Richard Andrew Couperthwaite

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https://richardcouperthwaite.github.io/

Education

Texas A&M University College Station, TX
Ph.D. - Materials Science and Engineering *Aug. 2017 – August 2021*

Thesis Title | *Efficient Bayesian-based Materials Design*

Texas A&M University College Station, TX
Materials Informatics & Design Certificate *Jan. 2018 – Jul. 2021*

University of the Witwatersrand Johannesburg, South Africa
MSc. Eng. - Metallurgical Engineering *Jan. 2015 – Jun. 2016*

Dissertation Title | *The effect of processing route on the structure and properties of Fe-Al based alloys*

University of the Witwatersrand Johannesburg, South Africa
BSc. Eng. - Metallurgical Engineering *Jan. 2006 – Dec 2009*

Experience

Graduate Research Assistant Aug. 2017 – Present
Texas A&M University *College Station, TX*

- Investigated surrogate modeling of thermodynamic model results for use in optimization frameworks
- Implemented high throughput calculations of a thermodynamic model and achieved at least an order of magnitude increase in speed
- Developed framework for Batch Bayesian Optimization of material properties that reduces the cost and time of the optimization by a factor of at least 10 when compared to traditional Bayesian Optimization
- Assisted in developing an optimization framework that uses a novel model fusion approach that was able to significantly decrease the cost and time required for optimization

Senior Materials Science Research Engineer Jan. 2017 – July 2017
Mintek *Johannesburg, South Africa*

- Managed research project work and ensured all work and project reporting was completed on schedule.
- Drafted research proposals for funding applications, one application was approved for funding of R50,000.
- Managed X-Ray Diffractometer, and ensured full operational ability over several years, and facilitated an upgrade to the functionality of the machine to obtain faster results.
- Executed upgrade to EDX and EBSD system for Scanning Electron Microscope, ensuring simultaneous EDX/EBSD scanning was possible
- Trained users on both X-Ray Diffractometer and Scanning Electron Microscope

Materials Science Research Engineer Jan. 2010 – Dec. 2016
Mintek *Johannesburg, South Africa*

- Executed small project research work for external clients, and returned all reports to clients before deadline.
- Executed several research projects, drafting full internal reports and sections for external reports to funding agencies.
- Managed X-Ray Diffractometer and operated system for internal work, ensuring turnaround time from sample acquisition to sending results was on average less than a week.
- Operated SEM for most research projects in the physical metallurgy group and ensured prompt and accurate results.

Projects

Batch Bayesian Materials Optimization | *Python, Bayesian Optimization* Jan. 2020 – Present

- Implemented reification/fusion approach in Python. Class based structure handles most functions automatically.
- Implemented Batch Bayesian Optimization approach. Modified approach to work with model fusion approach.
- Developed novel combined framework in Python. New framework optimizes faster and at lower cost than traditional Bayesian optimization approach.
- Published initial results in JOM
- Published framework code in the Code Ocean Repository

Thermodynamic surrogate modeling | *Python, Matlab, Thermo-Calc* Aug. 2017 – Present

- Built Gaussian Process Surrogate Models for Thermo-Calc results. Aim to speed up calculations, and ensure that calculations are available without license requirements.
- Gaussian Process models proved to be accurate and significantly faster than Thermo-Calc calculations.
- Published results in Computational Materials Science Journal

AMD Application Development | *Python, Qt GUI, MongoDB, Gmail API* Jan. 2016 – present

- Built two standalone applications for the Advanced Materials Division (AMD) at Mintek
- The first application handles booking of time on the instruments within the division
- Emails are automatically sent to instrument operators and requesters to notify either about the original requests or changes thereto
- The second application assists with the generation of quotations for small project work, and the generation of report numbers for the completed work.
- Both applications rely on JSON databases, with the small project application interfacing to a MongoDB online database
- Both are written in Python and use the Gmail API for sending emails. The GUI was built in Qt and is controlled through the PyQt interface.

Fe-Al Alloy Research Project | *Powder Metallurgy, Mechanical Alloying, Sintering, Casting* Jan. 2012 – Aug. 2017

- Researched the effect of adding platinum group metals to Fe-Al intermetallic alloys.
- Evaluated the change in microstructure and properties when processing materials by mechanical alloying and sintering compared to melting and casting.
- Investigated use of powder materials for coating applications using cold spray coating.

