A laser-plasma platform for ultra-fast absorption spectroscopy: measuring the electron-ion equilibration rate of warm dense matter

Contact: b.kettle@imperial.ac.uk

B. Kettle, C. Colgan, E. Los, E. Gerstmayr, R. A. Baggott, R. Watt, S. J. Rose, S. P. D. Mangles
The John Adams Institute for Accelerator Science, Blackett Laboratory, Imperial College London, London SW7 2AZ

F. Albert
Lawrence Livermore National Laboratory, Livermore, California 94550, USA

K. Falk, M. Šmíd
Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstrasse 400, 01328 Dresden, Germany

A. G. R. Thomas
Center for Ultrafast Optical Science, University of Michigan, Ann Arbor, Michigan 48109-2099, USA

M. J. V. Streeter, N. Cavanagh, D. Riley, G. Sarri
Department of Physics and Astronomy, Queen's University Belfast, Belfast, BT7 1NN, United Kingdom

S. Astbury, P. P. Rajeev, C. Spindloe, D. Symes, C. Thornton
Central Laser Facility, STFC Rutherford Appleton Laboratory, Didcot, OX11 0QX, UK

O. Lundh, K. Svendsen
Department of Physics, Lund University, P.O. Box 118, S-22100, Lund, Sweden

Abstract

The K-edge absorption profile of a copper sample has been measured over a 200 eV spectral window on a single shot using the ultrafast x-rays from a laser-wakefield accelerator. This provides simultaneous snapshot details of the samples electronic and ionic configurations through the XANES (X-ray Absorption Near Edge Structure) and EXAFS (Extended X-ray Absorption Fine Structure) profiles. We discuss how, when combined with an appropriate sample heating technique, this unique x-ray source could be used to measure ultrafast processes in high density matter, for example the electron-ion equilibration rates of warm dense samples.

1 Introduction

In recent years laser-plasma based accelerators have provided access to gigaelectronvolt electron energies within laboratory scale facilities [1–3]. This has led to new avenues of research such as strong field QED studies [4, 5], electron-positron pair generation [6, 7] and new X-ray and Gamma ray source applications [8–11]. One growing area makes use of the keV x-ray emission that is generated in tandem with the accelerated beam as the electrons wiggle in the back of the plasma wakefield bubble [12, 13]. A key strength of this source is that it has a smooth, broadband synchrotron-like spectrum with a critical energy of 10's of keV, making it ideal for x-ray absorption spectroscopy (XAS) techniques such as X-ray Absorption Near-Edge Structure (XANES) and Extended X-ray Absorption Fine Structure (EXAFS) spectroscopy. In these techniques the scattering and interference of ejected photoelectrons from neighboring atoms manifest as modulations in the absorption profile near resonant edges. These modulations are directly linked to the local electronic and atomic structure of the sample. In fact the electron temperature, ion temperature, ionisation state and local atomic positions can be simultaneously measured. These techniques have been used with great success over the last few decades on synchrotron facilities worldwide to measure the structure of materials at ambient conditions [14].

The x-rays generated in laser-plasma accelerator sources have the added benefit of having a pulse duration comparable to the emitted electron bunch; usually 10's of femtoseconds [15–17]. This means it is possible for this ultrashort x-ray pulse to be coupled with other laser-plasma systems to investigate conditions not possible at synchrotron systems [18]. Recently single-shot XANES measurements using a laser-plasma accelerator source have been demonstrated [19], and previously multi-shot measurements of ultrafast phenomena have been made [18, 20].

