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Computational and Experimental Hugoniot of Ti64 to 600 GPa[1]

KYLE COCHRANE, PATRICIA KALITA, SETH ROOT, TOMMY AO, Sandia National Laboratories — We present the shock compression of Ti64 (Ti 90w% Al 6w% V 4w%), a widely used titanium alloy with excellent mechanical properties. The Hugoniot is a key parameter for building analytical equations of state. We use density functional theory (DFT) to calculate the principal Hugoniot up to 600 GPa and pair it with corresponding shock experiments. The DFT framework uses Mermin's generalizations to finite temperature. The equation of state values are obtained via ab initio molecular dynamics (AIMD) simulations and the Hugoniot is calculated with Erpenbeck's method using the Rankine-Hugoniot energy equation to 600 GPa. We use Sandia National Laboratories' Z-machine to magnetically launch aluminum flyers to between 11 km/s and 17 km/s which yields 250 GPa to 500 GPa in the Ti64. The simulations show very good agreement with Z data and with previous three stage gas gun data from Sandia's STAR facility up to 250 GPa.

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