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Theoretical Spall Strength and EOS of Ti, Zr and Hf in the Negative Pressure Region. K.D. JOSHI, SATISH C. GUPTA, Applied Physics Division, Bhabha Atomic Research Centre, Mumbai, India 400085 — Determination of tensile stresses from the particle velocity histories in materials unloaded from the shocked state has opened the possibility of understanding the material behaviour in the negative pressure regimes. In the present work, we have determined the theoretical spall strength (σ_s) along [0001] direction, and also the EOS in the negative pressure regime, for transition metals Ti, Zr and Hf from first principles using FP-LAPW method. The σ_s for hcp (α) and ω phases of these metals have been derived from the calculated total energy versus uniaxial strain along [0001] direction. The calculated σ_s for α phase of Ti, Zr and Hf are 22, 18 and 20 GPa, and for the ω phase are 24.2, 19.5 and 23.6 GPa, respectively. The ω phase is found to be harder than α phase in agreement with available experimental results. The trend in the group IV B indicates that σ_s for Ti is largest followed by Hf and then Zr for both α and ω structures. The theoretical σ_s for Ti is much higher than ~ 4.2 GPa measured at strain rates of $\sim 10^6$/s. This discrepancy could be associated with the material defects, which dominantly control the spalling at such strain rates. For determination of ideal σ_s, experiment should be performed at still higher stresses (and higher strain rates). The bulk modulus of 110, 96 and 115 GPa, respectively for Ti, Zr and Hf, determined from the theoretical EOS in the negative pressure region, are in good agreement with experiments.

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