

## Siddharth Maddali, Ph.D Computational scientist/engineer

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### Links (clickable in PDF):

| Google Scholar | arXiv | ORCID | Researchgate | Web of Science | Scopus |

## Education

1. Ph.D (physics)	Carnegie Mellon University, 2016
2. M.S (physics)	Carnegie Mellon University, 2011
3. M.Sc (physics)	Indian Institute of Technology Madras, 2009
4. B.Sc (physics, mathematics, electronics)	Bangalore University, 2007

## Experience

1. Senior Applied Physics/ML Scientist, Liminal Insights, Inc.	Feb 2025 - present
2. Applied physics/ML consultant, Liminal Insights, Inc.	Nov 2024-Feb 2025
3. Scientific consultant	Mar 2024 - Oct 2024
4. Research Scientist, KLA Corporation (KLA-Tencor)	2022 - 2024
5. Staff Scientist, Argonne National Laboratory	2019 - 2022
6. Post-doctoral researcher, Argonne National Laboratory	2017 - 2019
7. Post-doctoral researcher (ORISE fellow), National Energy Technology Laboratory	May 2016 - Nov 2016
8. Graduate Teaching/Research Assistant, Carnegie Mellon University	2009 - 2016
9. Intern, Physics department, National University of Singapore	May-Jun 2008

## Interests

- Computational methods:** Inverse problems, signal processing, harmonic analysis, optimization, data science, deep learning, high-performance computing, algorithms, scientific software development, quantum computing
- Physics:** Acoustics, materials characterization, light-matter interaction, crystallography, interfacial dynamics, time-resolved phenomena, photonics, metastructures/metamaterials
- Optics/imaging:** Scattering theory, computational electromagnetics, microscopy, X-ray science, inspection/metrolology/detection/sensing, spectroscopy

## Presentations

= link to abstract

### - Invited

- Advanced Photon Source Scientific Computation Seminar, Argonne National Laboratory, Lemont, IL (March 2022)
- Materials Science Division Colloquium, Argonne National Laboratory, Lemont, IL (October 2021)
- Workshop on Advanced Probes & Data Analytics for Enabling Single-Pulse Imaging under Dynamic Conditions, Santa Fe, NM (August 2019)
- The Minerals, Metals & Materials Society (TMS), San Antonio, TX (March 2019)
- LANS seminar series, Mathematics & Computer Science Division, Argonne National Laboratory, Lemont, IL ( Sept 2018)
- Department of physics, Carnegie Mellon University, Pittsburgh, PA (May 2018)

### - Contributed

- Gordon X-ray Science Seminar, Easton, MA (July-August 2019: seminar & poster; July-August 2017: discussion leader)
- Coherence: International workshop on phase retrieval and coherent scattering, Port Jefferson, NY (June 2018)
- Materials Research Society Spring Meeting & Exhibit, Phoenix, AZ (April 2018)

- 4. The Minerals, Metals & Materials Society (TMS), Orlando, FL (March 2015: Poster)
- 5. Materials Science & Technology (MS&T), Pittsburgh, PA (October 2014: seminar; October 2012: poster)

### - Misc. (co-author)

1. The Minerals, Metals & 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 & honors

- Oak Ridge Institute for Science & Education (ORISE) post-doctoral fellowship (2016)
- Indian Institute of Technology Madras Academic Merit Fellowship (2007 – 2009)
- Indian Institutes of Technology Joint Admission to M.Sc: AIR 5 (2007)
- Bangalore University undergraduate rank 5

## Research grants

- **ANL LDRD 2019-0042: Finding Critical Processes of Deformation in Structural Materials with Artificial Intelligence**  
**Role:** Principal investigator  
**Funding:** Argonne Laboratory-Directed Research & Development (LDRD)  
**Period:** 1<sup>st</sup> Oct 2020 – 30<sup>th</sup> Sept 2021 (1 year)  
**Amount:** \$100,000
- **ANL LDRD 2021-0012: Coherence-enhanced dark-field imaging for structural heterogeneity in materials**  
**Role:** Principal investigator  
**Funding:** Argonne Laboratory-Directed Research & Development (LDRD)  
**Period:** 1<sup>st</sup> Oct 2020 – 30<sup>th</sup> Sept 2023 (3 years)  
**Amount:** \$900,000

