Molecular Dynamics Modelling of Laser-Pulse Compression of a Dislocated Lattice in Tantalum

C.J. Ruestes[1,3*], T. Remington[1], E.M. Bringa[2,3], M.A. Meyers[1], B.A. Remington[4]

[1]*University of California, San Diego, USA*

[2]*CONICET, Argentina*

[3]*Instituto de Ciencias Básicas, Universidad Nacional de Cuyo, Mendoza, Argentina*

[4]*Lawrence Livermore National Laboratory, USA*

Research Objective: *Can dislocations travel supersonically?*

Using Tantalum as a model bcc metal, perform MD research in the areas of:

- Nano-indentation plasticity.
- Shock compression and release.
- Coupling to experiments.

GENERAL MODEL DESCRIPTION

- Software: LAMMPS (lammps.sandia.gov)
- Sample size: 100x100x75 cells . PBC in x,y dir.
- Loading along [001] direction. T=300 K
- Defects detected by CNA.

-Phase I – NANO INDENTATION

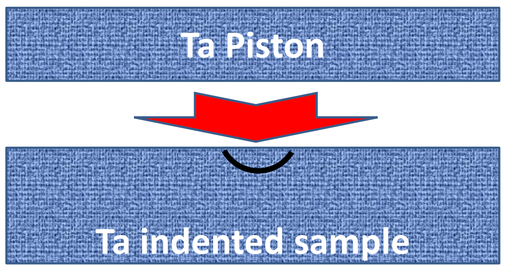
-Indenter: Spherical, 10 nm radius

- Indenter speed: 100 m/s
- Penetration depth: 7.5 nm

-Phase II – SHOCK COMPRESSION

-Piston: 100x100x50 cells

- Piston speed: 500 m/s

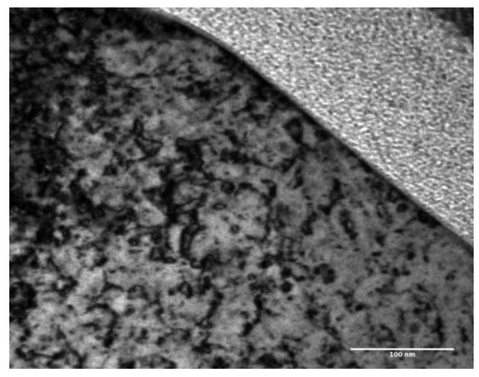


Shock simulation layout.