In this article we show we have extended the single-shot spectral range into the EXAFS region and present a platform for a laser-plasma accelerator based x-ray absorption spectroscopy that will be capable of measuring

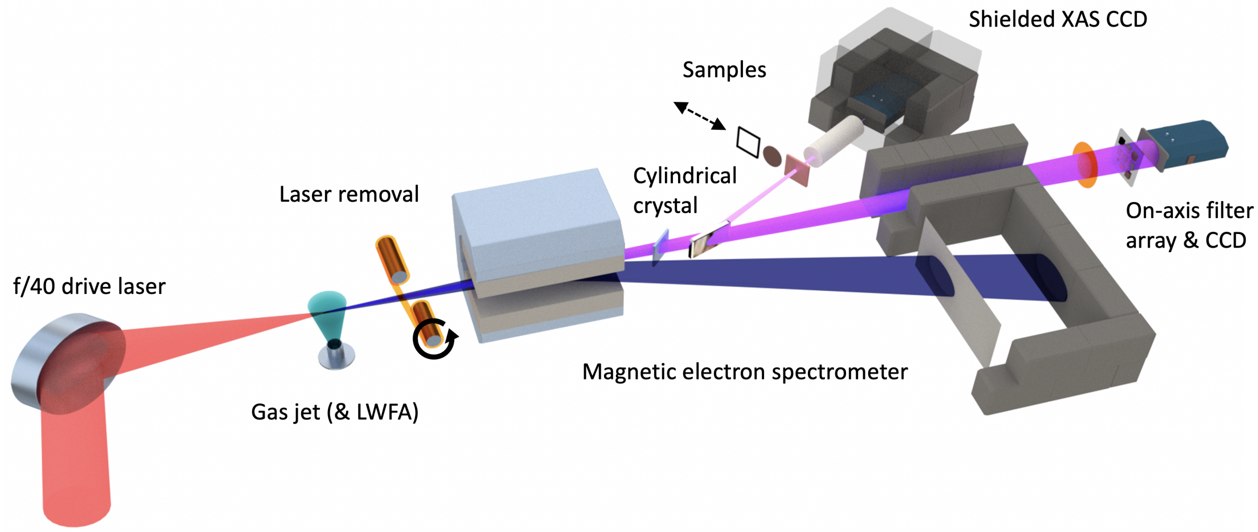

Figure 1: Overview of the experimental setup. An f/40 laser creates a LWFA in a high pressure gas jet, generating a beam of on-axis electrons and x-rays. The electrons are swept away by a dipole magnet and the x-rays are either diffracted off a cylindrical crystal through a sample and spectrally spread onto a shielded CCD, or alternatively (with the crystal translated out) straight onto a CCD through a multi-element filter array used to infer the broad spectral shape.

ultrafast processes in high energy density matter. Specifically, we propose how it can be used to investigate the electron-ion equilibration rate of warm dense copper.

Warm Dense Matter (WDM) exists near solid density with a temperature of 0.1-10's eV. In this regime there is a complex interaction between the thermal motion of the particles and their binding potential; degeneracy and quantum effects become apparent [21]. These complexities make it difficult to model and experimental measurements are crucial to understanding its behaviour. In particular the electron-ion coupling, or equilibration rate is a process which is not well understood, and is a highly sought after measurement [18, 22–24]. A range of models for this crucial parameter have been developed, including solid state approaches based on electron-phonon interactions [23], and plasma-based models which may incorporate collective effects [25]. Understanding the electronic and ion dynamics on an atomic scale allows macroscopic properties to be derived (optical, magnetic, transport, EOS, etc.). Due to the timsescales involved, in order to study this process an ultrashort duration x-ray probe must be used. This is where the unique properties of laser-plasma accelerator x-rays can excel. Detailed measurements of the electron-ion coupling with sub-ps resolution will provide much needed data to validate and refine the theoretical models.

