Baseline materials for characterizing the MUED configuration, their role verifying daily alignment and in operation and implementation of a non-destructive real-time machine learning diagnostic for ensuring beam stability

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Collaborators: Destry Monk, Salvador Sosa, Sandra Biedron, Manel Martinez-Ramon, Steve Conradson (UNM); David Martin, Michael Papka (ANL); Marcus Babzien, Mark Palmer, Robert Malone, Jing Tao, Kevin Brown, Mikhail Fedurin, Junjie Li (BNL); Alan Hurd, John Sarrao, Christine Sweeney, Rohit Prasankumar, Julian Chen (LANL).

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Funding secured through DOE EPSCoR program

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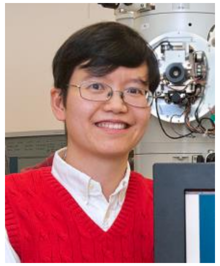

Jing Tao

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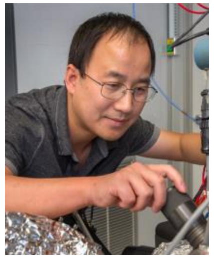

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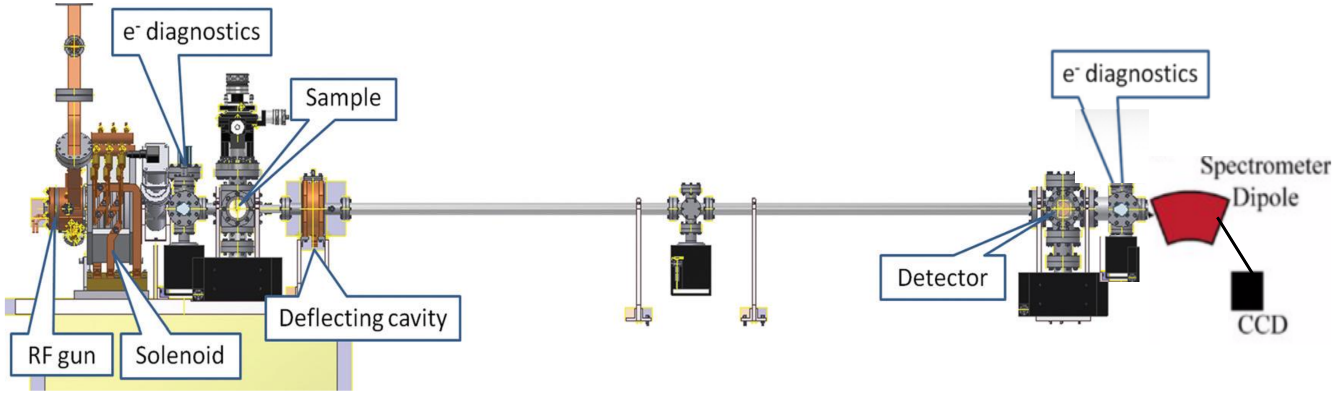
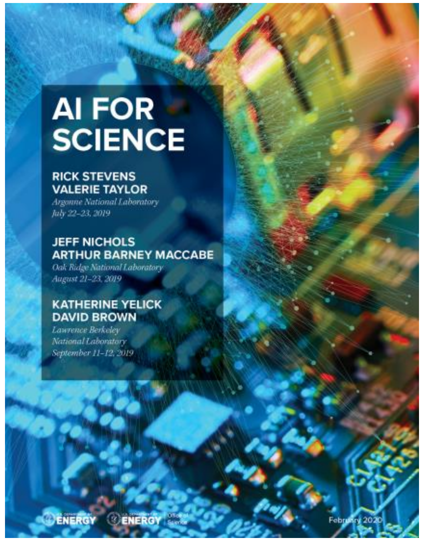
Two DOE facilities are involved: ATF and ALCF

Accelerator Test Facility (ATF)



Argonne Leadership Computing Facility (ALCF)



The combination of machine hardware, advanced computing for simulation, and data science for surrogate modelling, training of neural networks and data analysis is inspired by our past work and our participation on DOE meetings, workshops and reports such as AI for Science (*https://www.anl.gov/ai-for-science-report*).

Special Equipment Requirements and Hazards

Special equipment:

- A ***second camera*** will be eventually required for the last step of the suite of experiments as is the ***associated controls, sample holder etc***. Funding is secured for everything except for this last step.

Hazards:

- ***Black phosphorus*** is classified as a flammable solid and is harmful to aquatic life with long lasting effects. We will handle it with the necessary precautions.

