

Tom McAuliffe

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EDUCATION	Imperial College London , PhD - <i>Data-driven electron microscopy for alloy development</i> Sep 2017 – Present Completion expected in Summer 2020.
	University of Cambridge , 1st Class BA & MSci - <i>Natural sciences</i> Oct 2013 – Jul 2017
EXPERIENCE	PhD Research: Data-driven electron microscopy Sep 2017 – Present <ul style="list-style-type: none">▪ Data science techniques leveraged for novel physical insight and improved metal alloy development. My research has led to marked improvement in thermo-mechanical alloy properties, which when brought into service will improve jet engine efficiency. Patent is pending for new alloys developed as an outcome of my analysis pipeline in the scanning electron microscope.▪ Unsupervised ML for feature extraction of multimodal electron diffraction datasets, combining descriptors of metal alloy <i>structure</i> and <i>chemistry</i>. Correct data pre-treatment before modality combination, PCA, and NMF leads to physically meaningful latent feature extraction [1].▪ PCA, NMF, and autoencoder neural networks compared for understanding differences in almost physically indistinguishable datasets. This has been used to validate a new 'virtual' imaging mode, gathering intensity from solid angles of raised signal on a partial sphere constructed from the inverse gnomonic projection of measured (rectangular) patterns [2].▪ Fourier transforms and cross-correlation employed for comparison of, for example, a PCA reduced dataset basis to simulated templates. This permits efficient determination of crystalline structure and orientation [1-3].▪ Gradient descent with momentum implemented for optimisation of simulation hyperparameters. This has improved the fidelity of our simulations and crystallographic insight we can draw from comparison to measurements [2].▪ Elastic strain and stress tensors measured and calculated respectively using cross-correlation to track image properties across a region of interest. Comparable regions separated with NMF, and basis rotated to one of crystallographic interest. This was used to validate an important phenomenon in automotive steels [4].▪ Python, MATLAB, C++ software developed [7-9]. Available at http://github.com/tmcaul.
	Imperial College London: Undergraduate teaching Oct 2018 – May 2019 <ul style="list-style-type: none">▪ Tutored maths (including linear algebra, statistics, calculus) to undergraduates.▪ Led experimental practicals (one weekly lab and one longer, full-term project).▪ Co-supervised MSc student projects in alloy development and microscopy data analysis.
	Rolls-Royce PLC: External material surveillance Jul 2016 – Oct 2016 <ul style="list-style-type: none">▪ Quality control on outsourced forging and machining. New statistical process control template developed and implemented, ensuring tolerance according to a Gaussian distribution within an contracted parameter set.
	University of Warwick / Element 6: Optical data analysis Jul 2015 – Sep 2015 <ul style="list-style-type: none">▪ Spatial mapping of Raman spectra and optical microscopy quantification of synthetic diamond. Developed an automated crack identification algorithm for optical micrographs in MATLAB using convolution with edge filters.
SKILLS	<ul style="list-style-type: none">▪ Python - Experienced with <i>NumPy</i>, <i>PyTorch</i>, <i>Multiprocessing</i>, <i>SKLearn</i>, <i>Matplotlib</i>, <i>SciPy</i> packages <i>etc.</i> Two software packages (<i>ebspy</i>, <i>crosspy</i>) developed and released open-source.▪ MATLAB - Experienced with Machine Learning, Statistics, Parallel Computing toolboxes, <i>etc.</i> Five years' experience. Major contributions and refactoring of <i>AstroEBSD</i>, a widely used software package.▪ C++ - High-performance linear algebra and fast Fourier transforms implemented, using <i>eigen</i> and <i>fftw</i> packages. Porting functions from MATLAB has resulted in significant speedups (approx. 100 times).▪ Machine learning - Most experience with PCA, NMF, and neural networks. Unsupervised learning with <i>SKLearn</i>. Neural networks built with <i>PyTorch</i> (both with and without <i>fastai</i>) and MATLAB machine learning toolbox.▪ Computational linear algebra - I routinely analyse high-dimensionality data, perform orientation analyses, and implement data basis transformations. Experienced with SVD, eigen-decompositions, least-squares solutions.▪ Software development - Experienced with Github, VSCode, Jupyter Notebooks, <i>etc.</i>▪ Data handling and computation - Experienced with clustering, factor extraction, and feature ID. Proficient with <i>NumPy</i> / <i>PyTorch</i> for vectorisation, <i>Numba</i> for speedup, and <i>Multiprocessing</i> for parallelisation.