## Professional activity & outreach

- **Society membership:** American Physical Society (APS), the Materials Research Society (MRS), the Minerals, Metals & Materials Society (TMS)
- **Peer review:** US Department of Energy: Basic Energy Sciences (BES), Philosophical Magazine, Computational Materials Science, New Journal of Physics, Optics Letters, Crystals Research & Technology, Journal of Applied Physics, Physical Review {Letters, B, X}, Optics Letters, Journal of Applied Crystallography, Integrating Materials & 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:** Multiphysics simulations with the MOOSE (Multiphysics Object-Oriented Simulation Environment) Framework, Idaho National Laboratory
- **Editorship:** *Crystals* special issue: Synchrotron Studies of Materials

## Technical reports

1. R. Pokharel, C. Bolme, J. Bohon, A. Mandal, D. Pagan, F. Hofmann, **S. Maddali**, A. Rack, *Advanced probes & 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

Name	Relation	Organization	E-mail	Phone
Dr. Stephan Hruszkewycz	Supervisor	Argonne National Laboratory	shrus@anl.gov	+1 (630) 252-3214
Dr. Robert M. Suter	Ph.D advisor	Carnegie Mellon University	suter@cmu.edu	-
Dr. Anthony D. Rollett	Collaborator	Carnegie Mellon University	rollett@cmu.edu	+1 (412) 268-3177
Dr. Marc Allain	Collaborator	Aix-Marseille Univ/Inst. Fresnel	marc.allain@fresnel.fr	-

## Publications

- [1] 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**), 2024.
- [2] S. Kandel, **S. Maddali**, X. Huang, Y. S. G. Nashed, C. Jacobsen, M. Allain, and S. O. Hruszkewycz. Imaging extended single crystal lattice distortion fields with multi-peak bragg ptychography. *Opt. Express*, 32(11):19594–19610, May 2024.
- [3] **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. Concurrent multi-peak bragg coherent x-ray diffraction imaging of 3d nanocrystal lattice displacement via global optimization. *npj Computational Materials*, 9(1):77, May 2023.
- [4] 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*, 264:119541, Nov 2023.
- [5] 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.
- [6] 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*, 103:214103, Jun 2021.
- [7] 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*, 29(15):23019–23055, Jul 2021.
- [8] N. Bertaux, M. Allain, J. Weizerick, 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*, 29(22):35003–35021, Oct 2021.
- [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*, 53(2), Apr 2020.
- [10] 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*, 53(2), Apr 2020.
- [11] **S. Maddali**, M. Allain, P. Li, V. Chamard, and S. O. Hruszkewycz. Detector tilt considerations in bragg coherent diffraction imaging: A simulation study. *Crystals*, 10(12):1150, December 2020.
- [12] **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*, 14:024085, Aug 2020.
- [13] 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*, 10(12):1109, December 2020.
- [14] **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*, 99:053838, May 2019.

- [15] 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*, 9(1):6386, Apr 2019.
- [16] 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*, 27(13):18653–18672, Jun 2019.
- [17] N. Krishnamurthy, **S. Maddali**, J. A. Hawk, and V. N. Romanov. 9cr steel visualization and predictive modeling. *Computational Materials Science*, Mar 2019.
- [18] 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*, 3:063611, Jun 2019.
- [19] 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*, 26(4), Jul 2019.
- [20] 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*, pages 1–10, Oct 2019.
- [21] **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*, 8(1):4959, Mar 2018.
- [22] 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*, 2:086001, Aug 2018.
- [23] 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, Jul 2018.
- [24] 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*, 111(16):161602, Oct 2017.
- [25] **S. Maddali**, S. Ta'asan, and R. M. Suter. Topology-faithful nonparametric estimation and tracking of bulk interface networks. *Computational Materials Science*, 125:382–340, Dec 2016.
- [26] 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*, 3(1):32–42, Jan 2016.