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Molecular Dynamics Simulations of Transverse Effects in Shock-Compressed Fibre-Textured Tantalum Polycrystals PATRICK HEIGHWAY, University of Oxford, UK, ANDREW HIGGINBOTHAM, University of York, UK, DAVID MCGONEGLE, JUSTIN WARK, University of Oxford, UK — Whilst uniaxially shock-compressed crystas have zero total strain transverse to the shock propagation direction, this is a global, rather than local constraint. For individual grains, expansion or contraction can occur via the Poisson effect, or via plasticity. Neighbouring grains in a polycrystal may therefore 'push' one another transverse to the shock, causing transverse strain anisotropy. Here we discuss the results of multi-million atom molecular dynamics simulations of elementary fibre-textured tantalum polycrystals shock-compressed along the [110] direction. Below the elastic limit, we observe transverse stress waves driven by the Poisson effect that cause bending of the grain boundaries. In our quadcrystal geometry, the average transverse strains were 15% of the longitudinal strain, while the stress difference across the grain boundaries was of 2.5% of the peak pressure, representing a small deviation from the Reuss limit. Transverse motion of the boundaries is also visible in the plastic regime, but analysis of the stress-strain state of the bulk material is complicated by twin and dislocation nucleation. Work is currently being undertaken to quantify the transverse strain anisotropy of plastically deformed polycrystals at pressures in excess of 40 GPa.

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