- Other potential hazards include the ***laser*** of the MUED instrument and the ***cryogenic system*** necessary to cool the samples to the desired temperatures. We will work with the BNL collaborators to exercise the necessary precautions.

Experimental time request

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CY2021 Time Request

Capability	Setup Hours	Running Hours
UED Facility	36	84

Time Estimate for Remaining Years of Experiment (including CY2021)

Capability	Setup Hours	Running Hours
UED Facility	108	252

Overview of the proposal

We propose a suite of experiments that will span for a 3-year period aimed at characterizing baseline materials, optimizing their analysis and controlling alignment and stable operation of the instrument.

We will characterize baseline materials, automate the analysis, apply artificial neural network based models and contribute to the development of a MUED database. Analysis of the diffraction patterns will allow determination of the relevant beam parameters and enable to maintain beam stability during the experiment.

At a later stage, a chosen calibration sample will be placed in an extension of the beamline and will interact with the undiffracted beam, providing real-time feedback to the instrument systems.

We expect the proposed experiments move the MUED instrument forward to make it turn-key, high stability, and high-throughput.

Specifics objectives of the proposal

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Baseline materials

1. **Online** - Diffraction measurements of 3 calibration samples for the purpose of alignment of the system.
2. **Online** - For each of the baseline set of materials, measure the diffraction pattern with a variety of pump and delay parameter scans.

Specifics objectives of the proposal

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Automation of analysis and database creation

3. **Offline** - Perform materials analysis with the software available at BNL of these several baseline materials. Automation of the analysis. Place this into a database and begin the artificial neural network based models of the analysis.

Specifics objectives of the proposal

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Non-destructive real-time diagnostic

4. **Offline** - Replicate the diffraction experiment at the end of the beamline to use the undiffracted beam on one of the baseline materials so that it can serve as a non-destructive real-time machine learning diagnostic for ensuring beam stability in the MUED beamline.
5. **Online** – Commission the non-destructive diagnostic with the chosen baseline material and integrate into the machine model. Install, test and validate.

Specifics objectives of the proposal

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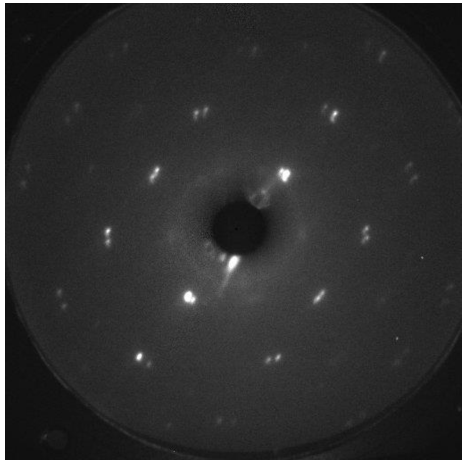
Characterization of baseline materials

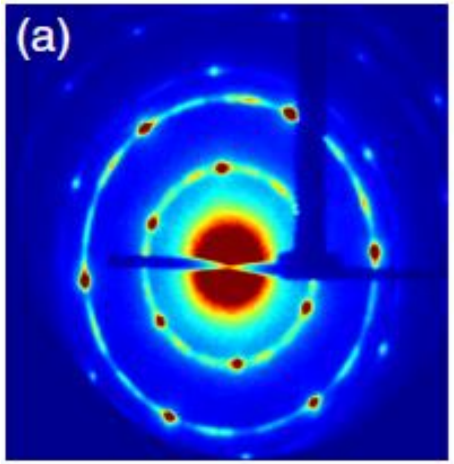
We identified 3 baseline materials:

- Black phosphorus thin films



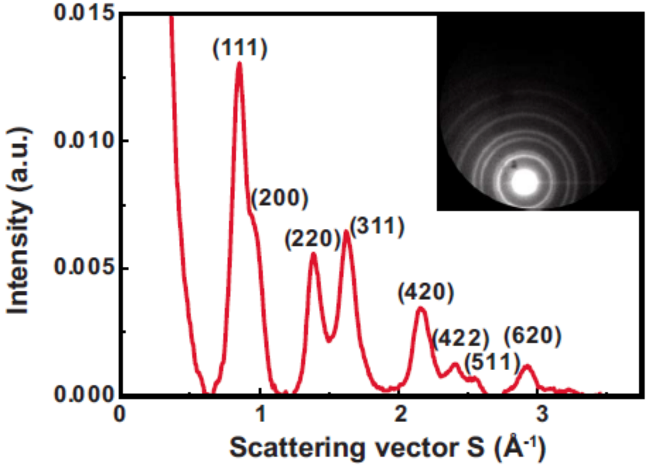
Courtesy of Junjie Li and Jing Tao, measured at BNL

- Graphite thin films



Harb, M., et al. PRB 93.10 (2016): 104104.

