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High –Pressure Synthesis and Characterization of Incompressible Titanium Pernitride[1] VENKATA BHADRAM, DUCK YOUNG KIM, TIMOTHY STROBEL, Carnegie Institution of Washington — We report the discovery of a new transition-metal pernitride, TiN_2, which was synthesized by reacting TiN with N_2 at 73GPa in a laser-heated diamond anvil cell (DAC). Our *in situ* pressure dependent x-ray diffraction studies suggest that TiN_2 is recoverable at ambient conditions in a crystal structure that contains single bonded nitrogen units (N_2 dumbbells) embedded in the metal lattice and exhibits high bulk modulus (in the range 360-385 GPa) which is usually observed in superhard materials. We have performed *ab initio* calculations to understand the electronic properties and bonding nature in TiN_2 and thereby elucidate the origin of incompressible behavior of this material which is rooted in the nearly filled anti-bonding states of the pernitride units. Although, study of transition metal pernitrides has been an active area of research for quite some time, most of the pernitrides synthesized so far are belong to noble metal group. To our knowledge, this is the first experimental report on TiN_2 which is the only light metal pernitride exhibiting bonding-mechanical property relation that is usually seen in heavy metal pernitrides.

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