Siddharth Maddali, Ph.D

Assistant Scientist (Materials Science Division)



























NOTE: Icons are clickable links.

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

Intern, National University of Singapore Department of Physics, May 2008

Research interests

X-ray sciences:

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:

Light-matter interaction Crystallography Meso/nanoscale structure & strain Interfacial dynamics in polycrystals

Computational methods:

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 (presenter)

- 1) Advanced Photon Source Scientific Computation Seminar, Argonne National Laboratory, Lemont, IL (March 2022)
- 2) Materials Science Division Colloquium, Argonne National Laboratory, Lemont, IL (October 2021) <u>□</u>
- 3) Workshop on Advanced Probes & Data Analytics for Enabling Single-Pulse Imaging under Dynamic Conditions, Santa Fe, NM (August 2019)
- 4) The Minerals, Metals and Materials Society (TMS), San Antonio, TX (March 2019)
- 5) LANS seminar series, Mathematics & Computer Science Division, Argonne National Laboratory, Lemont, IL (Sept 2018)
- 6) Department of physics, Carnegie Mellon University, Pittsburgh, PA (May 2018)

Select contributed (presenter)

- 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 Spring Meeting & Exhibit, 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)

Miscellaneous (co-author)

- 1) The American Physical Society (APS) March Meeting, Chicago, IL, 2022.
- 2) The Materials Research Society Spring Meeting & Exhibit, Phoenix, AZ, (April 2018).
- 3) The American Physical Society (APS) March Meeting, New Orleans, LA, 2017 🧵 📜

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 2023 (3 years)

Amount: \$900,000

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

Aug 2021 — present: Guest editor for *MDPI: Crystals* special issue: Synchrotron studies of materials.

Peer review R

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 , Optics Express , Journal of Applied Crystallography , Integrating Materials and Manufacturing Innovation

Organization

- 1) Workshop (Session chair): *Dark field x-ray microscopy for mesoscale phenomena in ordered materials at APS-U*: APS/CNM Users Meeting, Lemont, IL, USA (May 2022)
- 2) Workshop: Advances in Phase Retrieval Methods for High-Resolution X-ray Imaging , APS/CNM Users Meeting, Argonne National Laboratory, Lemont, IL, USA (August 2020)
- 3) Workshop: Advanced Probes and Data Analytics for Enabling Single Pulse Imaging Under Dynamic Conditions, Santa Fe, NM, USA (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. Online LAUL DMMSC

[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.

References

Dr. Stephan O. Hruszkewycz (postdoc mentor/supervisor)

Synchrotron Studies of Materials

Materials Science Division

Argonne National Laboratory

Chicago, IL (USA)

Dr. Robert M. Suter (Ph.D advisor)

Department of physics
Carnegie Mellon University
Pittsburgh, PA (USA)

Dr. Anthony D. Rollett (collaborator, materials science)

Department of Materials Science and Engineering
Carnegie Mellon University
Pittsburgh, PA (USA)

Dr. Marc Allain (collaborator, computation/mathematics)

☐ Institut Fresnel

Aix-Marseille University

Grenoble, France

Publications

- [1] (**Under review**) M. Hill, P. Schmiedeke, C. Huang, **S. Maddali**, X. Hu, S.O. Hruszkewycz, J.J. Finley, G. Koblmueller and L. Lauhon, *3D Bragg coherent diffraction imaging of extended nanowires: defect formation in highly strained InGaAs quantum wells*, 2022.
- [2] (**Under review**) **S. Maddali**, T.D. Frazer, N. Delegan, K.J. Harmon, S.E. Sullivan, M. Allain, W. Cha, A. Dibos, I. Poudyal, S. Kandel, Y.S.G. Nashed, F.J. Heremans, H. You, Y. Cao and S.O. Hruszkewycz, *A differentiable forward model for the concurrent, multi-peak Bragg coherent x-ray diffraction imaging problem, 2022. preprint arXiv:2208.00970*
- [3] N. Bertaux, M. Allain, J. Weizeorick, J.-. Park, P. Kenesei, S.D. Shastri, J. Almer, M.J. Highland, **S. Maddali** and S.O. Hruszkewycz, *Sub-pixel high-resolution imaging of high-energy x-rays inspired by sub-wavelength optical imaging*, *Opt. Express*, vol. 29, number 22, pp. 35003–35021, Oct 2021. Doi 10.1364/0E.438945
- [4] S. Kandel, **S. Maddali**, Y.S.G. Nashed, S.O. Hruszkewycz, C. Jacobsen and M. Allain, *Efficient ptychographic phase retrieval via a matrix-free Levenberg-Marquardt algorithm*, **Opt. Express**, vol. 29, number 15, pp. 23019–23055, Jul 2021.

 preprint arXiv:2103.01767 DOI 10.1364/0E.422768
- [5] M.J. Wilkin, S. **Maddali, S.**O. Hruszkewycz, A. Pateras, R.L. Sandberg, R. Harder, W. Cha, R.M. Suter and A.D. Rollett, *Experimental demonstration of coupled multipeak Bragg coherent diffraction imaging with genetic algorithms*, *Phys. Rev. B*, vol. 103, number, pp. 214103, Jun 2021. DOI 10.1103/PhysRevB.103.214103
- [6] Y. Cao, D. Sheyfer, Z. Jiang, **S. Maddali**, H. You, B.X. Wang, Z.G. Ye, E.M. Dufresne, H. Zhou, G.B. Stephenson and S.O. Hruszkewycz, *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.

