EXAFS Study of Laser Shocked Metals Below 1 Mbar

OMEGA shot 21238

Initial target size

EXAFS

Ti K edge

Photon energy (keV)

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EXAFS is used to measure compression and temperature in shocked Ti and V and a phase transformation in Ti

- V (z = 23): no phase transformation
  Ti (z = 22): $\alpha$-Ti to $\omega$-Ti phase transformation in $\mu$sec shocks

- An EXAFS spectrum from uncompressed and compressed V ($\sim 0.4$ Mbar) was analyzed by FEFF EXAFS code and favorably compared with LASNEX simulations.

- Uncompressed Ti was successfully analyzed, but compressed Ti shows EXAFS of stronger damping than expected for the predicted temperature.

- FEFF analysis with the $\alpha$-Ti and $\omega$-Ti phases clearly shows that the expected transformation does take place.

- 1-D compression is ruled out as the reason for this discrepancy.

**Summary**
EXAFS is modulations in x-ray absorption due to interference of the ejected electron wave function with reflections from neighboring atoms.

- Phase is $k_{\text{electron}}R$.
- Modulation frequency depends on $R$ and, hence, on density.
- For higher temperatures, vibrations reduce coherence, leading to faster damping of modulation.
EXAFS modulations in the x-ray absorption coefficient depend on the density and temperature

- Model for modulations in reduced x-ray absorption coefficient above the $K$ edge:

\[
\chi(k) = \sum_j N_j F_j(k) \exp \left[ -2\sigma^2 k^2 - 2R_j/\lambda(k) \right] \sin \left[ 2kR_j + \phi_j(k) \right]/kR_j^2
\]

Damping due to lattice vibrations
\[
\sigma^2 = f(T/\theta_D)
\]

Electron mean free path

Modulations due to neighboring atoms

- For shock heating, compression increases $\theta_D \sim h\nu_m/k_B$

($\nu_m$, the maximum lattice frequency $\sim \rho^{1/3}$).
The Debye-Waller term, $\sigma^2$, depends on temperature and compression.

![Graph showing the relationship between $\sigma^2$ (Å²) and temperature (K) for different compression values.]

Compression = 1.0

EXAFS is observed in thick metal foils backlit by a spherical target implosion.
Raw EXAFS film image of unshocked Ti shows expected modulation (shot 27499)
ASBO measures shock-arrival time at back of Ti; speed (through Hugoniot) confirms EXAFS compression.
The increased modulation period indicates shock compression (0.4 Mbar) in V

![Absorption vs Photon energy graph](image)

- Red line: 30142 (unshocked)
- Green line: 30143 (shocked)
EXAFS in shocked vanadium (0.4 Mbar) shows greater decay of modulations due to shock heating.
The FEFF fit of the EXAFS spectrum for unshocked vanadium shows solid density and $T = 430$ K.
The FEFF fit of the EXAFS spectrum for shocked vanadium (0.4 Mbar) indicates ×1.14 compression, $T = 770$ K.

Calculated and measured parameters for shocked vanadium

Laser of intensity of 0.5 TW/cm² yielding a pressure of ~0.45 Mbar

<table>
<thead>
<tr>
<th>LASNEX parameter ranges</th>
<th>EXAFS measurement</th>
<th>Shock-speed measurement</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.19±0.05</td>
<td>980±160 K</td>
<td>1.14±0.01</td>
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A 0.4-Mbar shock in Ti reduces the EXAFS modulation dramatically.
FEFF fits to the Ti EXAFS data show shock induced compression of \( \sim 1.2 \times \)

Unshocked: compression = 1, 
T = 380 K

Shock: compression = 1.2, 
T = 2100 K
At high pressures (0.02 to 0.1 Mbar) Ti undergoes an \(\alpha\)-Ti to \(\omega\)-Ti phase transformation.

- \(\alpha\)-Ti: 2.3 Å higher
- \(\omega\)-Ti: 1.4 Å higher

\[2.3 \, \text{Å} \quad \text{higher}\]
\[1.4 \, \text{Å} \quad \text{higher}\]
Evidence for $\alpha$-Ti to $\omega$-Ti phase transformation: fitting FEFF code to data, assuming $T = 900$ K

Electron wave number ($\text{Å}^{-1}$)

Data (28958)

$\alpha$-Ti

$\omega$-Ti

$\chi(k) = (\mu - \mu_0) / \mu_0$
Ti EXAFS spectra at reduced irradiances support the observation of a phase transformation.

![Graphs showing EXAFS spectra at different shock irradiances](image-url)

- **Shock irradiance = 0**
  - Normalized signal
  - Photon energy (keV)
  - 0 Mbar

- **Shock irradiance = 0.12 TW/cm²**
  - Normalized signal
  - Photon energy (keV)
  - ~ 0.12 Mbar

- **Shock irradiance = 0.23 TW/cm²**
  - Normalized signal
  - Photon energy (keV)
  - ~ 0.25 Mbar

- **Shock irradiance = 0.40 TW/cm²**
  - Normalized signal
  - Photon energy (keV)
  - ~ 0.35 Mbar
EXAFS of shocked Ti (0.4 Mbar) cannot be fitted with either 1-D (pole-figure-averaged) or 3-D compression at the predicted $T = 0.09$ eV.
In-situ diffraction of shocked metals on OMEGA measures compression*

In-situ diffraction using monochromatic point source shows uniform compression

Single crystal Ti, 0.1 Mbar

Compressed Uncompressed
In-situ diffraction shows compression (a) increases with pressure, (b) is 3-dimensional

Ti single crystal shocked along c-axis

\[ \frac{d_0 - d}{d} \]

\begin{itemize}
  \item This work
  \item Predicted uniaxial
  \item Predicted isotropic
\end{itemize}

Pressure (Mbar)
Initial L-shell EXAFS measurements are encouraging.

OMEGA shot 29443, 5-μm Ta

EXAFS above the LIII-absorption edge of Ta; spectrum similar to synchrotron data; can be amplified by a thicker Ta foil.
EXAFS has been used to study shock compression in V and Ti and to demonstrate phase transformation in Ti.

- *K*-shell EXAFS of shocked materials has been performed on OMEGA using an implosion as a backlighter.

- The measured compression and temperature of V (up to 0.4 Mbar) is in good agreement with predictions.

- The measured compression of Ti (up to 0.4 MBar) is in good agreement with predictions, but the damping can only be explained by assuming a transformation from the $\alpha$ to $\omega$ phase.

- In development:
  - Diffraction measurement of $\alpha$- to $\omega$-phase transformation in Ti
  - $L$-shell EXAFS measurements of very high-Z elements on OMEGA
  - EXAFS applied to isentropically compressed targets