity impacts in terms of geometrically necessary dislocations, much like in classic indentation theory [2]. Even larger simulations are in progress, in addition to indentation simulations.

Acknowledgements

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