

# High-Resolution X-Ray Spectrometer for X-Ray Absorption Fine Structure Spectroscopy

D. A. Chin,<sup>1,2</sup> P. M. Nilson,<sup>2</sup> D. Mastrosimone,<sup>2</sup> D. Guy,<sup>2</sup> J. J. Ruby,<sup>3</sup> D. T. Bishel,<sup>1,2</sup> J. F. Seely,<sup>4</sup> F. Coppari,<sup>3</sup> Y. Ping,<sup>3</sup> J. R. Rygg,<sup>1,2,5</sup> and G. W. Collins<sup>1,2,5</sup>

<sup>1</sup>Department of Physics and Astronomy, University of Rochester

<sup>2</sup>Laboratory for Laser Energetics, University of Rochester

<sup>3</sup>Lawrence Livermore National Laboratory

<sup>4</sup>Syntek Technologies

<sup>5</sup>Department of Mechanical Engineering, University of Rochester

Two extended x-ray absorption fine structure (EXAFS) flat crystal x-ray spectrometers (EFX's) were designed and built for high-resolution x-ray spectroscopy over a large energy range with flexible, on-shot energy dispersion calibration capabilities. EFX uses a flat silicon [111] crystal in the reflection geometry as the energy dispersive optic covering the energy range of 6.3 to 11.4 keV and achieving a spectral resolution of 4.5 eV with a source size of 50  $\mu\text{m}$  at 7.2 keV. A shot-to-shot configurable calibration filter pack and Bayesian inference routine were used to constrain the energy dispersion relation to within  $\pm 3$  eV. EFX was primarily designed for x-ray absorption fine structure (XAFS) spectroscopy and provides significant improvement to the OMEGA XAFS experimental platform at the Laboratory for Laser Energetics. EFX is capable of performing EXAFS measurements of multiple absorption edges simultaneously on metal alloys and x-ray absorption near-edge spectroscopy to measure the electron structure of compressed  $3d$  transition metals.

Two EFX spectrometers were designed and built for OMEGA. Diagrams of the physical housing of EFX are shown in Fig. 1, where Fig. 1(a) highlights the different components of EFX and Fig. 1(b) shows a photograph of EFX. The primary components of the spectrometer are a flat silicon [111] crystal and flat image-plate detector, which is loaded into EFX through the back of the housing, opposite the x-ray source. The crystal and detector are held in an aluminum housing with an entrance port for the x rays on one side, as shown in Fig. 1(a). Four crystals were built for EFX: three 170-mm-long Si [111] crystals and one 110-mm-long Si [111] crystal. A blast shield to protect the crystal and a filter pack to characterize the energy dispersion are held in the front of EFX. To reduce noise, EFX has a 3.175-mm-thick, external tungsten shell and a 12.7-mm-thick, tungsten line-of-sight block that protects the detector from the x-ray source.

The performance of EFX was tested on OMEGA by simultaneously measuring EXAFS from multiple K edges of an alloy material. Invar ( $\text{Fe}_{64}\text{Ni}_{36}$ ) foil was placed in the front-end filter pack of the EFX and the EXAFS spectrum from the Fe and Ni K edges was measured. The resulting spectra are shown in Fig. 2(a). By measuring two edges simultaneously, we are able to analyze both the iron and nickel K edges, allowing for more information to be extracted from a single shot.

The improved spectral resolution of EFX allows for x-ray absorption near-edge spectrometry (XANES) measurements to be made on OMEGA. Figure 2(b) shows the XANES from an iron foil in the front end of the EFX. A spectrum measured by an x-ray spectrometer (XRS) on the same shot is also shown for reference. XRS has been previously used to measure EXAFS on OMEGA<sup>1</sup> but was not able to perform XANES measurements. To highlight the key XANES features, the spectrum from iron measured at a synchrotron<sup>2</sup> is shown in the inset. The improved resolution of EFX is shown in the spectrum's steeper slope and ability to begin to capture the white line (point A) and central modulation (point B), which can be used to distinguish structural changes and melting in iron.<sup>3</sup> XANES pre-edge features have also been shown to increase with increasing compression,<sup>4</sup> meaning

