AI for Materials Science: Tuning Laser-Induced Graphene Production

Lars Kotthoff, Vivek Jain, Alexander Tyrrell, Hud Wahab, and Patrick Johnson
Artificially Intelligent Manufacturing Center
larsko@uwyo.edu

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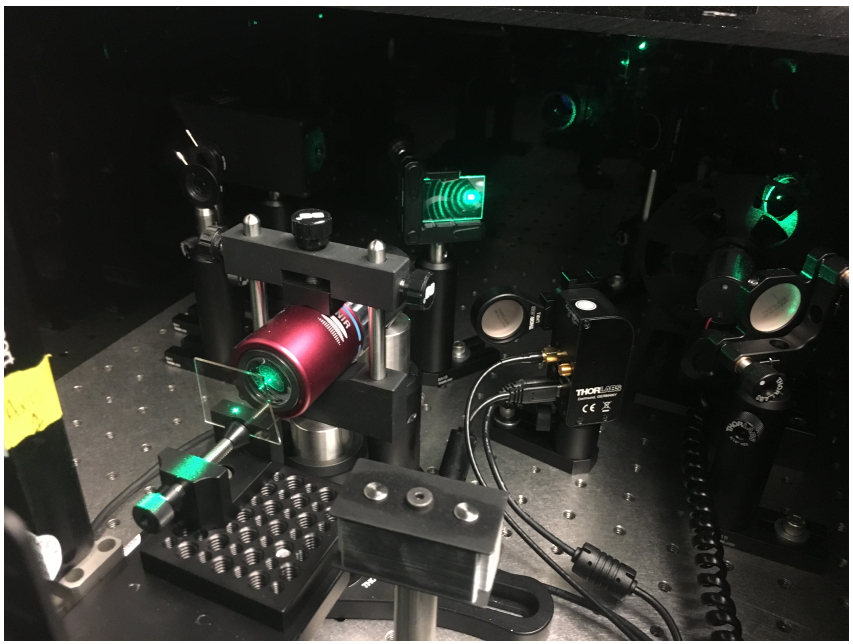
Automated Parameter Tuning

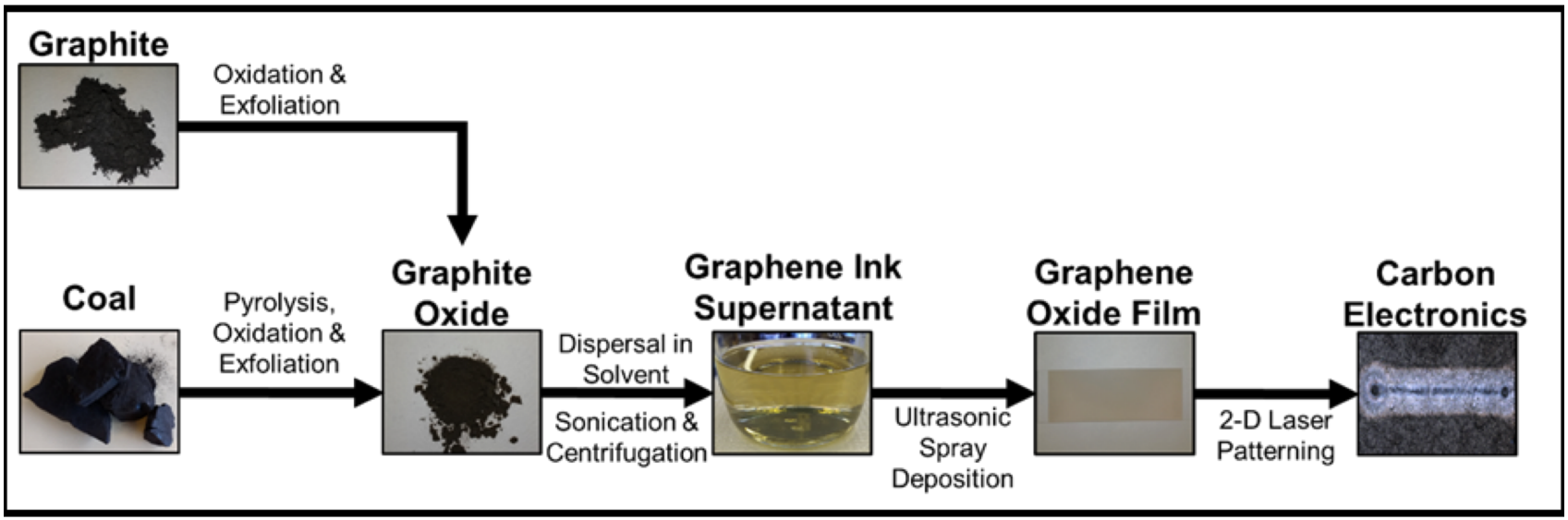
- ▷ treat tunable process as black box – no knowledge of inner workings required
- ▷ intelligently and iteratively select parameter settings likely to improve performance
- ▷ mature techniques used in many areas of AI

