

# Siddharth Maddali, Ph.D

## Computational Scientist



**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

**Research Scientist**, KLA Corp. (KLA-Tencor)

Broadband Plasma (BBP) division, **Nov 2022 - present**

**Assistant Scientist ( $\cong$  Assistant Professor)**, Argonne National Laboratory  
Synchrotron Radiation Studies of Materials group, **Oct 2019 - Oct 2022**

**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**

## Technical/research interests

Computational methods:

Inverse problems, phase retrieval, holography, wavefront engineering  
Signal processing and optimization  
Computational electromagnetics  
Data science, machine learning, reinforcement learning  
High-performance computing (HPC) and scientific software development

### **Electromagnetics/Optics/Imaging:**

Scattering theory, microscopy  
Incoherent & coherent diffraction imaging  
Dark field microscopy  
High-energy x-ray diffraction microscopy (HEDM)  
Multiscale characterization with x-rays & other light probes  
Detection and characterization below the diffraction limit  
Photon correlation spectroscopy (PCS), dynamic light scattering (DLS)

### **Condensed matter physics:**

Materials characterization  
Light-matter interaction  
Crystallography  
Micro/nanoscale structure, strain & defects  
Interfacial dynamics in polycrystals  
Time-resolved characterization  
Photonics, metastructures

# **Presentations**

□ = **link to accepted abstract**

## **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) □
- 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 Minerals, Metals and Materials Society (TMS) 2023, San Diego, CA, 2023.

□

2) The American Physical Society (APS) March Meeting, Chicago, IL, 2022. □

3) The Materials Research Society (MRS) Spring Meeting & Exhibit, Phoenix, AZ, 2018. □

4) 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)

IIT-JAM (Joint Admission to M.Sc at the Indian Institutes of Technology) all-India rank 5 (2007).

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:** 1<sup>st</sup> Oct 2020 — 30<sup>th</sup> 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:** 1<sup>st</sup> Oct 2020 — 30<sup>th</sup> Sept 2021 (1 year)

**Amount:** \$100,000

## **Professional activity**

### **Society membership**

American 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)

## Training / Professional development




Multiphysics simulations with the MOOSE (Multiphysics Object-Oriented Simulation Environment) Framework, Idaho National Laboratory



# 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.  [LANL DMMS](#)



[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](#)

# References

**Dr. Stephan O. Hruszkewycz**     
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 Mat. Sci. and Engg.  
Carnegie Mellon University

**Dr. Marc Allain**    
Collaborator, computation/mathematics  
Institut Fresnel  
Aix-Marseille University

# Publications

[26] K. J. Harmon, T. D. Frazer, P. Donahue, C. G. Carr, Y. Liu, A. Popescu, W. Cha, **S. Maddali**, S. M. Haile, Y. Cao and S. O. Hruszkewycz, *Operando ceria strain evolution via Bragg coherent diffraction imaging (In preparation)*

[25] S. Kandel, **S. Maddali**, M. Allain, X. Huang, Y. S. G. Nashed, C. Jacobsen and S. O. Hruszkewycz, *Imaging extended single-crystal lattice distortion fields with multi-peak Bragg ptychography (Submitted)*

preprint [arxiv:2312.14907](https://arxiv.org/abs/2312.14907)

[24] Z. Xu, Y.-F. Shen, S. K. Naghibzadeh, X. Peng, V. Muralikrishnan, **S. Maddali**, D. Menasche, A. R. Krause, K. Dayal, R. M. Suter and G. S. Rohrer, *Grain boundary migration in polycrystalline  $\alpha$ -Fe*, **Acta Materialia**, Nov 2023

DOI [10.1016/j.actamat.2023.119541](https://doi.org/10.1016/j.actamat.2023.119541)

preprint [arxiv:2311.11219](https://arxiv.org/abs/2311.11219)

Am score

[23] **S. Maddali**, T. D. Frazer, N. Deegan, 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, *Concurrent multi-peak Bragg coherent x-ray diffraction imaging of 3D nanocrystal lattice displacement via global optimization*, **npj Computational Materials**, May 2023

DOI [10.1038/s41524-023-01022-7](https://doi.org/10.1038/s41524-023-01022-7)

preprint [arxiv:2208.00970](https://arxiv.org/abs/2208.00970)

Am score

[22] M. O. Hill, P. Schmiedeke, C. Huang, **S. Maddali**, X. Hu, S. O. Hruszkewycz, J. J. Finley, G. Koblmuller and L. J. Lauhon, *3D Bragg Coherent Diffraction Imaging of Extended Nanowires: Defect Formation in Highly Strained InGaAs Quantum Wells*, **ACS Nano**, Nov 2022

DOI [10.1021/acsnano.2c06071](https://doi.org/10.1021/acsnano.2c06071)

Am score

[21] N. Bertaux, M. Allain, J. Weizeorick, J. -S. 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**, Oct 2021