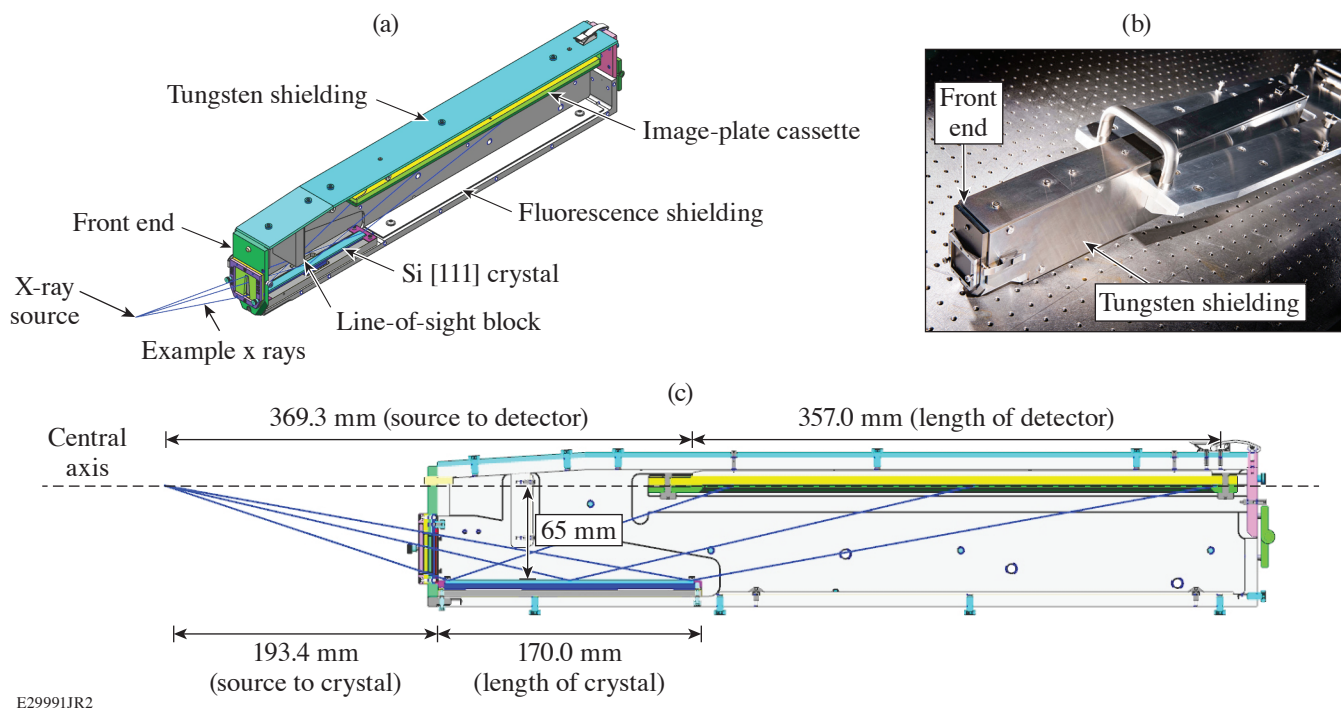


Figure 1  
 (a) Schematic of EFX showing the positions of the Si [111] crystal, the front end, and image-plate detector. (b) Photograph of EFX. (c) Cross section of EFX, highlighting the relevant distances for energy-dispersion calculations.

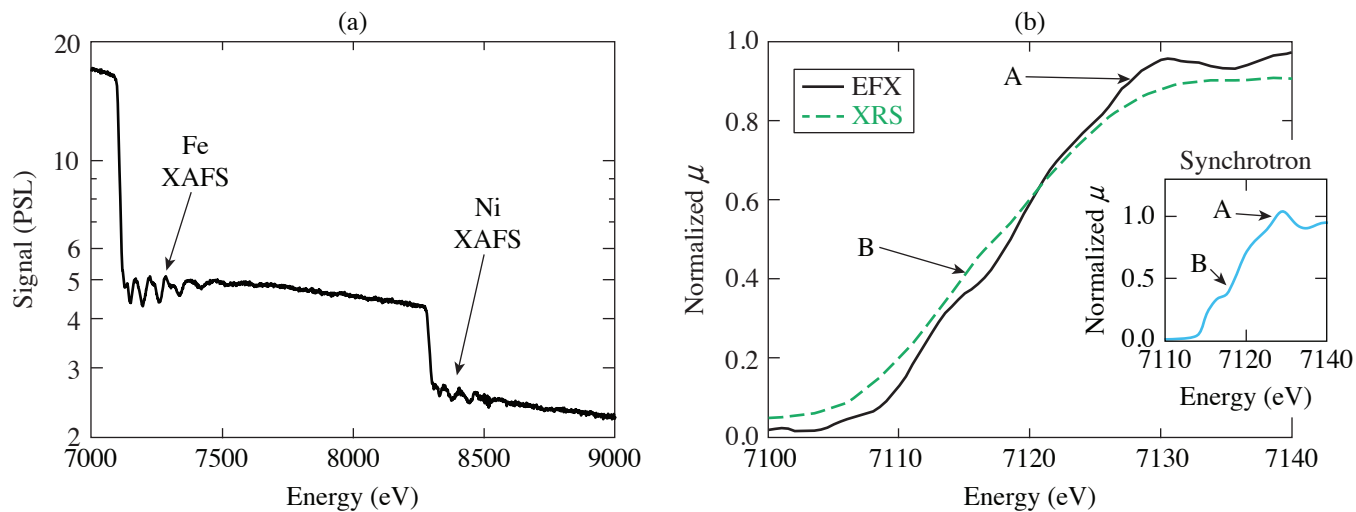


Figure 2  
 (a) Measured EXAFS spectra from Invar ( $\text{Fe}_{64}\text{Ni}_{36}$ ) showing the Fe and Ni K edges from shot 100646. The figure demonstrates the capability of EFX to perform EXAFS on multiple edges of the same alloy simultaneously. (b) Comparison of iron XANES data between an EFX spectrum (black solid line) and an XRS spectrum (green dashed line), both taken on shot 97178. The higher resolution of EFX allows it to capture more detail in the white line (point A) and the central modulation (point B). Inset: An iron synchrotron spectrum,<sup>2</sup> where the same A and B points are highlighted similar to (b).

that these features may become more apparent during laser-driven experiments. This improved resolution in the XANES region of the spectrum will allow for future electron structure measurements of compressed materials.<sup>4</sup>

This material is based upon work supported by the Department of Energy National Nuclear Security Administration under Award Number DE-NA0003856. D. A. Chin acknowledges DOE NNSA SSGF support, which is provided under Cooperative Agreement No. DE-NA0003960. This collaborative work was partially supported under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contracts No. DE-AC52-07NA27344.

1. Y. Ping *et al.*, *Rev. Sci. Instrum.* **84**, 123105 (2013).
2. International X-Ray Absorption Society: Fe Data, IXAS X-Ray Absorption Data Library, Accessed 10 May 2021, <https://xaslib.xrayabsorption.org/elem/>.
3. M. Harmand *et al.*, *Phys. Rev. B* **92**, 024108 (2015).
4. A. Sanson *et al.*, *Phys. Rev. B* **94**, 014112 (2016).