Optimizing Graphene Oxide Reduction

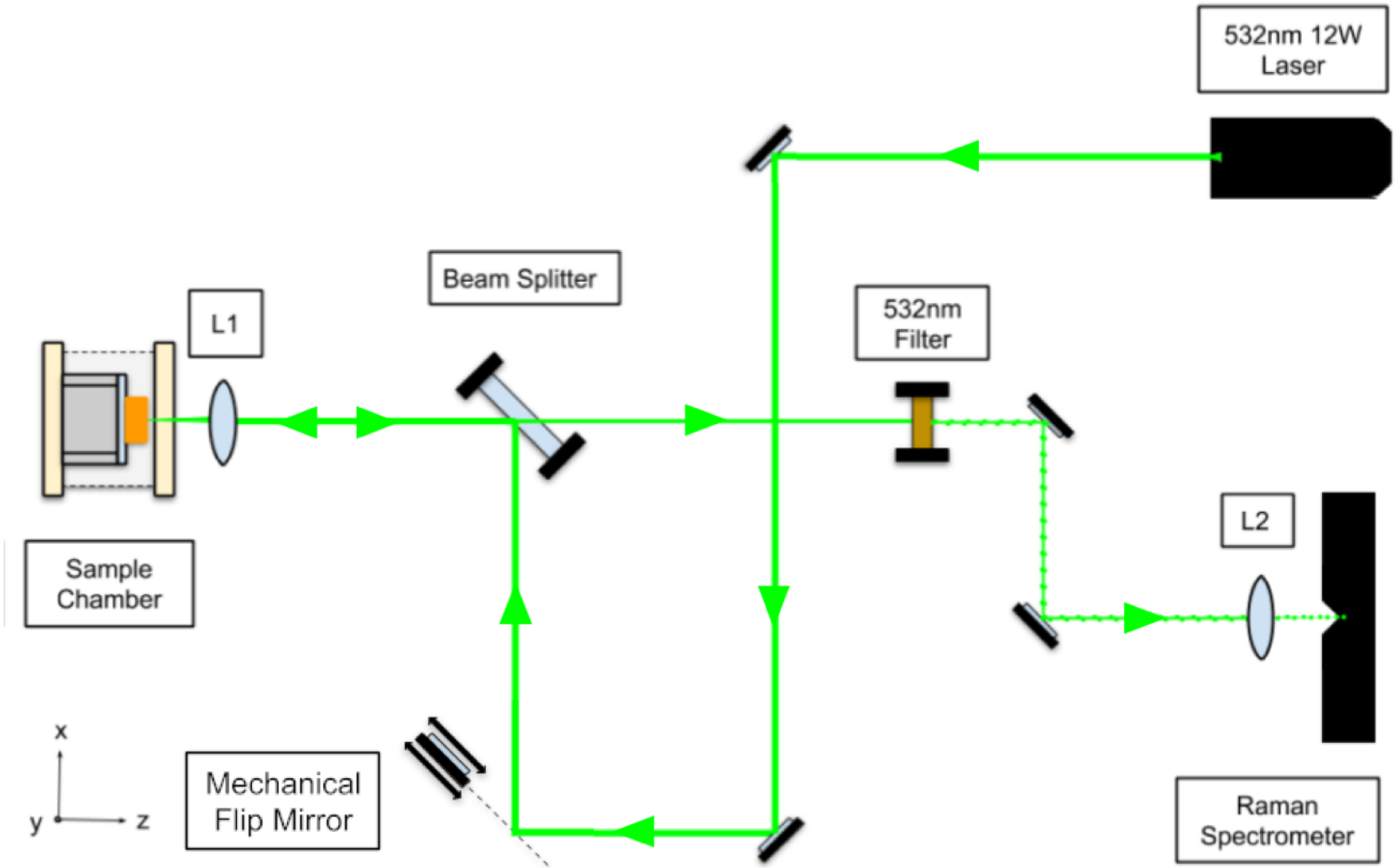
- ▷ reduce graphene oxide to graphene through laser irradiation
- ▷ allows to create electrically conductive lines in insulating material
- ▷ laser parameters need to be tuned carefully to achieve good results



