Phase Transition of Vanadium under High Pressure

Yang Ding

High Pressure Synergetic Center (HPSynC)
Carnegie Institution of Washington
### Structure sequence of transition metals

<table>
<thead>
<tr>
<th>3d</th>
<th>4d</th>
<th>5d</th>
</tr>
</thead>
<tbody>
<tr>
<td>hcp</td>
<td>bcc</td>
<td>hcp</td>
</tr>
<tr>
<td>Sc, Ti</td>
<td>V, Cr</td>
<td>Mn, Fe</td>
</tr>
<tr>
<td>Y, Zr</td>
<td>Nb, Mo</td>
<td>Tc, Ru</td>
</tr>
<tr>
<td>La, Hf</td>
<td>Ta, W</td>
<td>Re, Os</td>
</tr>
</tbody>
</table>

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<thead>
<tr>
<th>4d</th>
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</thead>
<tbody>
<tr>
<td>fcc</td>
<td>hcp</td>
</tr>
<tr>
<td>Co, Ni, Cu</td>
<td>Zn</td>
</tr>
<tr>
<td>Rh, Pd, Ag</td>
<td>Cd</td>
</tr>
<tr>
<td>Ir, Pt, Au</td>
<td>Hg</td>
</tr>
</tbody>
</table>

- **hcp** hexagonal close-packed
- **bcc** body-centered cubic
- **fcc** face-centered cubic

**Atomic number increases**
Structure and the d occupancy


Previous HP measurements on V

K. Takemura, 2000 Proceedings of the International Conference on High Pressure Science and Technology, AIRAPT-17 (Honolulu, July 1999),
Anomalous $T_c$ of V under P

M. Ishizuka, PRB 61, R3823 (2000)

N. Suzuki, JPCM 14, 10869 (2002)
Experimental settings at HPCAT

Energy
29.21 KeV
30.87 KeV

Beam size
~20 microns

DAC

16IDB station at HPCAT

HPSynC
High Pressure Synergetic Center at the Advanced Photon Source
Non-hydrostatic compression
Hydrostatic compression
Transition model
Comparison of diffraction patterns

K. Takemura, 2000
EOS and transition pressure

\[ <Q> = \frac{\alpha}{\alpha_0} - 1 = C(P - P_c)^{1/2} \]
What the origin for the transition?

\[ C_{44} \text{ softening} \quad C_{44} = \frac{\omega^2}{K^2} \]

Phonon softening?

\[ \text{s-d transition?} \]

It’s unlikely since
Chromium (3d54s1), \( C_{44} = 100 \text{ GPa} \)
Vanadium (3d34s3), \( C_{44} = 43 \text{ GPa} \)
Theoretical evidence

Fermi surface nesting
In the 3rd band
Kohn anomaly
Phonon soft mode
C\textsubscript{44} instability
Rhombohedral lattice distortion

Theoretical evidence

**Enthalpy of lattice**

![Graph showing enthalpy changes with pressure](image1)

B. Lee et al. PRB B 75, 180101R 2007

**Phonon softening**

![Graph showing phonon frequency changes with pressure](image2)

W. Luo et al. PNAS, 104, 16428, 2007
Summary and prospects

- A phase transition was observed at 63–69 GPa and room temperature in vanadium with synchrotron x-ray diffraction.

- The transition is characterized as a rhombohedral lattice distortion of the body-centered cubic vanadium, which represents a novel type of transition that has never been observed in elements.

- Instead of driven by the conventional s-d electronic transition mechanism, the phase transition could be associated with the softening of C44 trigonal elasticity tensor that originates from Fermi surface nesting.

- Can we measure the such phonon softening?

- Similar transition in Nb and Ta?
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