

# Dr. Siddharth Maddali

Post-Doctoral Researcher  
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## Education

- **Carnegie Mellon University** Pittsburgh, PA  
*PhD (Physics)* 2010 - Feb 2016
  - **PhD dissertation:** Computational mining of meso-scale physics from high-energy X-ray data sets
  - Advisor:** Dr. Robert M. Suter
- **Carnegie Mellon University** Pittsburgh, PA  
*MS Physics* 2009 - 2010
- **Indian Institute of Technology (IIT), Madras** Chennai, India  
*M.Sc Physics* 2007 - 2009
  - Master's thesis: Computational analysis of the vibrational modes of a solid sphere
- **Bangalore University** Bangalore, India  
*B.Sc. Physics* 2004 - 2007
  - Triple-major: physics, mathematics, electronics

## Experience

- **Post-doctoral researcher** Argonne National Laboratory  
*Synchrotron Radiation Studies* January 2017 - present
- **Post-Doctoral Research Associate (ORISE)** National Energy Technology Laboratory  
*Computational Materials Research* May 2016 - November 2016
- **Graduate Research Assistant** Carnegie Mellon University  
*Computational/experimental materials research* 2012 - Feb 2016
- **Graduate Teaching Assistant** Carnegie Mellon University  
*Physics for Science Students* 2009 - 2012
- **Intern, Department of Physics** National University of Singapore  
*Summer Internship Program for Indian Students (SIPIS)* May 2008

## Skills

### 1. Software

- **Expert:** C, C++, Python, GNU/Linux, scripting/automation, Matlab/Octave, Mathematica, L<sup>A</sup>T<sub>E</sub>X
- **Intermediate:** Parallelization with MPI, Arrayfire, Git, Tensorflow, scikit-learn
- **Miscellaneous:** Building software libraries and wrappers

### 2. Physics and mathematics

- **Expert:** Crystallography, X-ray physics & optics, materials science, statistics, mechanics, thermodynamics and statistical mechanics, quantum physics, electromagnetic theory, condensed matter/solid state physics
- **Intermediate:** Convex optimization, inverse problems, signal detection and processing, compressed sensing, machine learning

## Software projects

- **Hierarchical smooth** (C++): A module for topology-faithful surface smoothing for grain interface meshes obtained from 3D images of polycrystal materials<sup>1</sup>. Designed as a standalone library, and to work in conjunction with DREAM.3D<sup>2</sup>.
- **Fast Phasing Library (FPL)** (C++, GPU): Collaborated on FPL<sup>3</sup>, a phase retrieval program for Bragg coherent diffractive imaging (BCDI) data built on top of the Arrayfire GPU computational library<sup>4</sup>.
- **Phaser** (Python, Tensorflow): A Python module for running BCDI reconstructions on CPU & GPU<sup>5</sup>.
- **RegisterMic** (C++, MPI): A small, parallelized image registration program for 2D microstructure images obtained from high-energy diffraction microscopy measurements, written in C++/MPI.

## Research Interests

- Scientific software development (<https://github.com/siddharth-maddali>)
- Computational science (inverse problems, signal processing, optimization)
- Data science and machine learning
- Microstructure/nanostructure imaging
- Mesoscale phenomena and physics
- X-ray physics, coherent diffraction imaging, ptychography

## Publications

- [1] **S. Maddali**, J. S. Park, H. Sharma, S. D. Shastri, P. Kenesei, J. Almer, R. Harder, M. J. Highland, Y. S. G. Nashed, and S. O. Hruszkewycz. High-energy coherent x-ray diffraction microscopy of polycrystal grains: first steps towards a multi-scale approach, 2019. arXiv:1903.11815 [cond-mat.mtrl-sci] (under review).
- [2] N. Krishnamurthy, , **S. Maddali**, J. A. Hawk, and V. N. Romanov. 9cr steel visualization and predictive modeling. *Computational Materials Science*, 2019.
- [3] **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, 2018.
- [4] 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.
- [5] N. Krishnamurthy, **S. Maddali**, A. Verma, L. Bruckman, J. Carter, R. French, V. Romanov, and J. Hawk. Data analytics for alloy qualification. Technical Report NETL-PUB-21550, 2017.
- [6] N. Krishnamurthy, **S. Maddali**, V. Romanov, and J. Hawk. Segmentation of 9cr steel samples based on composition and mechanical property. volume 62. APS, 2017.
- [7] N. Krishnamurthy, **S. Maddali**, V. Romanov, and J. Hawk. Predictive analysis of the influence of the chemical composition and pre-processing regimen on structural properties of steel alloys using machine learning techniques. volume 62. APS, 2017.

