

Investigating the Structure and Temperature of Matter at Extremes using X-ray Free Electron Lasers

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Most of the matter in our universe, including within the Earth, exists at high pressures and temperatures. Therefore, understanding the behaviour of matter at extremes is essential for understanding many applications, including geophysics, planetary science and astrophysics, shock and plasma physics, warm dense matter research and pathways to fusion energy. This PhD project will involve using X-ray Free Electron Lasers (XFELs) to explore the complex behaviour that simple systems exhibit when they are driven far from ambient conditions.

Typically, extreme states are created in the laboratory through a variety of methods: by shock compression using nanosecond laser drivers [1], by isochoric heating via femtosecond laser excitation [2], by laser-generated proton beam heating [3], or by direct heating using a high intensity, femtosecond X-ray beam [4]. Due to the time-resolved nature of the methods used, the created states are highly transient, existing for a few picoseconds to a few nanoseconds, and have a large density of free electrons, making them challenging to probe using optical techniques. XFEL light sources, such as the [LCLS](#), USA, and the [European XFEL](#), Germany, have revolutionised how such experiments are performed. Crucially, these XFELs provide extremely bright X-rays (> 5 keV) with pulse durations much shorter than an atomic vibration (10s fs in duration) which are capable of penetrating and probing the highly-ionised, short lived states.

One of the most fundamental properties of a material is its structure, and knowledge of this is essential to our understanding of the high-pressure behaviour of materials. As such, a major focus of extreme conditions research at XFELs has been the measurement of the static structure factor, $S(Q)$, via X-ray diffraction. By performing such measurements, our international collaboration has provided unprecedented insight into many different physical phenomena including the occurrence of ultrafast solid-solid and solid-liquid phase transitions, the dynamic strength and failure of materials, the formation of “diamond rain” in Neptune and Neptune-like exoplanets [5-7]. However, while these observations have provided important insight, they are currently limited. In such studies, the density of the state achieved is often determined by combining diffraction observations with calculations, with neither density nor temperature measured directly. This project will focus on developing X-ray diffraction measurements at even higher X-ray energies to provide quantitative insight into the states obtained, and to pursue the development of a model independent temperature diagnostic using inelastic X-ray scattering methods.

Inelastic X-ray Scattering (IXS) is an umbrella term covering many photon in-photon out processes, covering a range of physical phenomena depending on the energy transfer range one chooses to investigate, and allows the direct measurement of the dynamic structure factor, $S(Q, \omega)$. In the millielectronvolt energy transfer range one can measure phonon modes in a solid or (ion-) acoustic modes in a liquid or plasma state, allowing the direct measurement of the material sound speed and bulk or ion temperature [8-10].

Project: This project will focus on performing laser-driven shock compression or ultrafast femtosecond laser heating techniques to generate high density and temperature states in fundamental elemental systems such as silicon, gold, bismuth etc. The evolution of solid-solid and solid-liquid phase transformations will be probed by using X-ray diffraction techniques at state-of-the-art XFELs. In addition, inelastic X-ray scattering techniques will be used to provide insight into the temperature, sound speed, and viscosity of matter at extreme conditions. Experiments will be conducted in large international collaborations at XFEL facilities in Europe and the US. Beamtime at these large-scale facilities is awarded on a highly competitive basis, and experiments are scheduled

with typically one week of set up time and three to five days of access to the X-ray beam to perform the data acquisition.

Specifically, this project will involve learning how to:

- Plan and implement experiments combining high intensity long and short pulse laser systems with X-ray Free Electron Lasers while working in a large international collaboration,
- Perform time-resolved X-ray diffraction and inelastic X-ray scattering measurements from matter at extreme conditions to measure structure, density, temperature, and sound speed to characterise the evolution of physical properties, and
- Critically evaluate, analyse, and interpret the data obtained.

Details of funding: DfE, 3 years

To apply: please register on the Queen's University applications portal

https://dap.qub.ac.uk/portal/user/u_login.php

Deadline: 10th February 2023

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