

# Siddharth Maddali, Ph.D

## Computational scientist/engineer

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 siddharthmaddali



## Experience

- **Liminal Insights, Inc.** **Emeryville, CA, USA**
  - **Applied Physics/Machine Learning Consultant** Nov 2024 – present
    - Developing ultrasound characterization techniques for structural defects in lithium batteries.
    - Building physics-inspired ML models for deployment on ultrasound-based battery inspection equipment.
- **Independent** **Fremont, CA, USA**
  - **Scientific Consultant** Feb 2024 – Nov 2024
    - Provided technical consulting for investors in emerging semiconductor technologies.
    - Built an AI-powered tool for automated land area survey trained on drone-based multi-spectral images.
- **KLA Corporation (KLA-Tencor)** **Milpitas, CA, USA**
  - **Research Scientist** Nov 2022 – Jan 2024
    - Developed methods for sensitivity enhancement in semiconductor wafer inspection processes.
- **Argonne National Laboratory** **Chicago, IL, USA**
  - **Staff Scientist** Oct 2019 – Sep 2022
    1. Led the computational development and worked on the **first demonstration** of the X-ray MR-BCDI imaging technique.
    2. Led the design of future imaging experiments at DoE facilities with physics-based signal processing techniques.
    3. Built software libraries for 3D X-ray image reconstruction: `Phaser`, `mrbcdi`.
    4. Raised \$900k seed funding for computational R&D and novel microscopy infrastructure.
    5. Proposed, executed novel proofs of concept in materials research (US, France).
    6. Published work in high-impact scientific journals, mentored junior researchers, organized/chaired international workshops.
  - **Postdoctoral researcher** Jan 2017 – Sep 2019
    1. **First demonstration** of multi-scale, high-energy coherent diffraction imaging (HEDM) of 3D materials.
- **National Energy Technology Laboratory** **Pittsburgh, PA, USA**
  - **Postdoctoral Researcher: ORISE Fellow** May 2016 – Nov 2016
    1. Developed guidelines for machine learning-driven materials discovery of novel, function-optimized alloys.
- **Carnegie Mellon University** **Pittsburgh, PA, USA**
  - **Graduate teaching/research assistant** Aug 2009 – Feb 2016
    1. Dissertation on mining meso-scale materials physics from high-energy synchrotron data.
    2. Created `HierarchicalSmooth`: mesh smoothing software for physical interface networks.
    3. Taught mechanics & electromagnetism to undergraduate science majors.

## Education

- **Ph.D, & M.S., Physics** (Dissertation area: materials science) **Pittsburgh, PA, USA**
  - *Carnegie Mellon University* Aug 2009 – Feb 2016
- **M.Sc, Physics** **Chennai, TN, India**
  - *Indian Institute of Technology Madras (IIT-M)* Aug 2007 – May 2009
- **B.Sc, Physics, mathematics, electronics** **Bengaluru, KA, India**
  - *Bangalore University* June 2004 – May 2007

## Technical skills

- **Science & Engg.:** Geometric + Fourier optics, ultrasound/acoustic methods, microscopy, image formation (Hopkins, Abbe), diffraction gratings, X-ray science, condensed matter + materials physics, electromagnetics, mechanics, statistical physics, semiconductors, experimental design, quantum sciences
- **Math/computation:** Linear algebra, reconstruction, optimization, signal processing, control theory, inverse problems, simulations, statistics, probability, FDTD (meep), RCWA, computational geometry, differential equations
- **Software:** Python scientific stack (numpy, scipy, matplotlib, scikit-learn, pandas + more), Matlab, Linux, git, bash,  $\LaTeX$ , HPC + parallel computing (MPI), GPU development, PyTorch, Tensorflow, C++, Docker, Qiskit
- **AI/ML:** LLMs, retrieval augmented generation (RAG), data science, applied statistics, machine learning, deep learning for computer vision, CNNs, NeRF, structure for motion

## Awards & Grants

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1. ANL LDRD Research grant: *Coherence-enhanced dark-field X-ray microscopy* (Role: PI; \$930,000).
2. ANL LDRD Research grant: *detecting critical microstructural processes with AI* (Role: PI; \$100,000).
3. ANL LDRD Research grant: *COHED: Coherence for high-energy diffraction* (Role: postdoc)
4. Oak Ridge Institute for Science & Education (ORISE) post-doctoral fellowship (2016).
5. Indian Institute of Technology Madras Academic Merit Scholarship (2007 – 2009).
6. IIT Joint Admission to M.Sc (IIT-JAM) All-india rank 5 (out of  $\simeq 4000$ ) (2007).
7. Bangalore University undergraduate rank 5 (2007).

## Professional Activities & Outreach (link to full CV)

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- **Editorship:** *Crystals* special issue: Synchrotron Studies of Materials
- **Select invited talks:** The Minerals, Metals, Materials Society (TMS), Advanced Photon Source.
- **Society membership:** American Physical Society, Materials Research Society, TMS.
- **Select peer review:** US Department of Energy, American Physical Society, Optica.
- **Select workshop organization:** Advanced Photon Source User Meetings.

## Select publications (link to full CV)

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1. **Maddali, S.**, Frazer, T.D., Deegan, N. *et al*, *Concurrent multi-peak Bragg coherent x-ray diffraction imaging of 3D nanocrystal lattice displacement via global optimization*, **npj Computational Materials** 9, 77 (2023).
2. Wilkin, M., **Maddali, S.**, Hruszkewycz, S., Pateras, A., Sandberg, R., Harder, R., Cha, W., Suter, R., & Rollett, A. *Experimental demonstration of coupled multi-peak Bragg coherent diffraction imaging with genetic algorithms*, **Phys. Rev. B**, 103, 214103. (2021).
3. **Maddali, S.**, Allain, M., Cha, W., Harder, R., Park, J.S., Kenesei, P., Almer, J., Nashed, Y., & Hruszkewycz, S., *Phase retrieval for Bragg coherent diffraction imaging at high x-ray energies*, **Phys. Rev. A**, 99, 053838 (2019).
4. **Maddali, S.**, Park, J.S., Sharma, H., Shastri, S., Kenesei, P., Almer, J., Harder, R., Highland, M., Nashed, Y., & Hruszkewycz, S., *High-Energy Coherent X-Ray Diffraction Microscopy of Polycrystal Grains: Steps Toward a Multiscale Approach*, **Phys. Rev. Appl.**, 14, 024085 (2020).
5. Kandel, S., **Maddali, S.**, Allain, M., Hruszkewycz, S. O., Jacobsen, C., & Nashed, Y. S. G., *Using automatic differentiation as a general framework for ptychographic reconstruction*, **Opt. Express**, 27(13):18653–18672 (2019).


## Languages


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English (fluent), Hindi (fluent), Tamil (intermediate), Telugu (intermediate), Marathi (intermediate), Kannada (intermediate), French (beginner)


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### Links (clickable in PDF):

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

## Education

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|---|---|
| 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

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





## Interests

- 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
- Optics/imaging:** Scattering theory, computational electromagnetics, microscopy, X-ray science, inspection/metrolgy/detection/sensing, spectroscopy, dynamic light scattering
- Physics:** Materials characterization, ultrasound/acoustics, light-matter interaction, crysallography, interfacial dynamics, time-resolved phenomena, photonics, metastructures/metamaterials


## 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. 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*, 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. 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. 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*, 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.