# Siddharth Maddali, Ph.D

### **Research Scientist (BBP Division)**















### **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:**

Metrology, anomaly detection 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)  $\equiv$
- 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**: 1st Oct 2020 — 30th 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 R

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. DOI 10.2172/1456238

### **References**

Dr. Stephan O. Hruszkewycz ⊕ 🖾 📞

Supervisor Synchrotron Studies of Materials Materials Science Division Argonne National Laboratory Chicago, IL (USA)

**Dr. Anthony D. Rollett ⊕** ⊠ **८** Collaborator, materials science

Dr. Robert M. Suter 

Ph.D advisor
Department of physics
Carnegie Mellon University
Pittsburgh, PA (USA)

**Dr. Marc Allain ⊕** ⊠ Collaborator, computation/mathematics

Institut Fresnel Aix-Marseille University Grenoble, France

### **Publications** 3

- [1] M.O. Hill, P. Schmiedeke, C. Huang, **S. Maddali**, X. Hu, S.O. Hruszkewycz, J.J. Finley, G. Koblm {"u}ller and L.J. Lauhon, 3D Bragg Coherent Diffraction Imaging of Extended Nanowires: Defect Formation in Highly Strained InGaAs Quantum Wells, **ACS Nano**, vol., number, pp., Nov 2022.
- [2] (**Under review**) **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, *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.
- [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 10.1364/06.422768
- [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.
- [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. [20] [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.

  Description arXiv:1903.11815 DOI 10.1103/PhysRevApplied.14.024085
- [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**, vol. 53, number 2, pp., Apr 2020. Preprint arXiv:1909.05353
- [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.
- [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. preprint arXiv:1811.06181 DOI 10.1103/PhysRevA.99.053838

- [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 10.1038/s41598-019-42797-4
- [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. Preprint arXiv:1902.03920 DOI 10.1364/0E.27.018653
- [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 10.1016/j.commatsci.2019.03.015]
- [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. [OI] 10.1103/PhysRevMaterials.3.063611*
- [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, number 4, pp. , Jul 2019. [DOI 10.1107/S15000577519003606]
- [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. [OII 10.1109/JPHOTOV2019.2942487]
- [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]
- [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. 

  DOI: 10.1038/s41598-018-25040-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.2.036001
- [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 In2O3 epitaxial films*, *Applied Physics Letters*, vol. 111, number 16, pp. 161602, 2017. [50] 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 DOI 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. [OI 10.1107/S2052252515019995]

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