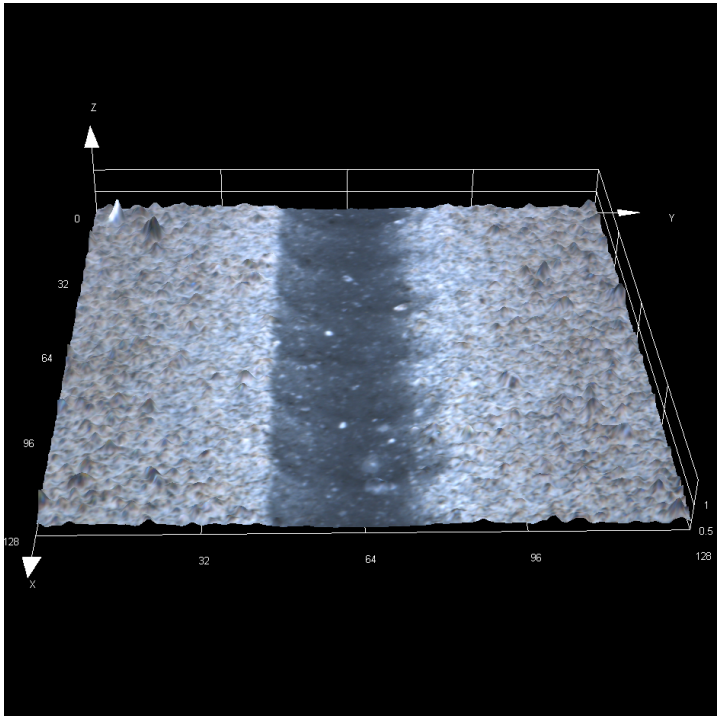
From Graphite/Coal to Carbon Electronics

