

Abstract Submitted
for the SHOCK13 Meeting of
The American Physical Society

Molecular Dynamics Modelling of Laser-Pulse Compression of a Ta single crystal with dislocations¹ CARLOS J. RUESTES, ICB-UNCUYO & University of California, San Diego, La Jolla, CA 92093, USA, TANE P. REMINGTON, University of California, San Diego, La Jolla, CA 92093, USA, EDUARDO M. BRINGA, ICB-UNCUYO & CONICET, Mendoza 5500, Argentina, MARC A. MEYERS, University of California, San Diego, La Jolla, CA 92093, USA, BRUCE A. REMINGTON, Lawrence Livermore National Laboratory, Livermore, CA 94550, USA — The nanoindentation of a defect-free Ta [001] single crystal is studied by Molecular Dynamics simulations. The potential by Li et al [PRB 67 (2003)], an EFS potential [J Phys Condens Matter 18(2006)], and a recent EAM potential by Ravelo et al [AIP Conf Proc 1426 (2012)] are tested and their results analyzed in terms of dislocation slip planes. Dislocations emitted from the indented zone interact forming prismatic loops. The Ta dislocated structure is then subjected to shock compression induced by a piston hitting the sample at various speeds. The shock-induced dislocation generation and motion mechanisms are studied in order to compare to on-going experiments.

¹This research was funded by ANPCyT PRH, PICT2008-1325, PICT2009-0092, SecTyP UNCuyo 06/M035 and UC Research Lab grants

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Date submitted: 27 Feb 2013

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