2 Experimental Setup

The experiment was conducted using the Gemini Laser at the Central Laser Facility (U.K.). An overview of the experimental setup can be seen in figure 1. The drive laser (800 nm) was focused using an f/40 geometry onto a 15 mm diameter gas jet nozzle. As this pulse propagates through the gas, it drives the laser wakefield accelerator (LWFA), expelling electrons from atoms and creating a charge cavity in the wake of the laser pulse. A 99% He and 1% N mix was used to promote ionisation injection of electrons into the charge cavity for acceleration to GeV energies [26, 27]. The nozzle was operated at 100 bar backing pressure, providing an estimated plasma density of $\approx 3 \times 10^{18}$ cm^{-3}. Each laser pulse (provided at 0.05 Hz) had a duration of 45 ± 5 fs and contained 9 ± 1 J. These pulses were focused to a spot of 46 ± 3 μm $\times$ 43 ± 3 μm FWHM, with the central FWHM containing 44 ± 3% of the energy. This provided an on-target intensity of $8 \pm 2 \times 10^{18}$ W/cm^2 and a laser strength parameter of $a_0 \approx 1.9$.

After the LWFA the residual drive laser was blocked by a refreshable tape drive (25 μm Kapton), and the electron beam was diagnosed with a 0.3 Tm magnetic spectrometer that dispersed the beam onto an imaged lanex screen. The remaining broadband x-ray beam is reflected off a cylindrical HAPG (Highly Annealed Pyrolytic Graphite) crystal, onto a well shielded x-ray CCD (*XAS CCD*). The crystal spectrally disperses the x-rays in one axis, while spatially focusing them in the other axis. The crystal was tilted 11.8° from the x-ray axis to observe x-rays in the 9 keV region, and was placed 825 mm from the gas jet (x-ray source). The CCD is also 825 mm from the crystal to maintain a 1-to-1 focus with the cylindrical crystal (required for optimal spectral resolution when using mosaic crystals such as HAPG). An additional single layer of aluminium foil (10 ± 2 μm) was

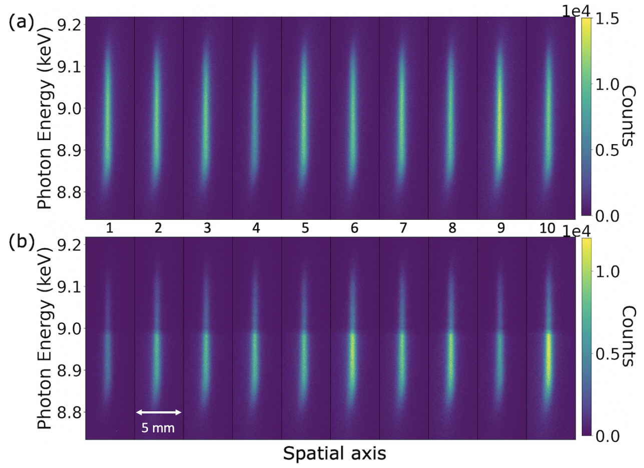

Figure 2: (a) Raw XAS CCD data for ten consecutive shots. The x-rays are spatially focused to a line, and spectrally spread in the vertical axis. (b) The next 10 consecutive shots, but with a 4 μm copper foil placed in the x-ray beam. The K-edge absorption is clear, and the LWFA x-rays are performing in a stable manner.

placed in front of the crystal at 45°, to further protect the crystal from laser damage in the case of the tape drive failing. The combined transmission of the Kapton tape and aluminium foil is over 80% at 9 keV. The x-ray CCD was an Andor DX435, with a 2048 x 1024 chip with 13 μm pixels, covered by an additional 10 ± 2 μm aluminium foil layer to prevent light leaks. Various copper samples were placed on a translation stage before the entrance to the CCD, so that their absorption can be measured. By temporarily moving the crystal out of the way, it was also possible to infer the full broadband spectrum of the x-rays using an on-axis CCD with an elemental filter array placed in front. This technique is now common place for measuring the critical energy of the synchtron-like spectrum [9, 12, 28, 29]

3 Results

Figure 2 (a) and (b) depicts XAS CCD data for 10 example shots from two consecutive runs. For these shots the electron beams contained an average charge of 128 ± 46 pC (standard deviation), and had maximum energies (90th percentile) of 717 ± 99 MeV. The total XAS CCD counts for each run (proportional to total photon number in our 9 keV photon region) had a standard deviation of 13% and 25% respectively (relative to the mean). For a preceding run of shots (not shown), the on-axis filtered x-ray CCD provided estimates of the mean critical energy of the broadband spectra as 28 ± 3.7 keV. The x-ray beam had a divergence (FWHM) of 14 ± 1 mrad (witnessed by the on-axis camera).