DOI 10.3390/cryst10121109

- [7] **S. Maddali**, M. Allain, P. Li, V. Chamard and S.O. Hruszkewycz, *Detector Tilt Considerations in Bragg Coherent Diffraction Imaging: A Simulation Study, Crystals*, vol. 10, number 12, pp. 1150, December 2020. preprint arXiv:2008.01843 DOI 10.3390/cryst10121150
- [8] **S. Maddali**, J. Park, H. Sharma, S. Shastri, P. Kenesei, J. Almer, R. Harder, M.J. Highland, Y. Nashed and S.O. Hruszkewycz, *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.

 [DOI 10.1103/PhysRevApplied.14.024085]
- [9] **S. Maddali**, P. Li, A. Pateras, D. Timbie, N. Delegan, A.L. Crook, H. Lee, I. Calvo-Almazan, D. Sheyfer, W. Cha, F.J. Heremans, D.D. Awschalom, V. Chamard, M. Allain and S.O. Hruszkewycz, *General approaches for shear-correcting coordinate transformations in Bragg coherent diffraction imaging. Part I, Journal of AppliedCrystallography, vol. 53, number 2, pp., Apr 2020. preprint arXiv:1909.05353

 DOI 10.1107/S1600576720001363*
- [10] P. Li, **S. Maddali**, A. Pateras, I. Calvo-Almazan, S. Hruszkewycz, W. Cha, V. Chamard and M. Allain, *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. preprint arXiv:1909.05354*
- [11] **S. Maddali**, M. Allain, W. Cha, R. Harder, J. Park, P. Kenesei, J. Almer, Y. Nashed and S.O. Hruszkewycz, *Phase retrieval for Bragg coherent diffraction imaging at high x-ray energies*, *Phys. Rev. A*, vol. 99, number, pp. 053838, May 2019.

 [Preprint arXiv:1811.06181] [DOI 10.1103/PhysRevA.99.053838]
- [12] I. Calvo-Almazan, M. Allain, **S. Maddali**, V. Chamard and S.O. Hruszkewycz, *Impact and mitigation of angular uncertainties in Bragg coherent x-ray diffraction imaging*, **Scientific Reports**, vol. 9, number 1, pp. 6386, 2019. DOI 10.1038/s41598-019-42797-4
- [13] S. Kandel, **S. Maddali**, M. Allain, S.O. Hruszkewycz, C. Jacobsen and Y. Nashed, *Using automatic differentiation as a general framework for ptychographic reconstruction*, *Opt. Express*, vol. 27, number 13, pp. 18653–18672, Jun 2019.

 [Preprint arXiv:1902.03920 DOI 10.1364/0E.27.018653
- [14] N. Krishnamurthy, **S. Maddali**, J.A. Hawk and V.N. Romanov, *9Cr steel visualization and predictive modeling*, **Computational Materials Science**, vol., number, pp., 2019. Dol 10.1016/j.commatsci.2019.03.015
- [15] Y. Shen, **S. Maddali**, D. Menasche, A. Bhattacharya, G.S. Rohrer and R.M. Suter, Importance of outliers: A three-dimensional study of coarsening in α -phase iron, **Phys. Rev. Materials**, vol. 3, number, pp. 063611, Jun 2019. DOI 10.1103/PhysRevMaterials.3.063611
- [16] A. Ulvestad, S.O. Hruszkewycz, M.V. Holt, M.O. Hill, I. Calvo-Almazan, **S. Maddali**, X. Huang, H. Yan, E. Nazaretski, Y.S. Chu, L.J. Lauhon, N. Rodkey, M.I. Bertoni and M.E. Stuckelberger, *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.
- [17] I. Calvo-Almazan, A.P. Ulvestad, E. Colegrove, T. Ablekim, M.V. Holt, M.O. Hill, **S. Maddali**, L.J. Lauhon, M.I. Bertoni, X. Huang, H. Yan, E. Nazaretski, Y.S. Chu, S.O. Hruszkewycz and M.E. Stuckelberger, *Strain Mapping of CdTe Grains in Photovoltaic Devices*, *IEEE Journal of Photovoltaics*, vol., number, pp. 1-10, 2019.
- [18] A. Ulvestad, W. Cha, I. Calvo-Almazan, S. Maddali, S.M. Wild, E. Maxey, M.

- Dupraz and S.O. Hruszkewycz, *Bragg Coherent Modulation Imaging: Strain- and Defect- Sensitive Single Views of Extended Samples*, 2018 preprint arXiv:1808.00115
- [19] **S. Maddali**, I. Calvo-Almazan, J. Almer, P. Kenesei, J. Park, R. Harder, Y. Nashed and S.O. Hruszkewycz, *Sparse recovery of undersampled intensity patterns for coherent diffraction imaging at high X-ray energies*, *Scientific Reports*, vol. 8, number 1, pp. 4959, 2018. preprint arXiv:1712.01108 DOI 10.1038/s41598-018-23040-y
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