Curriculum Vitae

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. Scientific consultant — 2024 - present
2. Research Scientist, KLA Corporation (KLA-Tencor) — 2022 - 2024
3. Staff Scientist, Argonne National Laboratory — 2019 - 2022
4. Post-doctoral researcher, Argonne National Laboratory — 2017 - 2019
5. Post-doctoral researcher (ORISE fellow), National Energy Technology Laboratory — May 2016 - Nov 2016
6. Graduate Teaching/Research Assistant, Carnegie Mellon University — 2009 - 2016
7. Intern, Physics department, National University of Singapore — May-Jun 2008

Interests

1. **Computational methods**: Inverse problems, phase retrieval, holography, wavefront engineering, signal processing, optimization, data science, deep learning, high-performance computing, algorithms, scientific software development, quantum computing
2. **Optics/imaging**: Scattering theory, computational electromagnetics, microscopy, X-ray science, inspection/metrology/detection/sensing, spectroscopy, dynamic light scattering
3. **Physics**: Materials characterization, light-matter interaction, crysallography, interfacial dynamics, time-resolved phenomena, photonics, metastructures/metamaterials

Presentations

🔗 = link to abstract

- **Invited**
  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 & 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)
- **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 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: 1st Oct 2020 – 30th 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: 1st Oct 2020 – 30th 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 α-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. 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*, 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 α-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.