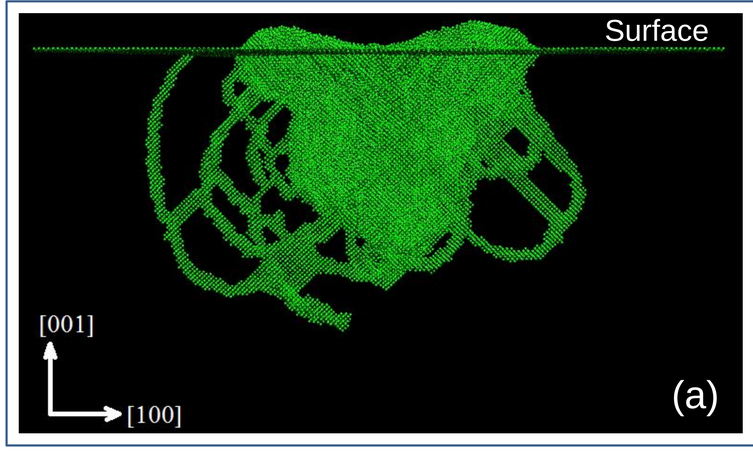
TANTALUM - B.C.C. MODEL DESCRIPTION

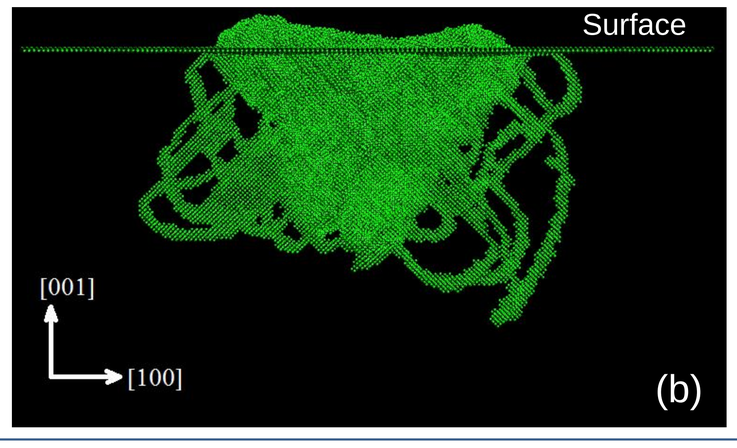
- Potential I: EAM-Li [PRB 67 (2003)]
- Potential II: extended Finnis-Sinclair EAM [J. Phys. Condens. Matter 18 (2006)]
- Potential III: EAM-Ravelo [AIP Conf. Proc. 1426 (2012)]

Berkovich Tip, Ta nanoindentation Micrograph



TANE, feel free to put here or describe whatever you want, even changing the figure.

