

# 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

Americal Physical Society (APS), Materials Research Society (MRS), The

## 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.  

[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**     
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**   

**Dr. Marc Allain**  

Collaborator, materials science  
Department of Mat. Sci. and Engg.  
Carnegie Mellon University  
Pittsburgh, PA (USA)

Collaborator, computation/mathematics  
Institut Fresnel  
Aix-Marseille University  
Grenoble, France

# 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](#)

[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](#)

preprint [arxiv:2311.11219](#)

Am score  0

[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](#)

preprint [arxiv:2208.00970](#)

Am score  13

[22] M. O. Hill, P. Schmiedeke, C. Huang, **S. Maddali**, X. Hu, S. O. Hruszkewycz, J. J. Finley, G. Koblmüller 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](#)

Am score  4

[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](#)

Am score  1

[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](#)

preprint [arxiv:2103.01767](#)

Am score  0

[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](#)

Am score  2

[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](#)

preprint [arxiv:1903.11815](#)

Am score  1

[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](#)

preprint [arxiv:1909.05353](#)

Am score  3

[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](#)

Am score  1

[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](#)


preprint [arxiv:2008.01843](#)

Am score  3











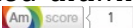
[14] P. Li, **S. Maddali**, A. Pateras, I. Calvo-Almazan, S. O. Hruszkewycz, W. Cha, V. Chamard and M. Allain, *General approaches for shear-correcting coordinate transformations in Bragg coherent diffraction imaging. Part II*, **Journal of Applied Crystallography**, Apr 2020

DOI [10.1107/S1600576720001375](#)

preprint [arxiv:1909.05354](#)

Am score  3



- [13] I. Calvo-Almazan, A. P. Ulvestad, E. Colegrove, T. Ablekim, M. V. Holt, M. O. Hill, **S. Maddali**, L. J. Lauhon, M. I. Berton, 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) 
- [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. Berton 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) 