- Polycrystalline gold films



Ligges, M., et al. APL 94.10 (2009): 101910.

✓ Material samples are available to use at BNL

✓ All these materials have previously been measured by MUED and good quality diffraction patterns were obtained.

Characterization of baseline materials

- Initial measurements will be conducted at room temperature with no pumping.
- Collected diffraction patterns + readouts of the instruments will be used to construct a machine learning model to align the system.
- This connects with proposal UED-308096 by Salvador Sosa Guitron.
- We want this virtual diagnostic to provide spot size and charge given the setpoints of the instrument.
- Ideally, we would like to operate on <u>single-shot</u> mode (see goals of proposal UED-308096).

Goal: to be able to dial in and maintain, based on the various rapid measurements, the desired spot size and charge at the sample.

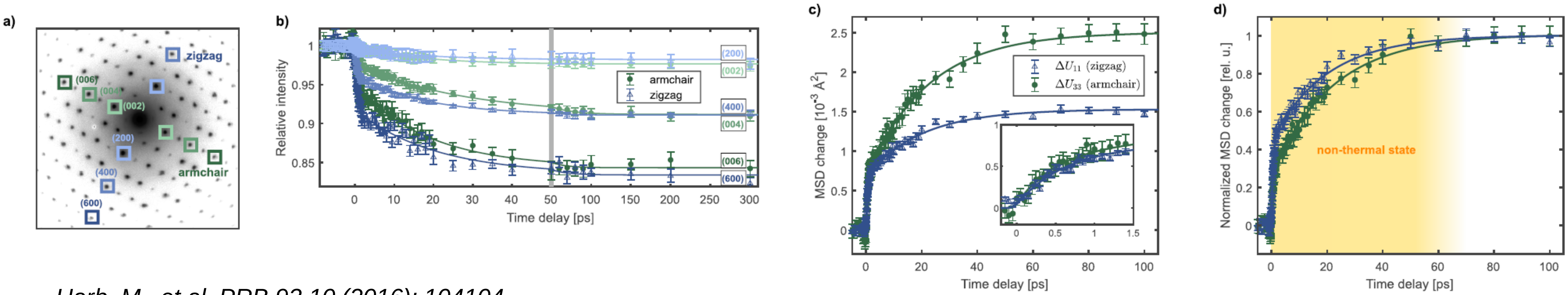
Characterization of baseline materials

- We will also fully characterize these materials systems employing different laser fluences, pulse delays and sample temperature.

- For graphite, it aligns with some experiments of proposal UED-308101 by Hisato Yamaguchi.

- Faster alignment and improved control of electron beam achieved before will provide better quality measurements, allowing further research on these material systems.

- *Example:* lattice dynamics black phosphorus previously analyzed with 70 keV UED



Harb, M., et al. PRB 93.10 (2016): 104104.

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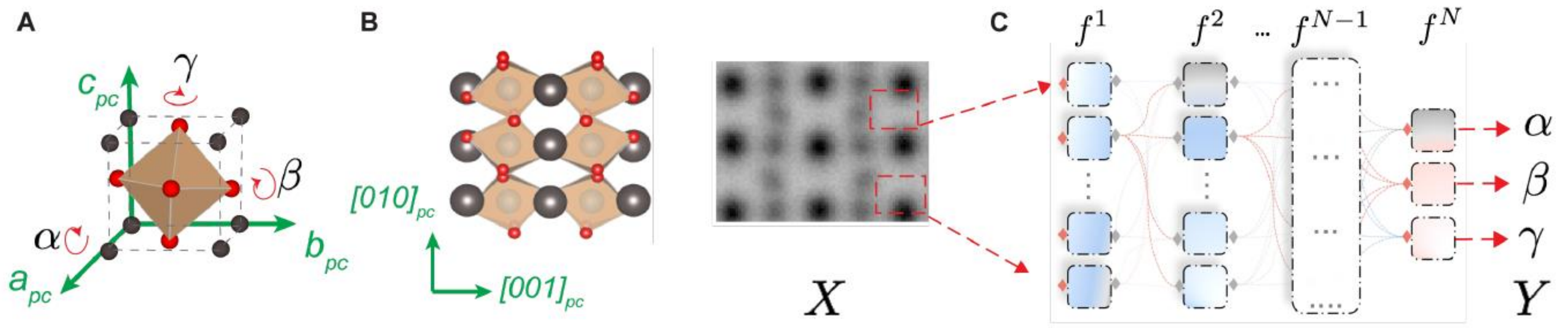
Automation of analysis and database creation

3. **Offline** - Perform materials analysis with the software available at BNL of these several baseline materials. Automation of the analysis. Place this into a database and begin the artificial neural network based models of the analysis.

