

Dr. Siddharth Maddali

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 (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 in imaging, 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) Advanced Photon Source Scientific Computation Seminar, Argonne National Laboratory, Lemont, IL (March 2022)
- 2) *New materials characterization capabilities with high-energy coherent X-rays*, Argonne Materials Science Division Colloquium, Lemont, IL (October 2021)
- 3) Workshop on *Advanced probes and 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) 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 2022 (2 years)

Amount: \$630,000

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

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.  

[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.

 [10.2172/1456238](https://doi.org/10.2172/1456238)

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)

References

Dr. Stephan O. Hruszkewycz

Synchrotron Studies of Materials

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Argonne National Laboratory

Chicago, IL (USA)



Dr. Robert M. Suter

Department of physics

Carnegie Mellon University

Pittsburgh, PA (USA)



Dr. Anthony D. Rollett

Department of Materials Science and Engineering

Carnegie Mellon University

Pittsburgh, PA (USA)



Dr. Marc Allain

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. Koblmuehler 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/OE.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/OE.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 multi-peak 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. preprint [arXiv:1903.11815](#) 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 Applied Crystallography**, 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](#) DOI [10.1107/S1600576720001375](#)

[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/OE.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. DOI [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. DOI [10.1107/S1600577519003606](#)

[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. DOI [10.1109/JPHOTOV.2019.2942487](https://doi.org/10.1109/JPHOTOV.2019.2942487)

[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](https://arxiv.org/abs/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](https://arxiv.org/abs/1712.01108) DOI [10.1038/s41598-018-23040-y](https://doi.org/10.1038/s41598-018-23040-y)

[20] S.O. Hruszkewycz, **S. Maddali**, C.P. Anderson, W. Cha, K.C. Miao, M.J. Highland, A. Ulvestad, D.D. Awschalom and F.J. Heremans, *Strain annealing of SiC nanoparticles revealed through Bragg coherent diffraction imaging for quantum technologies*, **Phys. Rev. Materials**, vol. 2, number , pp. 086001, Aug 2018. DOI [10.1103/PhysRevMaterials.2.086001](https://doi.org/10.1103/PhysRevMaterials.2.086001)

[21] M.J. Highland, S.O. Hruszkewycz, D.D. Fong, C. Thompson, P.H. Fuoss, I. Calvo-Almazan, **S. Maddali**, A. Ulvestad, E. Nazaretski, X. Huang, H. Yan, Y.S. Chu, H. Zhou, P.M. Baldo and J.A. Eastman, *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. DOI [10.1063/1.4997773](https://doi.org/10.1063/1.4997773)

[22] **S. Maddali**, S. Ta'asan and R.M. Suter, *Topology-faithful nonparametric estimation and tracking of bulk interface networks*, **Computational Materials Science**, vol. 125, number , pp. 382-340, 2016. preprint [arXiv:1601.04699](https://arxiv.org/abs/1601.04699) DOI [10.1016/j.commatsci.2016.08.021](https://doi.org/10.1016/j.commatsci.2016.08.021)

[23] L. Renversade, R. Quey, W. Ludwig, D. Menasche, **S. Maddali**, R.M. Suter and A. Borbely, *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.

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