For figure 2 the vertical axis is spectrally dispersed, with higher photon energies at the top of the image, and the colour scheme is proportional to the x-ray flux onto the CCD. Figure 2 (a) has no sample in the path of the beam and is a direct measurement of the beam spectrum. Figure 2 (b) has a 4 μm copper sample placed in the beam path. In these shots the absorption drop due to the K-edge is clearly evident. By averaging over the spectral profiles of the direct signal shots in (a), an average reference profile can be found. By dividing the copper filter profiles of (b) by this reference profile one can infer the absorption profile of the sample (the known transmission before the edge is used to anchor the magnitude of the reference profile). Once an absorption profile is found, a normalised absorption is calculated by fitting below and above the copper K-edge, subtracting the former, before dividing by the latter. The process is a standard XANES and EXAFS procedure, and we follow the method outlined in our previous work [19].

Figure 3 depicts the resulting normalised absorption data for the copper sample. The profile covers a 200 eV range, and demonstrates a marked increase in signal-to-noise over the 2019 publication [19]. The profile for a single shot is given in red, and the average profile for the 10 shot run is given in black. Both are compared to the absorption profile of a similar sample scanned at the Diamond synchrotron facility (green), and the same reference convolved with the simulated instrument function for our system (blue). In our case a simulated instrument response [30] indicates a spectral resolution of ≈ 5 eV (FWHM). The inset, figure 3 (b), gives a closer look at the profile close to the edge. The difference in the pre-edge magnitude (at $\approx$ 8985 eV) is currently being investigated further.

4 Discussion

The two most important alterations to the experimental setup (compared to the results of 2019) were the switch to a spatially focusing cylindrical crystal, and the appropriate handling of the electron beam noise (by sweeping the beam into a shielded dump and separately enclosing the XAS CCD in a shielded enclosure). Both these factors contributed to greatly increased signal-to-noise, and stretching the spectral range of the absorption profile. This has made it possible to measure both the XANES and EXAFS profiles on a single-shot, a powerful capability when probing the physics of targets heated to extreme conditions, especially when this measurement is made over an ultrafast snapshot duration of tens of femtoseconds or less.

As an example case study for how this ultrafast x-ray absorption spectroscopy source can be implemented, we have simulated the electron-ion coupling of warm dense copper at 1 eV. Figure 4 depicts the simulated absorption spectra (using ABINIT [31]) for (i) a cold copper foil, (ii) a copper foil with $T_e = 2$ eV and cold ions, and (iii) a copper foil with $T_e = T_i = 1$ eV (equilibrated). A 3 eV instrument function is applied. The increased

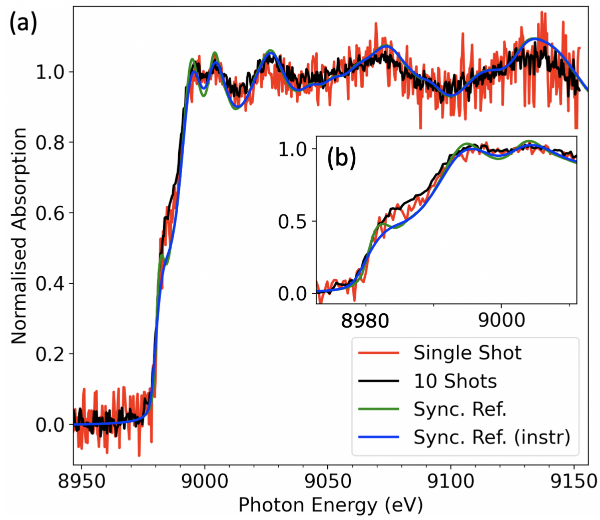

Figure 3: (a) Normalised absorption profile of the 4 μm copper foil. Data is shown for a single shot (red) and the average of the ten shots given in figure 2 (black). Both are compared to a synchrotron reference (green) and the same reference which has been convolved with our simulated instrument response (blue). (b) A zoomed view of the near edge profile.

