

Discovery of Semiconducting Titanium Nitride (Ti₃N₄)

1/2018

Scientific Achievement

A long-sought-after phase of titanium nitride with stoichiometry Ti₃N₄ was discovered using diamond anvil cell experiments supported by *ab initio* calculations.

Significance and Impact

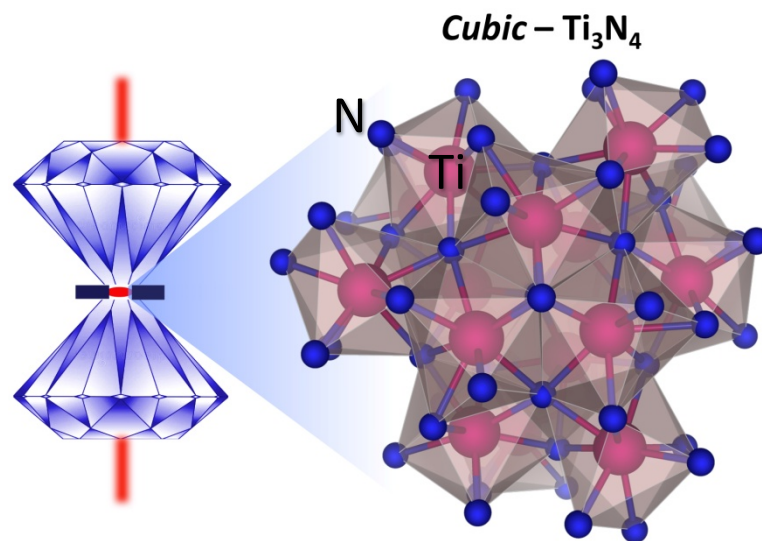
Ti₃N₄ is the first semiconducting titanium nitride with a calculated direct band gap of 0.9 eV.

Research Details

- Reaction between TiN and N₂ at 75 GPa and 2400 K resulted in the formation of cubic Ti₃N₄ with the Th₃P₄ type structure (*I-43d*), as characterized by synchrotron X-ray diffraction and Raman spectroscopy and supported by structure prediction calculations.
- Dynamically unstable at 1 atm, but may transition to defect rock salt structure upon decompression.
- InterEFRC collaboration between EFree and CNGMD.

Bhadram, V.S.; Liu, H.; Xu, E.; Li, T.; Prakapenka, V. B.; Hrubiak, R.; Lany, S.; Strobel, T. A., Semiconducting Cubic Titanium Nitride in the Th₃P₄ Structure, *Physical Review Materials (Rapid)*, In Press (Editor's Suggestion)

Facilities: APS, Argonne



Schematic depicting the high-pressure synthesis and polyhedral structural representation of cubic Ti₃N₄.



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