Dr. Siddharth Maddali

Assistant Scientist (Materials Science Division)



















Education

Doctor of Philosophy (**Ph.D**) in *physics* (Carnegie Mellon University, 2016)

Master of Science (M.S.) in *physics* (Carnegie Mellon University, 2010) Master of Science (M.Sc) in physics (Indian Institute of Technology Madras, 2009)

Bachelor of Science (B.Sc) in physics, mathematics, electronics (Bangalore University, 2007)

Experience

Assistant Scientist, Argonne National Laboratory Synchrotron Radiation Studies of Materials group, Oct 2019 - present

Post-doctoral researcher, Argonne National Laboratory Coherent diffraction imaging of materials structure, **Jan 2017 - Sept** 2019

Post-doctoral researcher, National Energy Technology Laboratory Materials discovery with machine learning, *May* 2016 - Sept 2016

Graduate research assistant, Carnegie Mellon University Department of Physics, 2012 - May 2016

Graduate teaching assistant, Carnegie Mellon University Department of Physics, 2009 - 2012

Research interests

X-ray sciences (imaging and characterization):

Coherent diffraction imaging (CDI) of tensor fields Coherent dark-field x-ray microscopy (DFXM) High-energy x-ray diffraction microscopy (HEDM) Multiscale characterization with x-ray probes X-ray photon correlation spectroscopy (XPCS)

Condensed matter physics:

Mesoscale/nanoscale structure and lattice strain Interfacial dynamics in polycrystals

Computational methods in physics:

Inverse problems, phase retrieval
Signal processing and optimization
Data science, machine learning, reinforcement learning -based
experimental control
High-performance computing and scientific software development

Presentations

Invited

- 1) Workshop on Advanced probes and data analytics for enabling singlepulse imaging under dynamic conditions, Santa Fe, NM (August 2019)
- 2) The Minerals, Metals and Materials Society (TMS), San Antonio, TX (March 2019)
- 3) Department of physics, Carnegie Mellon University, Pittsburgh, PA (May 2018)

Select contributed

- 1) Gordon X-ray Science Seminar, Easton, MA (July-August 2019: seminar & poster; July-August 2017: discussion leader)
- 2) Coherence: International workshop on phase retrieval and coherent scattering, Port Jefferson, NY (June 2018)
- 3) Materials Research Society, Phoenix, AZ (April 2018)
- 4) The Minerals, Metals and Materials Society (TMS), Orlando, FL

(March 2015: Poster)

5) Materials Science and Technology (MS&T), Pittsburgh, PA (October

2014: seminar; October 2012: poster)

Awards and honors

Oak Ridge Institute for Science and Education (ORISE) post-doctoral fellowship (2016)

The Indian Institute of Technology Madras Merit Scholarship (2007-2009)

Bangalore University overall rank 5 (2007)

Research grants

ANL LDRD 2021-0012: Coherence-enhanced dark-field imaging for structural heterogeneity in materials

Role: Principal investigator

Funding: Argonne LDRD (Laboratory Directed Research and

Development) program

Period: 1st Oct 2020 — 30th Sept 2021 (1 year)

Amount: \$300,000

ANL LDRD 2019-0042: Finding Critical Processes of Deformation in Structural Materials with Artificial Intelligence

Role: Principal investigator

Funding: Argonne LDRD (Laboratory Directed Research and

Development) program

Period: 1st Oct 2020 — 30th Sept 2021 (1 year)

Amount: \$100,000

Professional activity

Society membership

Americal Physical Society (APS), Materials Research Society (MRS), The Minerals, Metals and Materials Society (TMS)

Editorial

Jan 2020 — present: Topics editor for *MDPI: Crystals*

Peer review P

US Department of Energy: Basic Energy Sciences (BES) Program, Philosophical Magazine, Computational Materials Science, New Journal of Physics, Optics Letters, Physical Review X, Crystal Research and Technology, Journal of Applied Physics, Physical Review Letters, Physical Review B, IUCr Journal of Synchrotron Radiation

Organization

- 1) Workshop: Advances in Phase Retrieval Methodsfor High-Resolution X-ray Imaging, APS/CNM Users Meeting, Argonne National Laboratory, Lemont, IL (August 2020)
- 2) Workshop: Advanced Probes and Data Analytics for Enabling Single Pulse Imaging Under Dynamic Conditions , Santa Fe, NM (August 2019)

Technical reports

[1] R. Pokharel, C. Bolme, J. Bohon, A. Mandal, D. Pagan, F. Hofmann, S. Maddali, A. Rack, Advanced probes and data analytics for enabling 3-D imaging under dynamic conditions (LAUR-19-31832), Los Alamos National Laboratory, 2019.

