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The Design and Operation of a New Relativistic Ultrafast Electron Diffraction and Imaging (RUEDI) National Facility in the UK

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Transformative innovations in the science and technology of personalized medicine, energy storage, and clean growth start from achieving atomic and molecular understanding, and then control, of the fundamental (bio)-chemical interactions that determine each process. To generate the required level of understanding and control, the UK is currently investing in the design of a new national facility centered on the unique measurement capabilities offered by relativistic ultrafast electron diffraction and imaging (RUEDI). The underlying science and technology for RUEDI – ultrafast measurements and electron diffraction/imaging - are areas where John Spence made seminal contributions over the course of his career, and his work in these areas continues to guide the development of the science program for this new facility. Should RUEDI be successful in its goals, it will permit the direct observation of atomic/electronic motions directing the very chemistry we must control for the advances listed above.

RUEDI will enable observations that are the very essence of chemistry and by extension, the driving force for biological functions on their fundamental time and length scales. This will permit a determination of structure-function relations in biological systems as a means to better target drug development as well as create new biomimics, beyond mutagenesis, to harness biology in new ways. Catalysis and electrochemistry constitute a significant fraction of the global economy and RUEDI will be used to directly observe the electrical double layer in electrochemical systems and from it help develop new and improved energy storage systems. In addition, experiments will help determine the fundamental mechanisms leading to functionality in catalysts, enabling a more rational hunt for new catalysts and providing the impetus for developing new photocatalysts that will drive future renewable energy sources. The interplay between phonon and electron oscillations would also be directly observable and controllable with RUEDI, allowing it to uniquely probe new concepts in plasmonics and strongly coupled systems for electronic devices, sensors, probes and detectors that could transform the use of nanotechnology.

The working design of RUEDI (Figure 1) is based around a 4MeV RF source with a pulse duration of 10fs, coupled to both a diffraction and an imaging beam line. Multiple ultrabright electron sources will be developed/evaluated in concert to achieve ~femtosecond time resolution out to long time scales to fully capture all the atomic details related to form and function from surface chemistry, structure-function relationships in biology, to exotic forms of matter. The expectation is that the system will have a large enough number of electrons/pulse for single-shot imaging in addition to stroboscopic pump-probe methods. The diffraction capability will be similar to MeV systems used extensively around the world, but in RUEDI we will focus on fast precision rotation/translation ambient/cryo-stages in a UHV chamber. The imaging capability will be unique and involve the design and implementation of what will essentially be a 4MeV TEM. The imaging capabilities should permit sub-nm spatial resolution to be coupled with sub-ps temporal resolution for samples that can be up to ~1cm thick. Using in-situ stage designs for gases/liquids/heating/cryo, high temperature/pressure can be coupled with a wide range of optical excitations to probe many transient and non-equilibrium dynamic states in materials.

The methods and processes that are developed from the five novel RUEDI research themes – materials in extremes, the chemistry of change, internal/external fields, advanced energy technologies, and in-vivo biosciences will contribute to both local and national government policy/strategy for transportation, energy self-sufficiency and patient care. The facility will also help train scientists who can utilize the knowledge and methods to support existing businesses and form new start-ups that will lead to an overall expansion of the UK economy. As part of the development of the facility, RUEDI will involve artificial intelligence to help develop a digital twin for the instrument and to locate, assign and support users for the facility. In this presentation, we will discuss the main science goals of the new facility and the advances in electron diffraction, imaging, analytics and artificial intelligence that will be implemented to determine both the technical specifications of the instrument, and the functioning of the national facility [1].

References:

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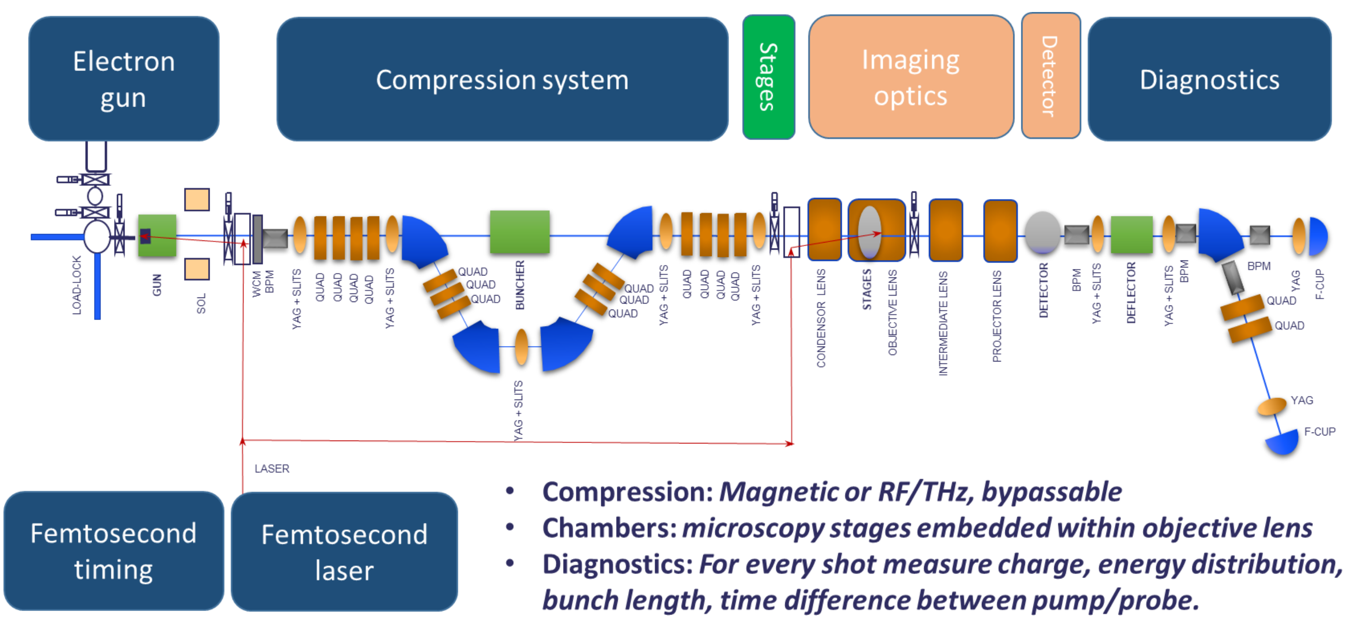

Figure 1: Initial working concept for the configuration of the 4MeV RUEDI system.

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