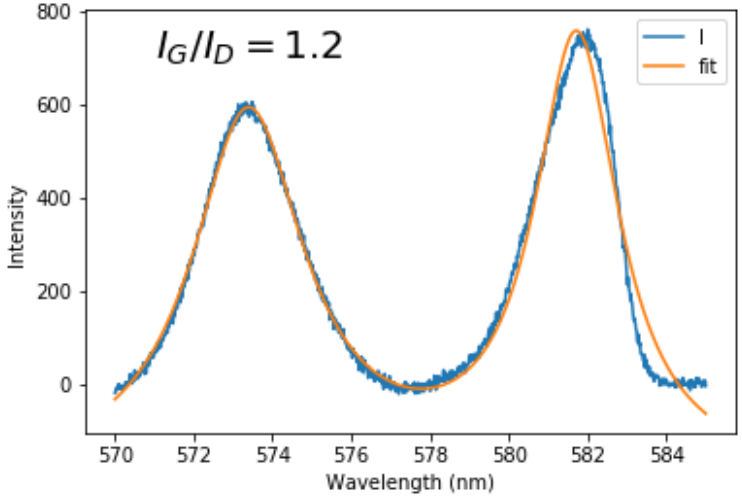


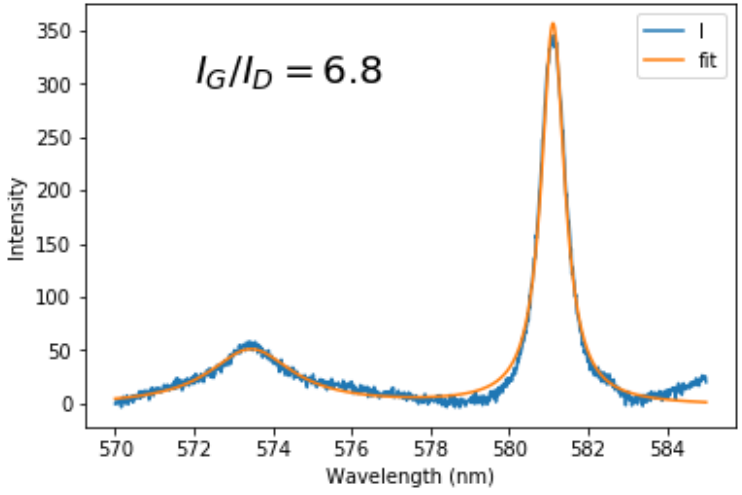
Experimental Setup



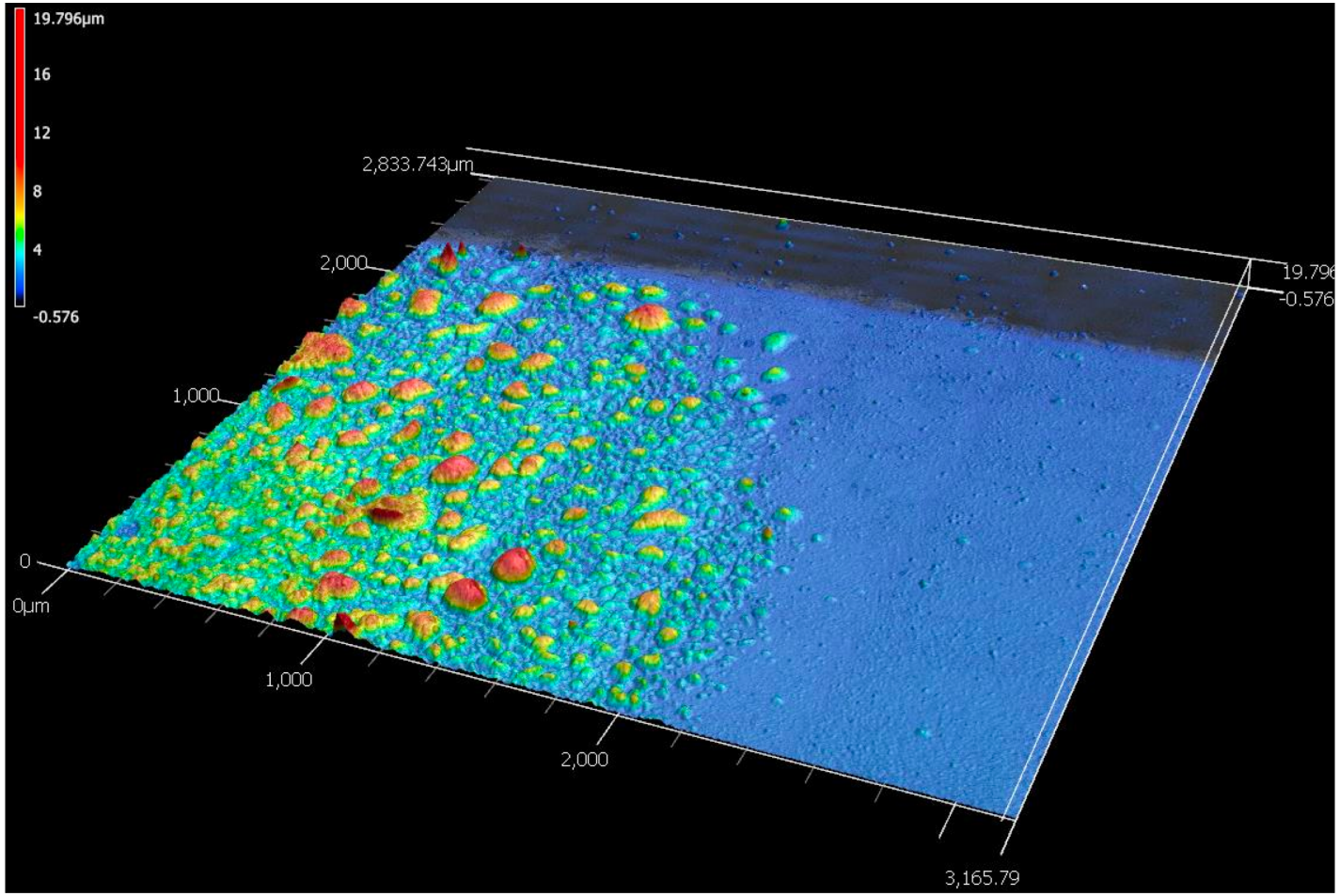