DOI [10.1364/OE.438945](https://doi.org/10.1364/OE.438945)

Am score

[20] 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**, Jul 2021

DOI [10.1364/OE.422768](https://doi.org/10.1364/OE.422768)

preprint [arxiv:2103.01767](https://arxiv.org/abs/2103.01767)

Am score

[19] 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**, Jun 2021

DOI [10.1103/PhysRevB.103.214103](https://doi.org/10.1103/PhysRevB.103.214103)

Am score

[18] **S. Maddali**, J.-S. 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**, Aug 2020

DOI [10.1103/PhysRevApplied.14.024085](https://doi.org/10.1103/PhysRevApplied.14.024085)

preprint [arxiv:1903.11815](https://arxiv.org/abs/1903.11815)

Am score

[17] **S. Maddali**, P. Li, A. Pateras, D. Timbie, N. Deegan, 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**, Apr 2020

DOI [10.1107/S1600576720001363](https://doi.org/10.1107/S1600576720001363)

preprint [arxiv:1909.05353](https://arxiv.org/abs/1909.05353)

Am score

[16] 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**, December 2020

DOI [10.3390/cryst10121109](https://doi.org/10.3390/cryst10121109)

Am score

[15] **S. Maddali**, M. Allain, P. Li, V. Chamard and S. O. Hruszkewycz, *Detector Tilt Considerations in Bragg Coherent Diffraction Imaging: A Simulation Study*, **Crystals**, December 2020

DOI [10.3390/cryst10121150](https://doi.org/10.3390/cryst10121150)

preprint [arxiv:2008.01843](https://arxiv.org/abs/2008.01843)

Am score

[14] P. Li, **S. Maddali**, A. Pateras, I. Calvo-Almazan, S. O. 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**, Apr 2020

DOI [10.1107/S1600576720001375](https://doi.org/10.1107/S1600576720001375)

preprint [arxiv:1909.05354](https://arxiv.org/abs/1909.05354)

Am score

[13] 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**, Oct 2019

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

Am score

- [12] 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**, Jul 2019  
DOI [10.1107/S1600577519003606](https://doi.org/10.1107/S1600577519003606) 
- [11] Yu-Feng Shen, **S. Maddali**, D. Menasche, A. Bhattacharya, G. S. Rohrer and R. M. Suter, *Importance of outliers: A three-dimensional study of coarsening in  $\alpha$ -phase iron*, **Phys. Rev. Materials**, Jun 2019  
DOI [10.1103/PhysRevMaterials.3.063611](https://doi.org/10.1103/PhysRevMaterials.3.063611) 
- [10] N. Krishnamurthy, **S. Maddali**, J. A. Hawk and V. N. Romanov, *9Cr steel visualization and predictive modeling*, **Computational Materials Science**, Mar 2019  
DOI [10.1016/j.commatsci.2019.03.015](https://doi.org/10.1016/j.commatsci.2019.03.015) 
- [9] 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**, Jun 2019  
DOI [10.1364/OE.27.018653](https://doi.org/10.1364/OE.27.018653) preprint [arxiv:1902.03920](https://arxiv.org/abs/1902.03920) 
- [8] 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**, Apr 2019  
DOI [10.1038/s41598-019-42797-4](https://doi.org/10.1038/s41598-019-42797-4) 
- [7] **S. Maddali**, M. Allain, W. Cha, R. Harder, J.-S. 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**, May 2019  
DOI [10.1103/PhysRevA.99.053838](https://doi.org/10.1103/PhysRevA.99.053838) preprint [arxiv:1811.06181](https://arxiv.org/abs/1811.06181) 
- [6] 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*, **arXiv**, Jul 2018  
preprint [arxiv:1808.00115](https://arxiv.org/abs/1808.00115)
- [5] 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**, Aug 2018  
DOI [10.1103/PhysRevMaterials.2.086001](https://doi.org/10.1103/PhysRevMaterials.2.086001) 
- [4] **S. Maddali**, I. Calvo-Almazan, J. Almer, P. Kenesei, J.-S. 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**, Mar 2018  
DOI [10.1038/s41598-018-23040-y](https://doi.org/10.1038/s41598-018-23040-y) preprint [arxiv:1712.01108](https://arxiv.org/abs/1712.01108) 
- [3] 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**, Oct 2017  
DOI [10.1063/1.4997773](https://doi.org/10.1063/1.4997773) 
- [2] 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**, Jan 2016  
DOI [10.1107/S2052252515019995](https://doi.org/10.1107/S2052252515019995) 
- [1] **S. Maddali**, S. Ta'asan and R. M. Suter, *Topology-faithful nonparametric estimation and tracking of bulk interface networks*, **Computational Materials Science**, Dec 2016  
DOI [10.1016/j.commatsci.2016.08.021](https://doi.org/10.1016/j.commatsci.2016.08.021) preprint [arxiv:1601.04699](https://arxiv.org/abs/1601.04699) 

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