Phonon dispersion of Molybdenum

$bcc$ Mo single crystal

Helium

Ruby

Rocking curve width: 0.1 – 0.3 degrees

Origin of H-point anomaly?

Pressure evolution of the H-point anomaly: experiment and theory

Gradual disappearance of H-point anomaly
  • reduced electron-phonon coupling
  • shift of Fermi level with respect to p-like bands
IXS in Earth science

The preliminary reference Earth model (PREM)

- Seismology (+ mineral physics)
- Geochemistry (+ petrology)

- density and elasticity
- partitioning and solubility
hcp iron: Raw spectra and phonon dispersion

\[ P = 55 \text{ GPa} \]

\[ V_P \text{ from initial slope of dispersion curve via sine fit} \]
Sound Velocities in the Core

- Linear dependence of $V_p (\rho)$: Birch law
- Inclusion of light elements needed!

G. Fiquet et al.; Science 291, 468 (2001)
Sound Velocities in the Core

\[ V_p = 3.00 \rho - 6977 \]
\[ V_p = 1.82 \rho - 4169 \]
\[ V_p = 1.67 \rho - 3285 \]
\[ V_p = 1.07 \rho - 1392 \]
\[ V_p = 0.94 \rho - 1466 \]
\[ V_p = 0.72 \rho + 1804 \]

FeS2, FeSi, FeO, FeS IV, Fe, Fe3C, IC, OC, Brown & McQueen
Simple composite model

Proposed composition of the core

\[
\rho = (1 - x) \rho_{Fe} + x \rho_{le} = \rho_{seismic}
\]

\[
V = \frac{V_{Fe} \cdot V_{le}}{(1 - x)V_{le} + xV_{Fe}} = V_{seismic}
\]

<table>
<thead>
<tr>
<th>Element</th>
<th>Fraction (wt%)</th>
<th>Compression (\rho/\rho_0)</th>
<th>Model Outer Core (wt%)</th>
<th>Model Inner Core (wt%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Si</td>
<td>2.3</td>
<td>1.28</td>
<td>2.8</td>
<td>2.8</td>
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<tr>
<td>O</td>
<td>1.6</td>
<td>1.33</td>
<td>minor</td>
<td>5.3</td>
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<tr>
<td>S^{2-}</td>
<td>9.7</td>
<td>2.51</td>
<td>minor</td>
<td>minor</td>
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<tr>
<td>S^{-}</td>
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<td>1.05</td>
<td>minor</td>
<td>minor</td>
</tr>
<tr>
<td>C</td>
<td>1.0</td>
<td>1.40</td>
<td>1.0</td>
<td>—</td>
</tr>
</tbody>
</table>
Determination of the phonon density of states

- Incoherent inelastic neutron scattering
  - sample volume: $10^{-4}$ mm$^3$
  - $f(Q)$ versus $b$

- Nuclear inelastic scattering
  - no need of Mössbauer isotope

**Prerequisites**

- Uniform sampling of the Brillouin zone
- Mutual annihilation of “selection rule”-terms
Test case: polycrystalline diamond

- $\Delta E = 3 \text{ meV}$
- Sum of 10 IXS spectra ($45 \text{ nm}^{-1} < Q < 60 \text{ nm}^{-1}$)

... and first applications

Ba$_8$Si$_{46}$

Te III at 15 GPa

I. Loa, A. Bosak, et al.; A. San Miguel, M. Koza, A. Bosak et al.