[2] N. Krishnamurthy, **S. Maddali**, A. Verma, L. Bruckman, J. Carter, R. French, V. Romanov, J. Hawk, *Data analytics for alloy qualification* (**NETL-PUB-21550**), **National Energy technology Laboratory**, 2017.

Conference presentations

[1] Krishnamurthy, N., **Maddali, S.**, Romanov, V. & Hawk, J., *Predictive* analysis of the influence of the chemical composition and pre-processing regimen on structural properties of steel alloys using machine learning techniques. **Bulletin of the American Physical Society**, APS, 2017, 62 (abstract)

[2] Krishnamurthy, N., **Maddali, S.**, Romanov, V. & Hawk, J., Segmentation of 9Cr Steel Samples based on Composition and Mechanical Property. **Bulletin of the American Physical Society**, APS, 2017, 62 (abstract)

Publications

- [1] Wilkin M. J., **Maddali S.**, Hruszkewycz S. O., Pateras A., Sandberg R. L., Harder R. J., Cha W., Suter R. M. and Rollett A. D., *Experimental demonstration of coupled multi-peak Bragg coherent diffraction imaging with genetic algorithms*, **Phys. Rev. B** (in press), May 2021.
- [2] (**Under review**) Bertaux N., Allain M., Weizeorick J., Park J.- S., Kenesei P., Shastri S. D., Almer J., Highland M. J., **Maddali S.** and Hruszkewycz S. O., *Sub-pixel high-resolution imaging of high-energy x-rays by sub-wavelength optical imaging*, 2021.
- [3] (**Under review**) Kandel S., **Maddali S.**, Nashed Y. S. G., Hruszkewycz S. O., Jacobsen C. and Allain Marc, *A matrix-free Levenberg-Marquardt algorithm for efficient ptychographic phase retrieval*, 2021.
- [4] Cao Y., Sheyfer D., Jiang Z., **Maddali S.**, You H., Wang B. X., Ye Z. G., Dufresne E. M., Zhou H., Stephenson G. B. and Hruszkewycz S. O., *The Effect of Intensity Fluctuations on Sequential X-ray Photon Correlation Spectroscopy at the X-ray Free Electron Laser Facilities*, **Crystals**, vol. 10, number 12, pp. 1109, December 2020. online
- [5] **Maddali S.**, Allain M., Li P., Chamard V. and Hruszkewycz S. O., *Detector Tilt Considerations in Bragg Coherent Diffraction Imaging: A Simulation Study, Crystals*, vol. 10, number 12, pp. 1150, December 2020. online
- [6] **Maddali S.**, Park J.-S., Sharma H., Shastri S., Kenesei P., Almer J., Harder R., Highland M. J., Nashed Y. and Hruszkewycz S. O., *High-Energy Coherent X-Ray Diffraction Microscopy of Polycrystal Grains: Steps Toward a Multiscale Approach*, **Phys. Rev. Applied**, vol. 14, number , pp. 024085, Aug 2020. online
- [7] **Maddali S.**, Li P., Pateras A., Timbie D., Delegan N., Crook A. L., Lee H., Calvo-Almazan I., Sheyfer D., Cha W., Heremans F. J., Awschalom D. D., Chamard V., Allain M. and Hruszkewycz S. O., *General approaches for shear-correcting coordinate transformations in Bragg coherent diffraction imaging. Part I, Journal of Applied Crystallography, vol. 53, number 2, pp., Apr 2020. online*
- [8] Li P., **Maddali S.**, Pateras A., Calvo-Almazan I., Hruszkewycz S.O., Cha W., Chamard V. and Allain M., *General approaches for shear-correcting coordinate transformations in Bragg coherent diffraction imaging. Part II*, **Journal of Applied Crystallography**, vol. 53, number 2, pp., Apr 2020. online