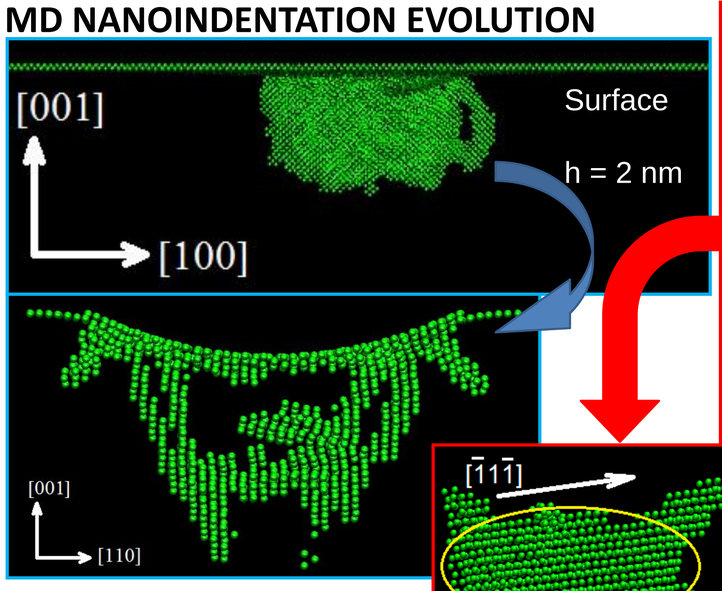


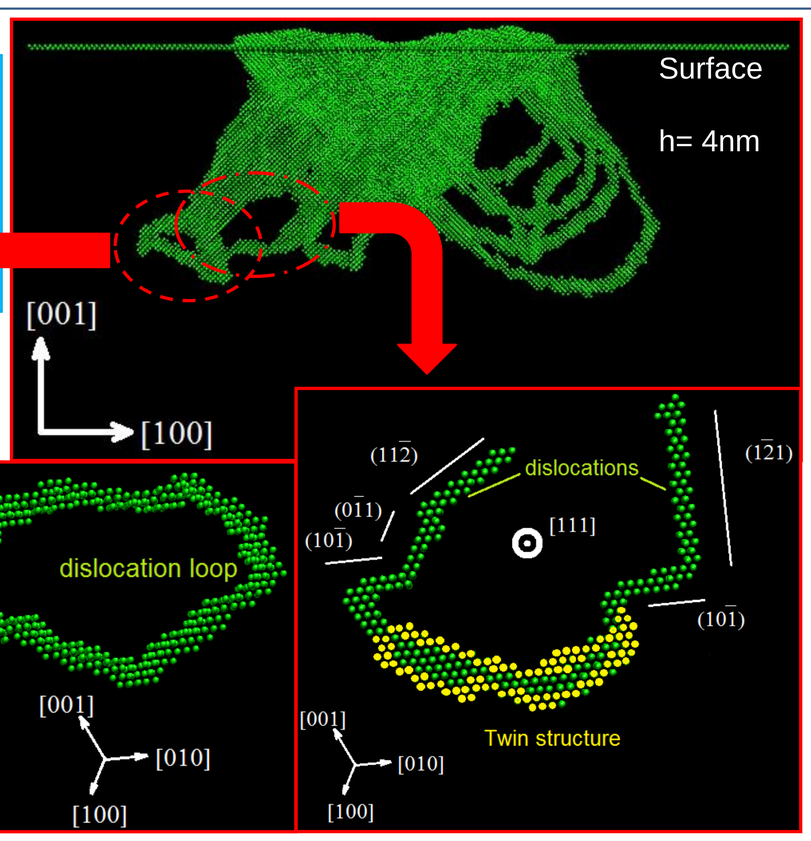


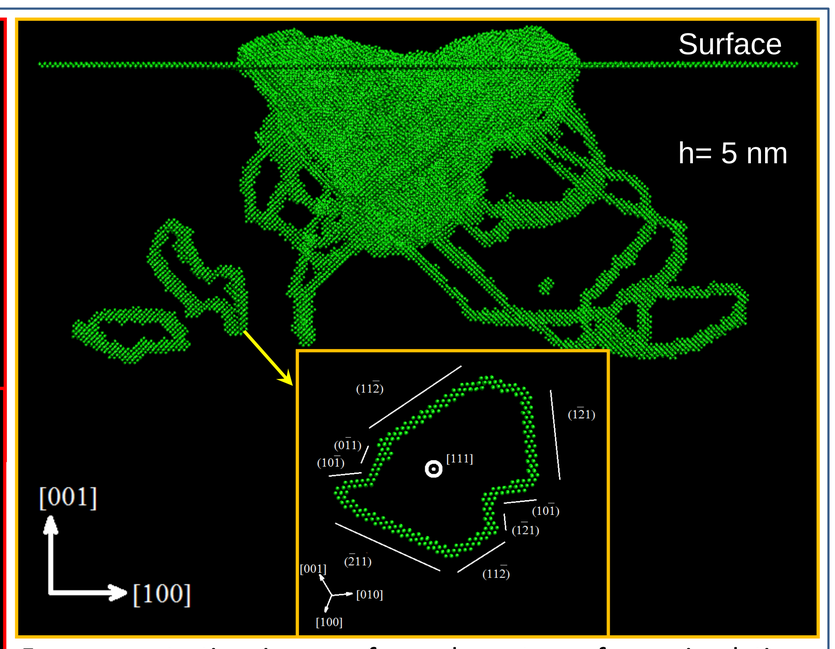
POTENTIAL COMPARISON – 5 nm penetration

(a) Image of non bcc atoms shows similar results as reported by Alcalá *et al* [PRL 109 (2012)] for their Ta nanoindentation MD using Li's EAM. Plasticity is triggered by nucleation and propagation of planar defects. **(b)** EFS potential results. While planar and linear defects are noticed as in (a), interaction leading to prismatic loops was indeed observed for a penetration depth of 7 nm and above, this being a major difference with Li's EAM output.