<sup>1</sup><https://github.com/siddharth-maddali/HierarchicalSmooth>

<sup>2</sup><http://dream3d.bluequartz.net/>

<sup>3</sup><https://bitbucket.org/ynashed/fpl/src/smaddali/>

<sup>4</sup><https://arrayfire.com/>

<sup>5</sup><https://github.com/siddharth-maddali/Phaser>

- [8] M. J. Highland, S. O. Hruszkewycz, D. D. Fong, Carol 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, 2017.
- [9] **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, 2016.
- [10] **S. Maddali**. *Computational Mining of Meso-Scale Physics From High-Energy X-Ray Data Sets*. PhD thesis, Carnegie Mellon University, 2016. Ph.D Thesis.
- [11] L. Renversade, R. Quey, W. Ludwig, D. Menasche, **S. Maddali**, R. M. Suter, and A. Borbély. Comparison between diffraction contrast tomography and high-energy diffraction microscopy on a slightly deformed aluminium alloy. *IUCrJ*, 3(1):32–42, 2016.
- [12] 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. Lauhono, N. Rodkey, M. I. Bertoni, and M. E Stuckelburger. Multimodal x-ray imaging of grain-level properties and performance in a polycrystalline solar cell. (accepted for publication in *Journal of Synchrotron Radiation*).
- [13] **S. Maddali**, M. Allain, W. Cha, R. Harder, J. Almer, P. Kenesei, J.-S. Park, Y. Nashed, and S. O. Hruszkewycz. Phase retrieval for bragg coherent diffraction imaging at high x-ray energies. arXiv:1811.06181v1 [cond-mat.mtrl-sci] (under review).
- [14] Y. F. 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. (under review).
- [15] S. Kandel, **S. Maddali**, M. Allain, S. O. Hruszkewycz, C. Jacobsen, and Youssef S. G. Nashed. Using automatic differentiation as a general framework for ptychographic reconstruction. (under review).
- [16] I. Calvo-Almazan, M. Allain, **S. Maddali**, V. Chamard, and S. O. Hruszkewycz. Impact mitigation of angular uncertainties in bragg coherent diffraction imaging. (accepted for publication in *Scientific Reports*).

## Presentations

- (Invited) **The Minerals, Metals & Materials Society (TMS)**, San Antonio, TX (Mar '19)
- **Advanced Photon Source User Science Seminar**, Lemont, IL (July '18)
- **Coherence: International Workshop on Phase Retrieval and Coherent Scattering**, Port Jefferson, NY (June '18)
- (Invited) **Dept. of Physics, Carnegie Mellon University**, Pittsburgh, PA (May '18)
- **Materials Research Society**, Phoenix, AZ (April '18)
- **Gordon X-ray Science Conference & Seminar**, Poster + Discussion leader, Easton, MA (Jul-Aug '17)
- **Dept. of Mathematics, Georgia Institute of Technology**, Seminar, Atlanta, GA (Nov '15)
- **The Minerals, Metals & Materials Society (TMS)**, Poster, Orlando, FL (Mar '15)
- **Materials Science & Technology (MS&T)**, Seminar, Pittsburgh, PA (Oct '14)
- **Materials Science & Technology (MS&T)**, Poster, Pittsburgh, PA (Oct '12)

## Workshops

- Multiphysics Object-Oriented Simulation Environment (**MOOSE**) - open-source finite element engine (Idaho National Laboratory)
- Center for Causal Discovery (**CCD**) Summer Course '16, Pittsburgh, PA (USA)
- Machine Learning for Materials Research (**MLMR**) 2016, College Park, MD (USA)

## Awards, Grants, Honours

Institute Freeship (tuition waiver scholarship), IIT-Madras . . . . . 2007 - 2009  
Ranked 5 in the nation-wide Joint Admission Test for M.Sc (JAM) for the IITs . . . . . 2007  
Ranked 5 in Bangalore University for overall academic performance . . . . . 2007

## Professional Activities

- **Member:** Americal Physical Society (APS), Materials Research Society (MRS), The Minerals, Metals & Materials Society (TMS)
- **Reviewer:** *Philosophical Magazine, Computational Materials Science*