- [9] **Maddali S.**, Allain M., Cha W., Harder R., Park J.-S., Kenesei P., Almer J., Nashed Y. and Hruszkewycz S. O., *Phase retrieval for Bragg coherent diffraction imaging at high x-ray energies*, *Phys. Rev. A*, vol. 99, number , pp. 053838, May 2019. online
- [10] Calvo-Almazan I., Allain M., **Maddali S.**, Chamard V. and Hruszkewycz S. O., *Impact and mitigation of angular uncertainties in Bragg coherent x-ray diffraction imaging*, *Scientific Reports*, vol. 9, number 1, pp. 6386, 2019. online
- [11] Kandel S., **Maddali S.**, Allain M., Hruszkewycz S. O., Jacobsen C. and Nashed Y., *Using automatic differentiation as a general framework for ptychographic reconstruction*, *Opt. Express*, vol. 27, number 13, pp. 18653–18672, Jun 2019. online
- [12] Krishnamurthy N., **Maddali S.**, Hawk J. A. and Romanov V. N., *9Cr steel visualization and predictive modeling*, **Computational Materials Science**, vol., number, pp., 2019. online
- [13] Shen Yu-Feng, **Maddali S.**, Menasche D., Bhattacharya A., Rohrer G. S. and Suter R. M., *Importance of outliers: A three-dimensional study of coarsening in \alpha-phase iron, Phys. Rev. Materials, vol. 3, number , pp. 063611, Jun 2019. online*
- [14] Ulvestad A., Hruszkewycz S. O., Holt M. V., Hill M. O., Calvo-Almazan I., **Maddali S.**, Huang X., Yan H., Nazaretski E., Chu Y. S., Lauhon L. J., Rodkey N., Bertoni M. I. and Stuckelberger M. E., *Multimodal X-ray imaging of grain-level properties and performance in a polycrystalline solar cell*, **Journal of Synchrotron Radiation**, vol. 26, number 4, pp. , Jul 2019. online
- [15] Calvo-Almazan I., Ulvestad A. P., Colegrove E., Ablekim T., Holt M. V., Hill M. O., **Maddali S.**, Lauhon L. J., Bertoni M. I, Huang X., Yan H., Nazaretski E., Chu Y. S., Hruszkewycz S. O. and Stuckelberger M. E., *Strain Mapping of CdTe Grains in Photovoltaic Devices*, **IEEE Journal of Photovoltaics**, vol., number, pp. 1-10, 2019. online
- [16] **Maddali S.**, Calvo-Almazan I., Almer J., Kenesei P., Park J.-S., Harder R., Nashed Y. and Hruszkewycz S. O., *Sparse recovery of undersampled intensity patterns for coherent diffraction imaging at high X-ray energies*, *Scientific Reports*, vol. 8, number 1, pp. 4959, 2018. online
- [17] Hruszkewycz S. O., **Maddali S.**, Anderson C. P., Cha W., Miao K. C., Highland M. J., Ulvestad A., Awschalom D. D. and Heremans F. J., *Strain*

annealing of SiC nanoparticles revealed through Bragg coherent diffraction imaging for quantum technologies, **Phys. Rev. Materials**, vol. 2, number , pp. 086001, Aug 2018. online

- [18] Highland M. J., Hruszkewycz S. O., Fong D. D., Thompson C, Fuoss P. H., Calvo-Almazan I., **Maddali S.**, Ulvestad A., Nazaretski E., Huang X., Yan H., Chu Y. S., Zhou H., Baldo P. M. and Eastman J. A., *In-situ synchrotron x-ray studies of the microstructure and stability of In2O3 epitaxial films*, **Applied Physics Letters**, vol. 111, number 16, pp. 161602, 2017. online
- [19] **Maddali S.**, Ta'asan S. and Suter R. M., *Topology-faithful* nonparametric estimation and tracking of bulk interface networks, *Computational Materials Science*, vol. 125, number , pp. 382–340, 2016. online
- [20] Renversade L., Quey R., Ludwig W., Menasche D., **Maddali S.**, Suter R. M. and Borbely A., *Comparison between diffraction contrast tomography and high-energy diffraction microscopy on a slightly deformed aluminium alloy*, *IUCrJ*, vol. 3, number 1, pp. 32–42, 2016. online

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