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High Pressure Studies of Titanium Hydride Up to 50 GPa with Synchrotron X-ray Diffraction
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Abstract
Titanium dihydride has the potential to play an important role in the efficiency of high density hydrogen storage. The structural instability of TiH₂ at high pressures makes an accurate characterization of its structure a vital part of understanding its behavior. A sample of TiH₂ was placed in a diamond anvil cell and studied from ambient pressure up to 53 GPa using in situ synchrotron x-ray diffraction at the Advanced Photon Source (APS) of Argonne National Laboratory (Sector 16, HPCAT). From data of the evolution of the structure with pressure, an equation of state was obtained to model the behavior of the unit cell of TiH₂ between 0 and 51 GPa.

Introduction
- Crystals change structure as pressure increases
- Change in structure results in new properties
- Diamond anvil cell (DAC) allows for high pressure in situ x-ray diffraction
- X-ray diffraction reveals information about the structure of the material
- Synchrotron x-rays allow for smaller samples to be studied due to high flux

Methods
Diamond Anvil Cell
- Rhenium gasket indented between two diamond culets
- Electric Discharge Machine (EDM) used to drill hole through center of indentation
- Sample placed on diamond culet in gasket hole

Synchrotron XRD
- DAC placed in x-ray beam
- Pressure increased in 1-2 GPa steps
- Diffraction patterns recorded for each step

Synchrotron Facility at Argonne National Laboratory

Data Analysis
- Circular pattern integrated to generate linear model using Fit2D
- Peak fitting used to find spacing between atoms
- Structure inferred from spacing

Results
- Peak splitting on diffraction pattern confirms phase change in material
- TiH₂ undergoes a structure change from face-centered cubic (fcc) to body-centered tetragonal (bct) before 1.3 GPa
- Remains bct up through 53.3 GPa

Conclusions
- TiH₂ transitions from fcc to bct between ambient pressure and 1.3 GPa and remains bct through 53 GPa
- Titanium hydride has a relatively high bulk modulus of 136 ± 3 GPa

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