

# Siddharth Maddali, Ph.D

Research Scientist (BBP 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

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

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

**Assistant Scientist**, 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**

## Research interests

### Optics/imaging:

Defect inspection using optical nanoscopy

Electromagnetic scattering

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 & other light probes

X-ray photon correlation spectroscopy (XPCS), dynamic light scattering (DLS)

### **Condensed matter physics:**

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

### **Computational methods:**

Electromagnetic simulations  
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 (□ = 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)  
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 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.  

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

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

## Publications

- [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)  { 1 }
- [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](https://doi.org/10.1021/acsnano.2c06071)  { 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](https://doi.org/10.1364/OE.438945)  { 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](https://doi.org/10.1364/OE.422768) preprint [arxiv:2103.01767](https://arxiv.org/abs/2103.01767)  { 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](https://doi.org/10.1103/PhysRevB.103.214103)  { 3 }
- [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)  { 0 }
- [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)  { 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](https://doi.org/10.3390/cryst10121109)  { 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](https://doi.org/10.3390/cryst10121150) preprint [arxiv:2008.01843](https://arxiv.org/abs/2008.01843)  { 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](https://doi.org/10.1107/S1600576720001375) preprint [arxiv:1909.05354](https://arxiv.org/abs/1909.05354)  { 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. 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)  { 1 }
- [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)  { 1 }
- [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)  { 1 }
- [10] N. Krishnamurthy, **S. Maddali**, J. A. Hawk and V. N. Romanov, *9Cr steel visualization and predictive modeling*, **Computational Materials Science**, Mar 2019

[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

[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

[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

[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

[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

[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

[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 In<sub>2</sub>O<sub>3</sub> epitaxial films*, **Applied Physics Letters**, Oct 2017

[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

[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