Analysis automation and database creation

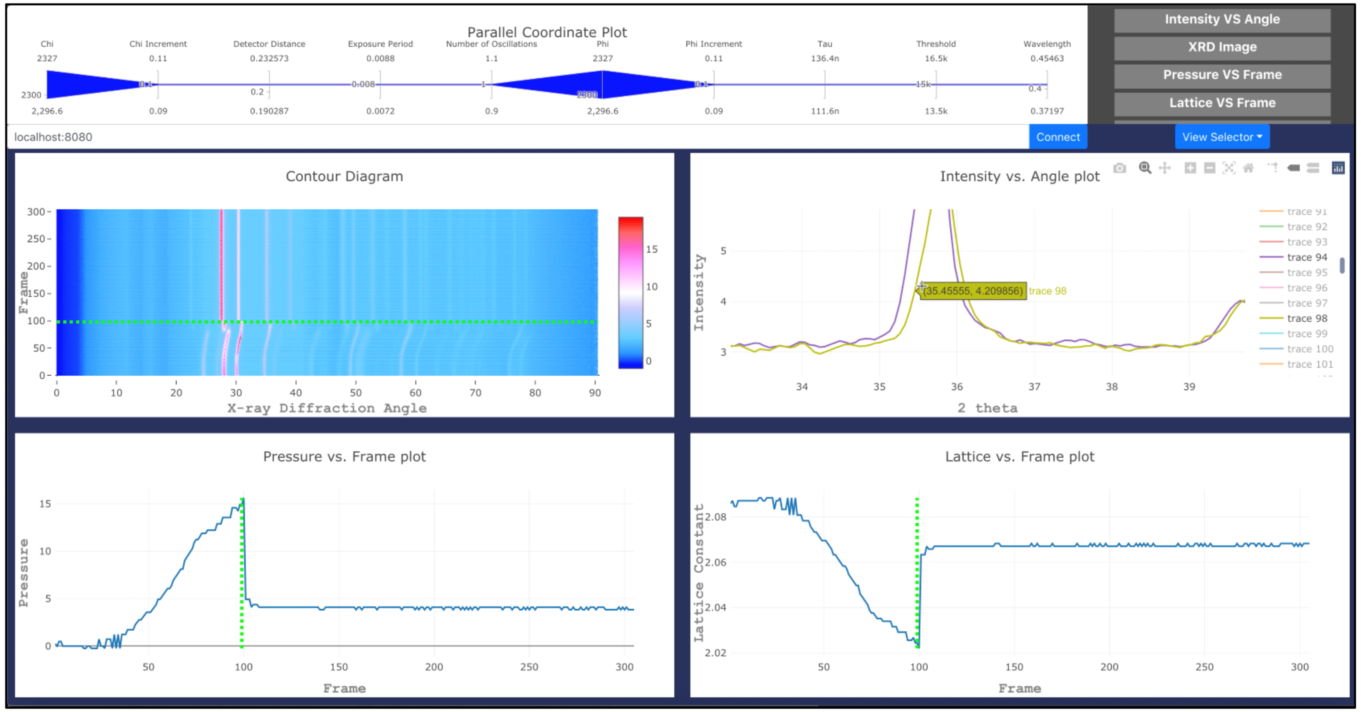
- *These proposed goals involve offline experiments (no instrument time).*
- Analysis of collected diffraction patterns with software available at BNL.
- Automation of this process can lead to real-time analysis (UED-308096). Similar control methodologies on lasers on the main ATF (building 820) proposed by Aasma Aslam (UED-308095).
- We will also implement artificial neural networked based models to extract relevant information and predict the materials structure.
- Relevant previous work on STEM by Nouamane Laanait (ex ORNL) et. al.:



Laanait, Nouamane, Qian He, and Albina Y. Borisevich. arXiv preprint arXiv:1902.06876 (2019).