Evaluation of Irradiated Material



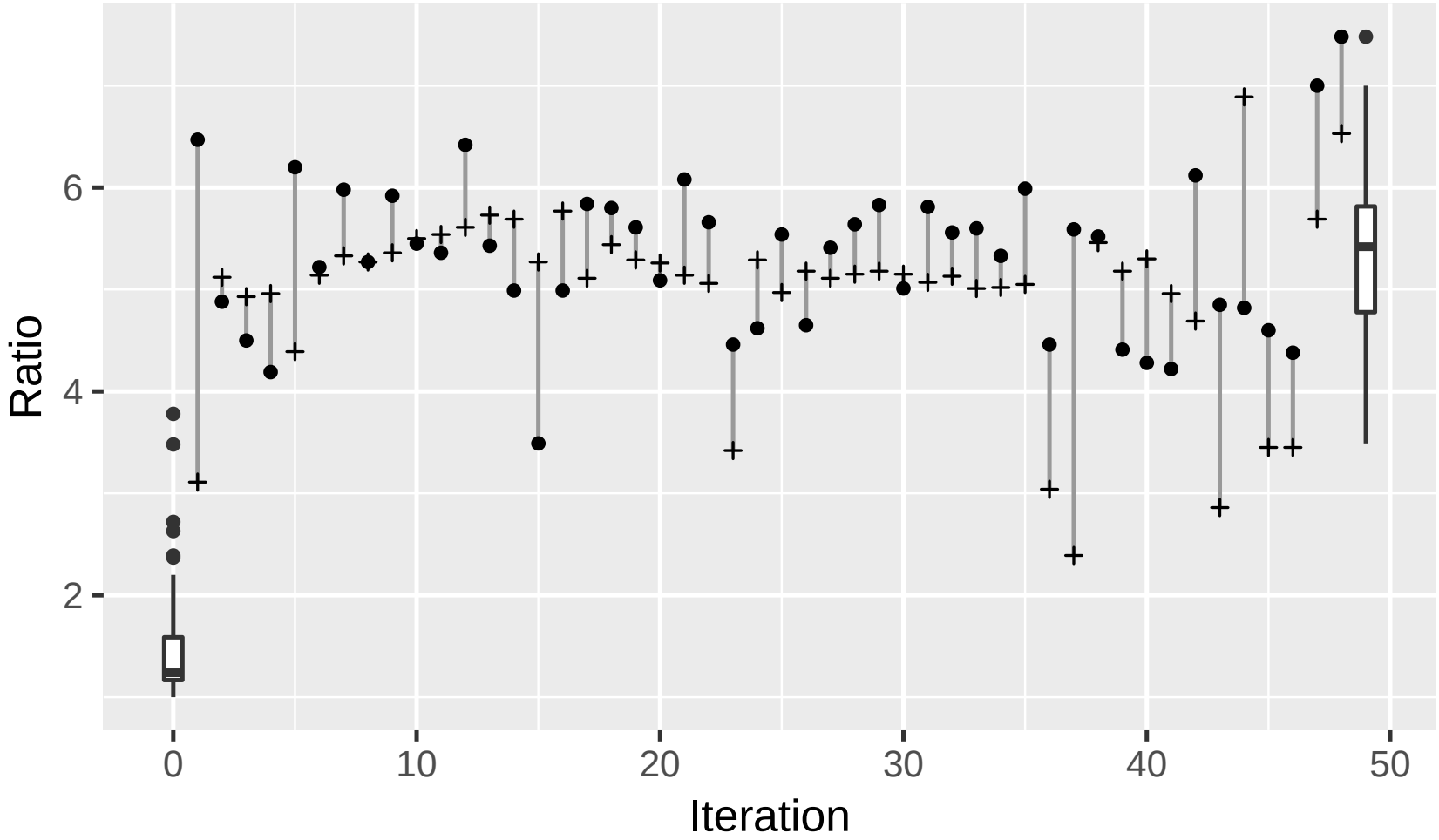




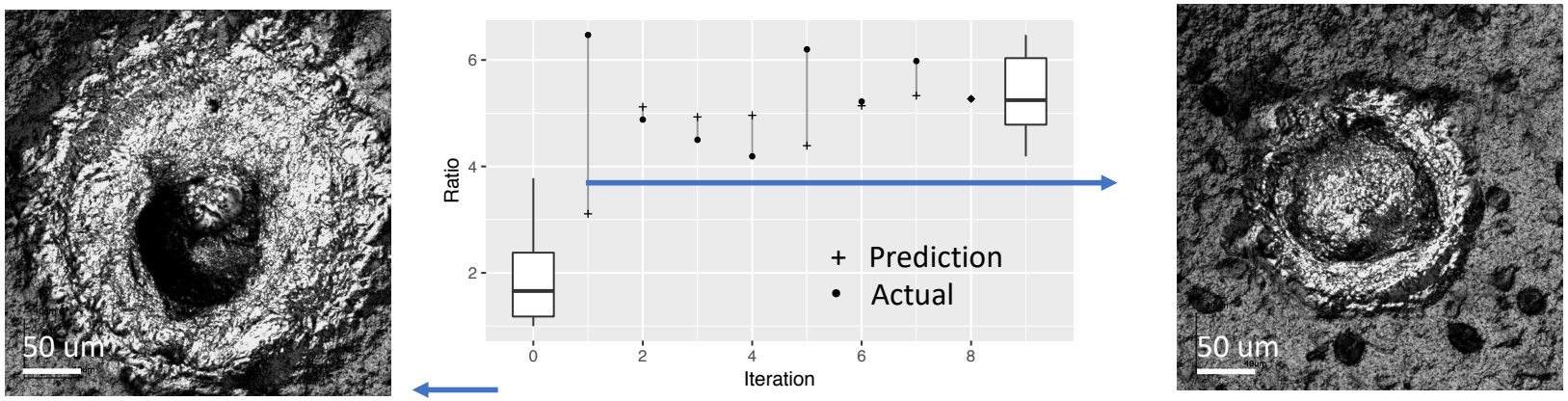
Morphology of Irradiated Material



