

# 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:** 1<sup>st</sup> Oct 2020 — 30<sup>th</sup> 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:** 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.

 [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

Materials Science Division

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










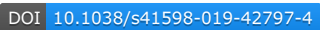





Grenoble, France



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## 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. 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, *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. 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**, vol. 53, number 2, pp. , Apr 2020.   DOI 
- [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.   DOI 
- [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.   DOI   
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- [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 
- [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.   DOI 
- [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 
- [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  $\alpha$ -phase iron*, **Phys. Rev. Materials**, vol. 3, number , pp. 063611, Jun 2019. DOI 
- [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,



[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 In<sub>2</sub>O<sub>3</sub> 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.

DOI [10.1107/S2052252515019995](https://doi.org/10.1107/S2052252515019995)