MD NANOINDENTATION EVOLUTION

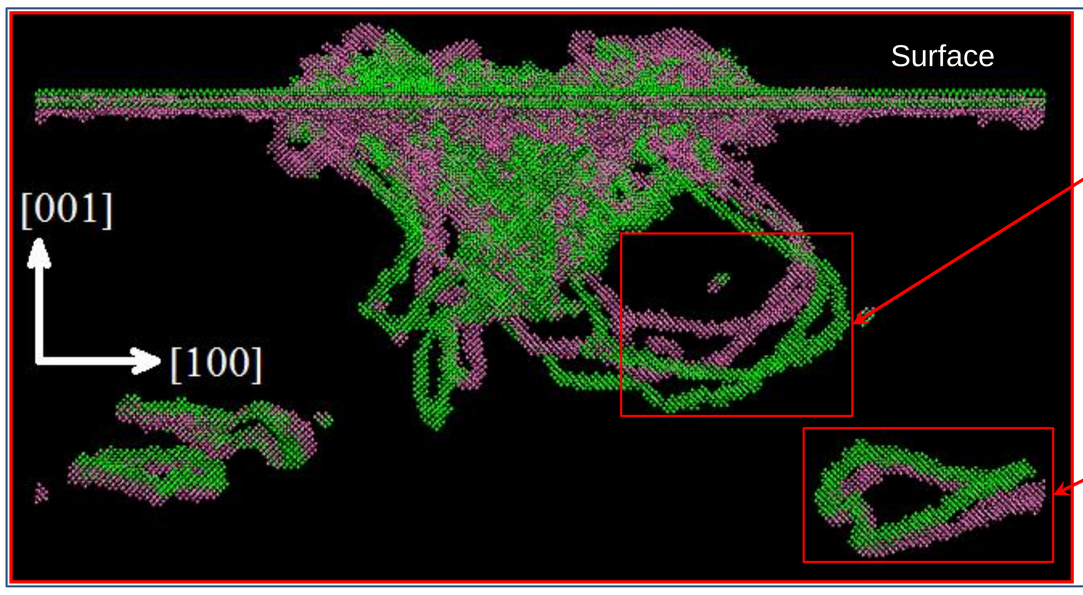


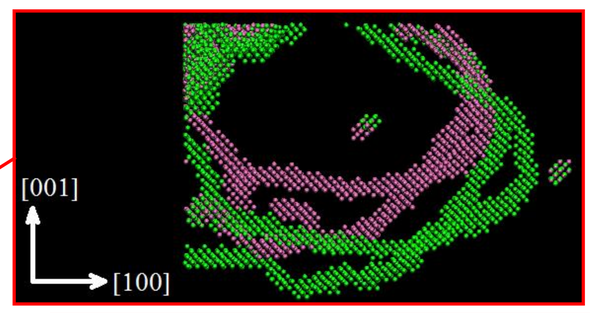


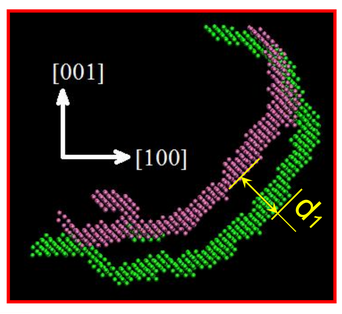


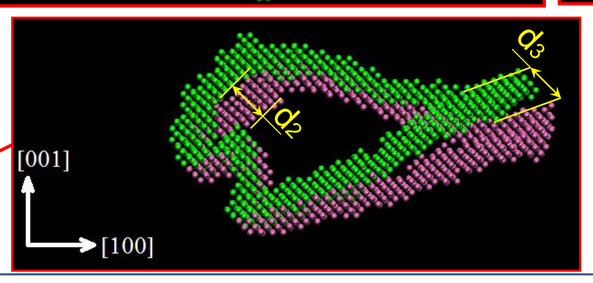
Plasticity initiates through a complex process involving nucleation, propagation and interaction of planar defects.

5 nm penetration image of non bcc atoms for a simulation using Ravelo's EAM potential [4]. Prismatic loops are already visible being formed by virtue of the interaction of {110} and {112} slip systems. For the highlighted loop, all the planes share the same [111] direction.









MD – SHOCK COMPRESSION

DISLOCATIONS VELOCITY CALCULATION EXAMPLES

Δt = 2 ps

d_1 = 16 Angs ⟹ V_1 = 800 m/s

d_2 = 14 Angs ⟹ V_2 = 700 m/s

d_3 = 22 Angs ⟹ V_3 = 1100 m/s

CONCLUSIONS AND FUTURE WORK:

- MD results qualitatively match the results shown in TEM micrographs of Berkovich tip nanoindentation tests.
- A model was successfully tested to study the laser-pulse compression of a dislocated lattice in Ta.
- An exhaustive study of the plasticity initiation and evolution is mandatory prior to extensive use of these potentials in nano-contact applications.
- The output of Ravelo's EAM shows a complex interaction of {110} and {112} slip systems leading to prismatic loops emission.
- Dislocations move at subsonic speeds that vary from 700 to 1100 m/s depending on the nature of the dislocation being analyzed.
- Future work will bridge the scale between experiments and MD by upscaling the simulations to 500 million atoms.

FUNDING & ACKNOWLEDGEMENTS:

C.J. Ruestes gratefully acknowledges NNSA support for attending NIF/Jupiter User Group Meeting 2013. E.M. Bringa thanks ANPCyT PICT-2008-1325. Calculation time at ICB-ITIC CPU Cluster (Universidad Nacional de Cuyo) is highly appreciated.

*Corresponding author. (cjruestes@hotmail.com)