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UPDATES IN EFFORTS TO DATA SCIENCE ENABLED MeV ULTRA-FAST ELECTRON DIFFRACTION SYSTEM

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Abstract

A MeV ultrafast electron diffraction (MUED) instrument is a unique characterization technique to study ultrafast processes in materials by a pump-probe method. This relatively new technology can be advanced further into a turn-key instrument by using data science and artificial intelligence (AI) techniques in conjunctions with high-performance computing (HPC). This can facilitate auto-mated operation, data acquisition and real-time or near-real-time processing. AI-based system controls can pro-vide real-time feedback on the electron beam which is currently not possible due to the use of destructive diagnostics. Deep learning can be applied to the MUED diffraction patterns to recover valuable information on subtle lattice variations that can lead to a greater understanding of a wide range of material systems. A data science enabled MUED facility will also facilitate the application of this technique, expand its user base, and provide a fully automated state-of-the-art instrument. We will pro-vide updates on research and development efforts the MUED instrument in the Accelerator Test Facility of Brookhaven National Laboratory.

INTORDUCTION

MeV ultrafast electron diffraction (MUED) is a pump-probe characterization technique for studying ultrafast processes in materials. The use of relativistic beams leads to decreased space-charge effects compared to typical ultrafast electron diffraction experiments employing energies in the keV range [1, 2]. Compared to other ultrafast probes such as X-ray free electron lasers, MUED has a higher scattering cross section with material samples and allows access to higher order reflections in the diffraction patterns due to the short electron wavelengths.

However, this is a relatively new technology and several factors contribute to making it challenging to utilize, such as beam instabilities which can lower the effective spatial and temporal resolution. In the past years, machine learning (ML) approaches to materials and characterization techniques have provided anew path towards unlocking new physics by improving existing probes and increasing the user's ability to interpret data. Particularly, ML methods can be employed to control characterization probes in near-real time, acting as virtual diagnostics, or ML can be deployed to extract features and effectively denoise acquired data. In this later case, convolutional neural network architectures such as auto encoder models are an attractive and more powerful alternative to conventional denoising techniques. The autoencoder models provide a method of unsupervised learning of latent space representation of data that can help reduce the noise in the data. By supplying a paired training dataset of "noisy" and "clean" data, these ML models can denoise measurements quite effectively [3, 4]. This method relies on the existence of an ideal dataset with no noise which can be obtained by simulation or by averaging existing noisy datasets. However, in some cases these are not accessible or practical to use. Generative adversarial networks (GANs) are a more suitable option when no "clean" data are available and have been proven to perform well for blind image denoising [5]. They can be trained to estimate and generate the noise distribution, thus producing paired training datasets that can be fed to an autoencoder model. These approaches can lead to increased resolution if employed to denoise, for example, diffraction patterns. In addition, deep convolutional neural network architectures can be used for data analysis. Laanait et. al., for instance, measured diffraction patterns of different oxide perovskites using scanning transmission electron microscopy and, by applying a custom ML algorithm, were able to invert the materials structure and recover 3-dimensional atomic distortions [6]. ML has yet to be applied to the MUED technique, where it can certainly enable advances that can further our understanding of ultrafast material processes in a variety of systems.

EXPERIMENTAL

The MUED instrument is located at the Accelerator Test Facility at Brookhaven National Laboratory. A schematic representation of the experimental setup is presented in Fig.1. The details of data collection are very briefly. described here. The femtosecond electron beams are generated using a frequency-tripled Ti:Sapphire laser that illuminates a copper photocathode, generating a high brightness beam. The electrons are then accelerated and

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compressed in a 1.6-cell RF cavity achieving energies up to 5 MeV. Current parameters of the electron beam source optimized for stability are presented in Table 1. The sample chamber is located down-stream from the source with a motorized holder for up to nine samples with cryogenic cooling capabilities and a window to allow laser pumping of the material. 4 meters down-stream, the detector system is located to collect the diffraction patterns. The detector consists of a phosphor screen followed by a copper mirror (with a hole for non-diffracted electrons to pass) and a CCD Andor camera of 512 pixels x 512 pixels with a large aperture lens. Suitable material systems for MUED require careful preparation with typical lateral sizes of 100 – 300 µm and roughly < 100 nm thickness to assure electron transparency. Laser fluency is adjusted to avoid radiation-induced damage of the probed material.

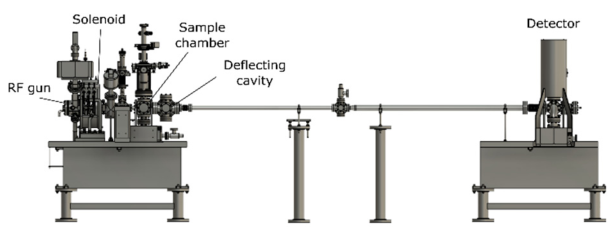

Figure 1: MUED beamline schematic.

Table 1: MUED Source Parameters for Typical Operation

Beam Energy	**3 MeV**
Number of electrons per pulse	1.25×10^6
Temporal resolution	180 fs
Beam diameter	100-300 µm
Repetition rate	5-48 Hz
Number of electrons per sec per μm^2	88-880

UPDATES AND FUTURE PLANS

In 2021, with COVID restrictions lifted, the team has had beam time at the facility, and future visits are being planned for 2022.

Our group uses VSim, a finite-difference time domain (FTDT) and particle-in-cell (PIC) code developed by Tech-X, to model different accelerator devices, including the radiofrequency gun of MUED. We are developing a surrogate model of the MUED beamline for advanced controllers, where VSim is used to model the active region of the copper gun that includes the power coupling waveguide and tuners. For the rest of the MUED beamline, we use elegant, a particle tracker developed at Argonne National Laboratory. Elegant is more suitable for modelling the beam phase space downstream through the solenoid, corrector magnets and collimators. With these combined tools we can model the un-diffracted electron beam all the way down to the detector. We drive the rf gun by defining a plane electromagnetic wave travelling through the waveguide at 2.856 GHz, it takes then about 100 rf cycles to fill the gun and establish the fields in the pi-mode.

During our last experimental run, we also worked on establishing a connection between the MUED facility at BNL and the computing resources at ALCF. We established this connection and will test streaming of data from BNL to ALCF in our next beamtime. This will also enable use of the method described above for all MUED users regardless of the material under study but limited to single crystal samples. We also developed scripts for data analysis that will also be accessible to users and can be run on ALCF.

Recently, we have presented two talks on our recent progress [7, 8]. Finally, a manuscript is in preparation on the research on the unsupervised anomaly detection for the MUED samples.

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