Bio-Ceramic Research Project | *Powder Metallurgy, Ceramic Testing* Jan. 2010 – Dec. 2011

- Research project looking to develop a new ceramic for biological applications.
- Characterized and tested sintered materials produced by collaborators

Academic Publications

Publications

- Khatamsaz, D., Molkeri, A., Couperthwaite, R., James, J., Arróyave, R., Allaire, D., Srivastava, A., Efficiently exploiting process-structure-property relationships in material design by multi-information source fusion. Acta Materialia 206, 2021 DOI: https://doi.org/10.1016/j.actamat.2020.116619
- Richard Couperthwaite, Abhilash Molkeri, Danial Khatamsaz, Ankit Srivastava, Douglas Allaire, Raymundo Arròyave, Materials Design Through Batch Bayesian Optimization with Multisource Information Fusion, JOM, 72, 4431–4443 (2020), DOI: 10.1007/s11837-020-04396-x
- Couperthwaite, Richard, Douglas Allaire, and Raymundo Arroyave. "Utilizing Gaussian Processes to Fit High Dimension Thermodynamic Data That Includes Estimated Variability." Computational Materials Science, (In Press, Corrected Proof, Available Online 20 November 2020) DOI: doi.org/10.1016/j.commatsci.2020.110133.
- R.A. Couperthwaite, L.A. Cornish, I.A. Mwamba, M.J. Papo, Effect of processing route on the microstructure and properties of an Fe-Al alloy with additions of precious metal, Materials Today: Proceedings, 2, 2015, 3932 – 3942
- R.A. Couperthwaite, L.A. Cornish, I.A. Mwamba, Cold-spray coating of an Fe-40 at.% Al alloy with additions of ruthenium, Journal of the SAIMM, Volume 116, 2016, 927-934

Conference Presentations

- Richard Couperthwaite, Abhilash Molkeri, Danial Khatamsaz, Ankit Srivastava, Douglas Allaire, Raymundo Arròyave, Model Reification with Batch Bayesian Optimization, TMS 2021 Conference, 15-18 March 2021, Remote Conference
- Richard Couperthwaite, Abhilash Molkeri, Danial Khatamsaz, Ankit Srivastava, Douglas Allaire, Raymundo Arròyave, Batch Reification Fusion Optimization (BAREFOOT) Framework, TMS 2021 Conference, 15-18 March 2021, Remote Conference
- R.A. Couperthwaite, R. Arroyave, A. Srivastava, D. Allaire, Model Reification with Batch Bayesian Optimization TMS 2021 Conference, 15-18 March 2021, Remote Conference
- R.A. Couperthwaite, R. Arroyave, I. Karaman, A. Srivastava, D. Allaire, A Model Fusion Approach to Modeling Microstructure Development during Heat Treatment, TMS 2020 Conference, 23-28 February 2020, San Diego, California, USA
- R.A. Couperthwaite, L. McClenny, J. James, V. Attari, R. Arroyave, U. Braga-Neto, Utilizing Convolutional Neural Networks for Prediction of Process and Material Parameters from Microstructural Images, TMS 2020 Conference, 23-28 February 2020, San Diego, California, USA

- R.A. Couperthwaite, R. Arroyave, I. Karaman, A. Srivastava, D. Allaire, Thermodynamic Design of Dual-Phase Steels Within and Information-Fusion Framework, TMS 2019 Conference, 10-14 March 2019, San Antonio, Texas, USA
- R.A. Couperthwaite, R. Arroyave, Estimation of Dual-Phase Steel Properties from Composition, CALPHAD XLVII, 27 May-01 June 2018, Queretaro, Mexico
- R.A. Couperthwaite, L.A. Cornish, I.A. Mwamba, Cold-spray coating of an Fe-40 at.% Al alloy with additions of ruthenium, AMI Ferrous and Base Metals Development Network Conference, 19-21 October 2016, Durban, South Africa
- R.A. Couperthwaite, I.A. Mwamba, L.A. Cornish, EBSD analysis of an FeAl alloy produced by two different methods, 53rd Annual Conference of the Microscopy Society of Southern Africa, 30 November – 3 December 2015, Pretoria, South Africa
- R.A. Couperthwaite, L.A. Cornish, I.A. Mwamba , M.J. Papo, Effect of processing route on the microstructure and properties of an Fe-Al alloy with additions of precious metal, 7th International Symposium On Macro- and Supramolecular Architectures and Materials, 24 – 26 November 2014, Johannesburg, South Africa

Technical Skills

Computational Methods

Languages: Python, Matlab
Developer Tools: Git, Code Ocean, Qt, MongoDB
Libraries: pandas, NumPy, SciPy, Matplotlib, Keras, PyQt, pymongo

Experimental Methods

Materials Characterization: Optical Microscopy, Hardness Testing, Tensile Testing
Scanning Electron Microscopy: Imaging, EDX, EBSD (Total exceeds 1000 user hours)
X-Ray Diffraction: Powder and Solid Sample, Phase Identification, Rietveld Refinement