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High pressure studies of titanium hydride up to 50 GPa with synchrotron x-ray diffraction

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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.

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

Data Analysis (cont’d)
• Peak fitting yields cell parameters
• Corresponding pressures and volumes can be fitted to Equation of State using following formula:
  \[ P = \frac{3}{2}K_0 \left( \frac{V}{V_0} \right)^{7/3} \left( \frac{1 + \frac{3}{4}K_0 - \frac{3}{2}V_0^{2/3}}{1 - \frac{3}{2}V_0^{2/3}} \right) \]
  where \( K_0 \) is the bulk modulus and \( V_0 \) is the volume at atmospheric pressure

Ko = 136 ± 3 GPa
Kp = 4.6 ± 0.2
V0 = 43.9

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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