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**Shock induced deformation twinning in tantalum MD simulations** MATTHEW SUGGIT, ANDREW HIGGINBOTHAM, GABRIELE MOGNI, JUSTIN WARK, University of Oxford, UK, EDUARDO BRINGA, Universidad Nacional de Cuyo, Mendoza, Argentina, PAUL ERHART, JAMES HAWRELIAK, BRUCE REMINGTON, LLNL, NIGEL PARK, AWE, Aldermaston, UK — Twinning is a potentially important deformation mechanism for shock compression of materials such as tantalum. We present large-scale molecular dynamics (MD) simulations of shock compression of tantalum employing an extended Finnis-Sinclair (EFS) potential[1]. For shock loading along the [100] axis, the plastic deformation mechanism is demonstrated to be twinning using the Fourier transform of the atomic positions, and a new per atom structure factor (PASF) method. Using this method, the atoms can be accurately separated into each twin variant and the stress and strain calculated individually. Locally, the individual twins support a large strain anisotropy and deviatoric stress, which is globally reduced towards the hydrostat. The mechanism of deformation twinning in the bcc structure is usually described by the successive displacement of (112) planes. In these simulations, the twinning mechanism is identified as the short range shuffling of alternate (112) planes after the large uniaxial compression due to the elastic precursor.

[1]X. D. Dai et al. J. Phys.: Condensed Matter, **18**, 4527 (2006).

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