EXAFS Detection of Laser Shock Compression

B. Yaakobi, T. R. Boehly, D. D. Meyerhofer, R. Epstein, and D. Salzman
Laboratory for Laser Energetics
University of Rochester

B. A. Remington and S. Pollaine
Lawrence Livermore National Laboratory

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EXAFS measurements of laser-shocked titanium have been made

- Laser-shocked metals have been recently studied in LLNL by x-ray diffraction (Bragg and Laue), observing elastic (1-D) and plastic (3-D) compressions. Extended x-ray absorption fine structure (EXAFS) can supplement such measurements.

- EXAFS can yield information on density and temperature.

- High-contrast EXAFS modulations of polycrystalline Ti absorber were obtained using a laser-imploded spherical target as backlighter.

- For a shock strength of ~0.5 Mbar we obtained EXAFS spectra that indicate compression of ~1.3, in agreement with simulations and measured shock speed.

- The decay rate of the EXAFS modulations (with wave number) is much faster than expected due the temperature rise and is attributed to increased crystal disorder, most probably due to the $\alpha$-Ti $\rightarrow$ $\omega$-Ti phase transformation.
EXAFS is modulations in x-ray absorption due to interference of the ejected electron wave function with reflections from neighboring atoms.

- If the two electron waves are
  - in phase: maximum absorption
  - out of phase: minimum absorption
- Phase is $k_{\text{electron}}R$.
- Modulation frequency depends on $R$ and, hence, on density.
- For higher temperatures, vibrations reduce coherence, leading to less modulation.

\[
\hbar^2 k_{\text{electron}}^2 / 2m = E_{\text{ph}} - E_K
\]
EXAFS model shows the dependence of modulations in the x-ray absorption coefficient on 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 $\theta_D \sim \hbar \nu_m/k_B$ ($\nu_m$, the maximum lattice frequency $\sim \rho^{1/3}$).

$$\hbar^2 k^2/2m = E_{ph} - E_K$$
Vibration amplitude increases with temperature but decreases with compression (through $\Theta_D$)
Fitting EXAFS model to experimental spectrum of cold, undriven target yields the expected $T, \rho$.

\[ k\chi = k(\mu - \mu_0)\mu_0 \]

Electron wave number ($\text{A}^{-1}$)
EXAFS is observed in thick metal foils backlit by a spherical target implosion.
Smooth x-ray continuum from imploding target is suitable for EXAFS measurement (shot 23134)
ASBO measures shock-arrival time at back of Ti; speed (through Hugoniot) confirms EXAFS compression.

Lateral nonuniformity is ±10% in speed, ±4% in pressure.
Heating of Ti foil (by radiation) to \( \sim 0.5 \text{ eV} \) causes EXAFS spectrum to disappear.
Preheat determination: fitting EXAFS spectrum of undriven target yields $T = 40$ meV

$$k' = k (\mu - \mu_0)\mu_0$$

$\chi$ $= k' (\mu - \mu_0)\mu_0$

Electron wave number (Å$^{-1}$)

Shot 27499
*LILAC* profiles (with QEOS) for Ti shocked by a 3-ns pulse at 0.5 TW/cm² are quite uniform axially
QEOS Hugoniot curves for Ti agree with measured pressure at room temperature (Vohra and Spencer)
EXAFS spectrum (unshocked target) before Fourier filtering shows good S/N ratio.
Longer EXAFS wavelength after shock passage indicates compression ($\times 1.3$)
EXAFS model fit yields compression of 1.3 (assumed 3-D); decay rate depends on T but includes the effect of Ti crystal phase transition.

\[ k \chi = k (\mu - \mu_0)^{\frac{1}{4}} \]

\[ \sigma^2 = 0.033 \text{ A}^2 \ (T = 0.25 \text{ eV}) \]

\[ \sigma^2 = \sigma^2 \text{ (thermal)} + \sigma^2 \text{ (disorder)} \]
Shock-compressed EXAFS spectrum fitted with model for 3-subshell \( \omega \)-Ti at \( C = 1.3 \) and \( T = 0.08 \) eV.
EXAFS is better suited for diagnosing isentropic compressions (ICE) than shocks because they access higher $\rho$, lower $T$. 

![Graph showing the comparison between EXAFS and shocks in terms of compression and temperature. The graph includes regions labeled 'High', 'Marginal', and 'Low' for both compression and temperature. The Hugoniot (Mbar) is also indicated.](image-url)
EXAFS is better suited for diagnosing isentropic compressions (ICE) than shocks because they access higher $\rho$, lower $T$. 

Regions of EXAFS observability in Ti

- High
- Marginal
- Low

![Graph showing regions of EXAFS observability in Ti with compression on the y-axis and temperature on the x-axis.](image)
$\chi^2$ analysis of EXAFS is used for finding best fit; error found from Hessian matrix (unshocked case)
High-contrast EXAFS modulations of polycrystalline Ti absorber have been demonstrated using a laser-imploded target as backlighter.

- For a shock strength of $\sim 0.5$ Mbar we obtained EXAFS spectrum that indicates compression of $\sim 1.3$, in agreement with simulations and shock-speed measurement.

- The decay rate of the EXAFS modulations (with wave number) is much faster than expected due to the temperature rise and is attributed to increased crystal disorder, most probably due to the $\alpha$-Ti $\rightarrow$ $\omega$-Ti phase transformation.

- Future experiments that can improve our understanding include:
  - simultaneous measurements of EXAFS and multidirectional diffraction on a single-crystal sample with no phase transformation.
  - use EXAFS in isentropic compression experiments (ICE) where higher density and lower temperature than in shocks make EXAFS a more-suitable technique.