Analysis automation and database creation

- We will incorporate the use of data visualization tools such as *Cinema:Bandit* (by Sweeney et. al. at LANL)



- Another similar framework developed at ORNL: *Universal Spectroscopic and Imaging Data (USID)*
  - Represents data in a standardized manner.
  - HDF5 data format to facilitate storage of large data.
  - Free open-source Python packages to access and analyze datasets.

Analysis automation and database creation

- All collected diffraction patterns will be stored in a newly created database.
- Team members at LANL have a ‘materials genome-like’ effort under the auspices of the Institute for Materials Science.
- They also have a data repository through the LANL library that they use for all of the LANL Office of Science Data Management Plans (DMPs).
- We will develop a long-term data storage strategy and implementation for archival storage.
- A mirror of the data will be on the Argonne Leadership Computing Facility where this materials data will be used to build models of various material genres to assist with the automated data analysis system based around machine learning.

Specifics objectives of the proposal

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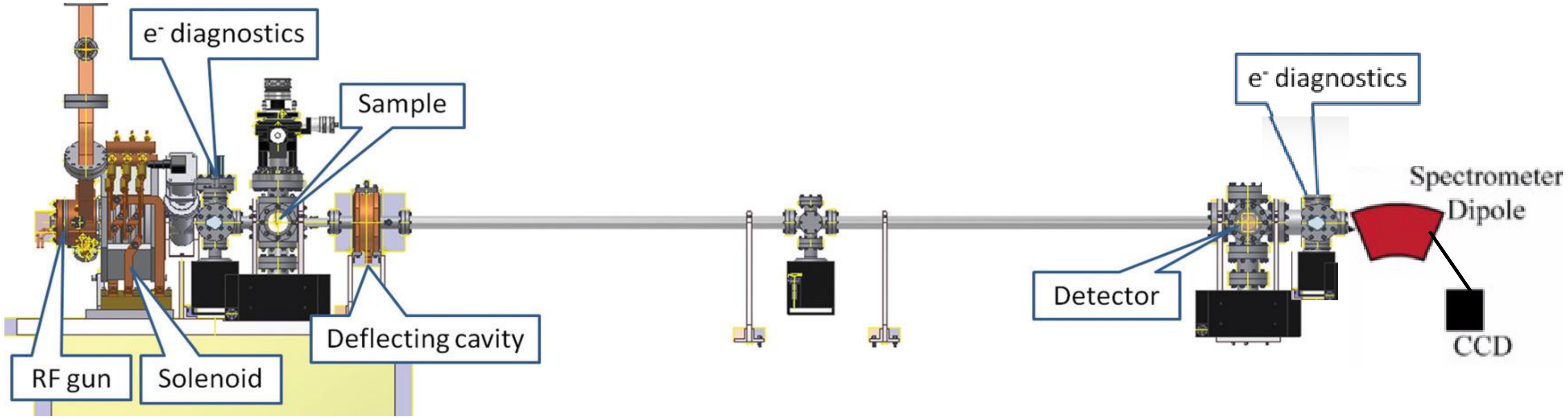
Non-destructive real-time diagnostic

4. **Offline** - Replicate the diffraction experiment at the end of the beamline to use the undiffracted beam on one of the baseline materials so that it can serve as a non-destructive real-time machine learning diagnostic for ensuring beam stability in the MUED beamline.

5. **Online** – Commission the non-destructive diagnostic with the chosen baseline material and integrate into the machine model. Install, test and validate.

Non-destructive real-time diagnostic

- Current setup utilizes undiffracted beam for diagnostics:

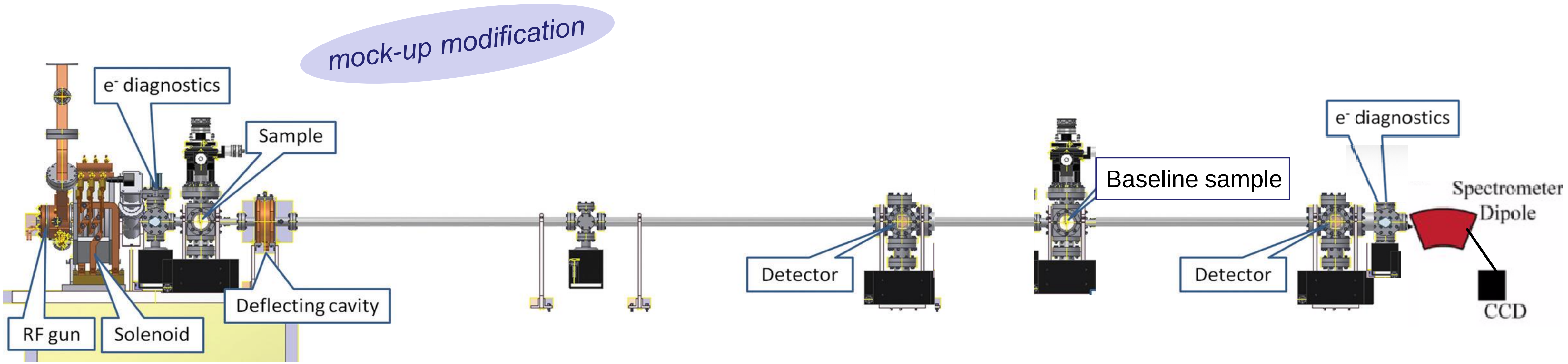


- 90% of incident beam is not diffracted, so how can we exploit this and our previous characterization of baseline materials?

- Purchase of a better-quality camera is planned, can we repurpose the existing camera?

Non-destructive real-time diagnostic

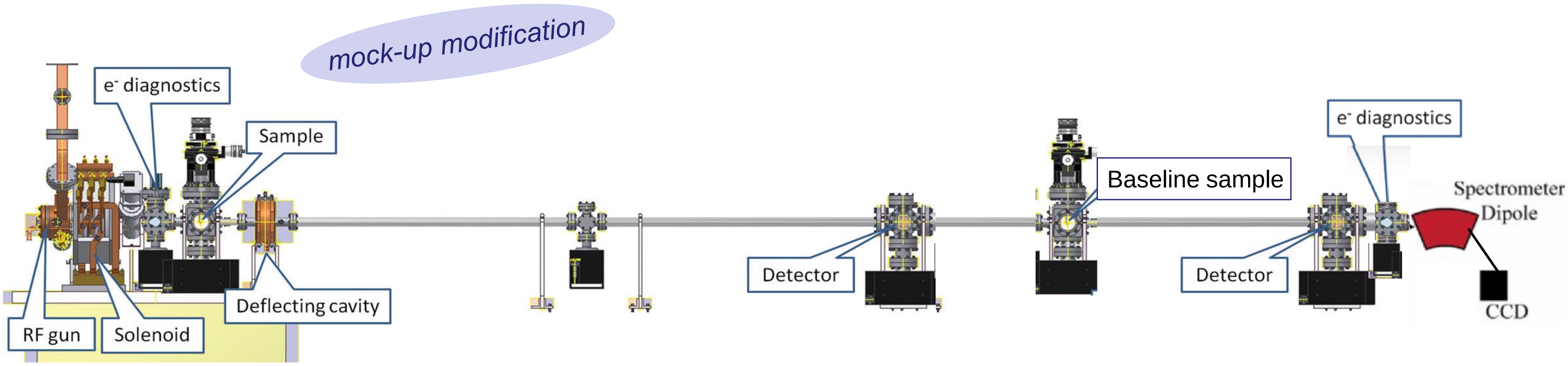
- We can add a second sample chamber containing one of our baseline materials that can interact with the undiffracted beam and use the collect diffraction patterns as a non-destructive real-time diagnostic (*Junjie Li at BNL*).



- We will leverage our previous characterization of the material.

- We can still keep electron beam diagnostics at the end of the beamline.

Non-destructive real-time diagnostic



- Collected diffraction patterns can be fed into our virtual diagnostic developed previously to infer beam parameters.

- Shot-to-shot control of the beam can be implemented using this diagnostic.

Goal: ensure beam stability during single shot measurements with minimum down time of the machine and minimum intervention of the operator

Non-destructive real-time diagnostic

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Ultimate goal: achieve single-shot capabilities for MUED

- Single-shot MUED would enable higher instrument throughput, measurement of samples that are susceptible to pump or probe damage, and potentially higher precision
- Integration of many shots to obtain good S/N ratio limits precision (high-frequency noise sources and systematic errors)
- The full suite of diagnostics described would enable complete pump-probe characterization (pump-probe delay, pump energy, probe charge, probe energy, probe position)
- Normalization of single diffraction patterns to remove these noise sources then becomes possible, improving the precision of each single image, with or without subsequent averaging

Thank you for your attention

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We appreciate all the support from our team members on the development of this proposal.

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