# An Ultraincompressible Titanium Pernitride ($TiN_2$)

5/2016

## Scientific Achievement

**Synthesis of a new transition metal pernitride, $TiN_2$, that is the only non-noble metal pernitride exists to date.**

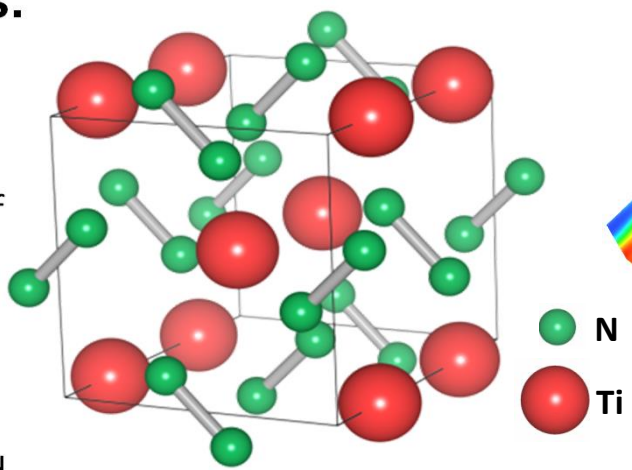
## Significance and Impact

**Titanium pernitride ($TiN_2$) is ultaincompressible (bulk modulus >360GPa) due to the presence of single bonded nitrogen units (pernitride ions) in its crystal lattice. The structure-property relation exhibited by $TiN_2$ is useful in discovering similar superhard materials.**

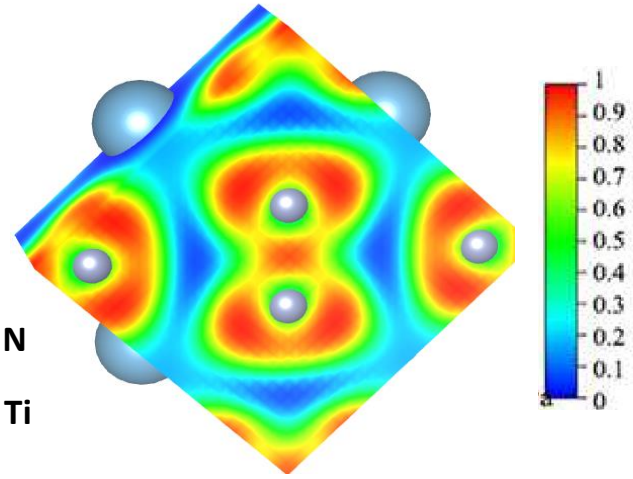
## Research Details

- Reaction between TiN and $N_2$ at 73GPa resulted in the formation of $TiN_2$. As synthesized $TiN_2$ was recovered at ambient conditions.
- $TiN_2$ was characterized by synchrotron x-ray diffraction, EDS on SEM, Raman spectroscopy, and first principles calculations made possible by the EFree ERFC.

Facilities: APS, Argonne




Crystal Structure




Electron Localization Function

Bhadram, V.S.; Kim, D.Y.; Strobel, T.A., High-pressure synthesis and characterization of incompressible titanium pernitride,. *chem mater (2016).* doi:10.1021/acs.chemmater.6b00042.

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