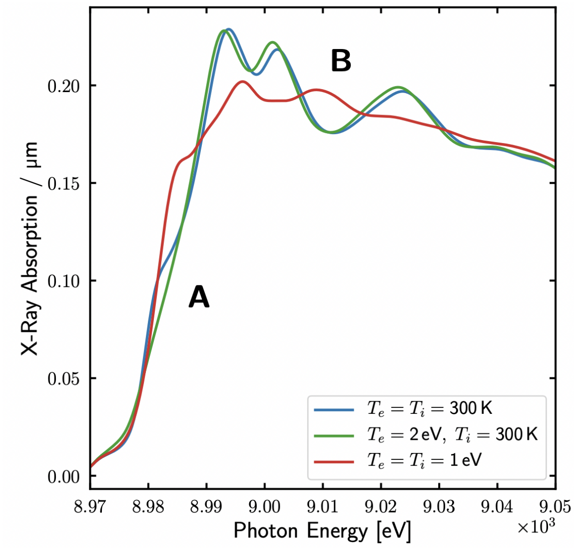

Figure 4: DFT simulations of copper XANES profiles for (i) a cold foil, (ii) a foil with $T_e = 2$eV and cold ions (i.e. non-equilibrium), and (iii) a foil with $T_e = T_i = 1$eV.

edge slope due to the electron temperature (Fermi level broadening) is clear in the latter two cases ("A"). However, the loss of the modulations due to ion heating is only evident in the final case ("B"). For any single spectrum, by comparing the edge slope with the modulation structure we can infer the electron and ion temperature simultaneously. In a proposed pump-probe experiment, one could use a picosecond laser-plasma x-ray source to radiatively heat a micron thick sample to the required $\approx$ eV temperatures, before any hydrodynamic expansion takes place. By taking shots at various temporal delays the electron and ion temperature history of the sample can be reconstructed, and the electron-ion equilibration rate inferred. This evidence can be used to identify the correct underlying theoretical coupling model. Such an experiment can be performed for various other elements by changing the photon probe energy (simple change in crystal angle). Alternatively similiar experiments can be used to investigate other ultrafast electronic and ionic processes such as bond-hardening [32] or non-thermal phase changes [33].

Development of this ultrafast x-ray absorption platform is on-going. Recent studies have shown that machine learning can be used to improve the electron accelerator stability [34]. Additionally, novel techniques that implement tailored density profiles for the LWFA gas target have shown that the on-shot x-ray flux can be increased by an order of magnitude [35]. In the future as more powerful laser systems come online, this will lead to higher electron energies, an increase in charge and an increase in the associated x-ray flux [36]. Already petawatt class (more than 4 times the drive laser energy used in this article) facilities exist, with repetition rates on order of 1 hertz (a x20 increase in data taking speed). This progress should allow laser-plasma accelerator based x-ray absorption platforms to compete with Synchrotron facilities, as well as offering the unique chance to investigate high energy density physics phenomena experimentally for the first time.

5 Conclusion

In conclusion, we have demonstrated that the x-rays from a LWFA source are sufficiently bright and stable to measure the absorption profile around the copper K-edge, over a 200 eV spectral window. The absorption profile is of high enough quality to make single-shot XANES and EXAFS measurements. Further to this, simulations show that it will be possible to make simultaneous but independent measurements of the electron and ion temperature of a rapidly heated copper sample. By performing a temporal scan and making use of the ultrashort duration of the LWFA x-rays this will allow the deduction of the electron-ion equilibration of warm dense copper. These measurements, with other possible ultrafast investigations, will help further our understanding of the complex state of WDM, which is fundamental to a range of fields including astrophysics, planetary science and fusion.

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