- **Data presentation** - Familiar with producing publication quality figures with Adobe Illustrator, Photoshop, Inkscape. Prefer data plotting in MATLAB or *Matplotlib*. Experienced with Excel.
- **Time management** - Five substantive papers, three software packages over course of PhD).
- **Teamwork** - Collaborated on many projects, both leading and providing analytical support. Have assisted in use of pipelines that I have developed, and co-developed pipelines with other researchers.

PUBLICATIONS

- [1] “Advancing characterisation with statistics from correlative electron diffraction and X-ray spectroscopy, in the scanning electron microscope,” - McAuliffe *et al* - *Ultramicroscopy*, 2020 - *Clustering and classification of hyperdimensional (and multimodal) electron microscopy datasets*.
- [2] “Spherical-angular dark field imaging and sensitive microstructural phase clustering with unsupervised machine learning” - McAuliffe *et al* - *ArXiv*, 2020 (under review) - *PCA, NMF, autoencoder neural network comparison for latent feature extraction in electron backscatter diffraction*.
- [3] “The Use of Scanning Electron Beam-based Phase Classification as a Crucial Tool in Alloy Development for Gas Turbine Engine Applications,” - McAuliffe *et al* - *Microscopy & Microanalysis*, 2019 - *Combination of multimodal data for material analysis*.
- [4] “4D-STEM elastic stress state characterisation of a TWIP steel nanotwin” - McAuliffe *et al* - *ArXiv*, 2020 (under review) - *Measurement of crystal lattice stress and strain tensors over a highly resolved spatial domain*.
- [5] “On the prediction and the formation of the sigma phase in CrMnCoFeNi high entropy alloys,” - Christofidou, McAuliffe *et al* - *Journal of Alloys & Compounds*, 2018 - *Measurement and modelling of modern aerospace alloys*.
- [6] “Interface characteristics in an alpha + beta titanium alloy,” - Ackerman *et al* - *Physical Review Materials*, 2020 - *Measurement and modelling of atomic coherence*.

SOFTWARE

ebspy: *Python analysis of electron backscatter diffraction data* - [7]

- Created and fully developed by me for loading, handling, and cleaning microscopy data. Provides normalisation, background correction, and pipelines to interface with SKLearn for ML characterisation.
- Used within my research group and others’ in the UK and abroad.

AstroEBSD: *Crystallographic analysis of electron microscopy data* - [8].

- Orientation determination, signal clustering, and structure classification with template matching in MATLAB.
- Initially developed in the group for Hough transforms and geometrical analysis of diffraction data.
- Recently updated with my contributions: an open-source PCA pipeline for analysis of correlative multimodal datasets, including Fourier cross-correlation of simulated templates for orientation ID.

crosspy: *Fourier image registration and subset tracking in Python* - [9].

- Co-created and developed for loading, handling, and analysing digital images for displacement tracking.
- Code for cross-correlation, displacement tracking, and data loading developed by me. Includes least-squares fitted polynomial plane for correcting out-of-image displacement. This massively improves fidelity of calculable displacements upon a second pass.
- Collaborated with co-creator for calculation of strain tensor components given the displacements.

ACHIEVEMENTS

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| ▪ Student Academic Choice Award Nominee, Imperial College
For undergraduate maths tutoring and supervision. | 2018 – 2019 |
| ▪ Armourers & Brasiers’ Guild Prize, City of London
Funding awarded to present internationally on electron microscopy and applied data science. | Jan 2019 |
| ▪ Institute of Materials, Minerals & Mining Prize
Awarded to University of Cambridge undergraduate with the most impressive research project. | Jul 2017 |
| ▪ Scholar of Jesus College, Cambridge
Elected as scholar of Jesus College for outstanding performance in Natural Sciences tripos. | Jul 2017 |
| ▪ CREST Gold Award & Nuffield Foundation ‘Best use of Maths’ Prize
Awarded by British Science Association for nanotube property Matlab modelling internship. | Oct 2012 |
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