Tuned Parameters

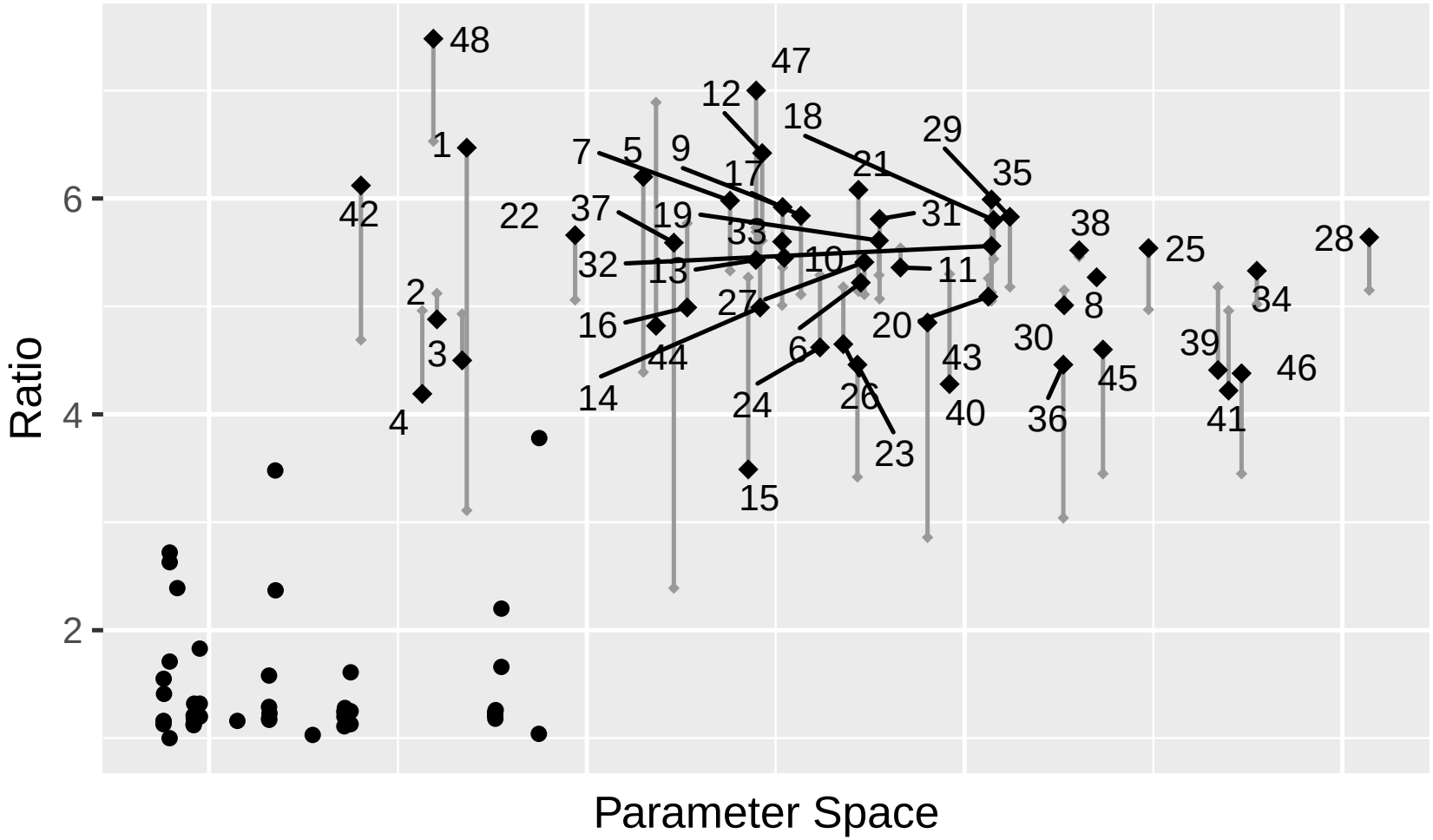


Tuned Parameters



- ▷ improvement of factor of two over best result in literature
- ▷ good results even with small amount of initial data (19 evaluations)
- ▷ code can be used by domain experts with no background in machine learning

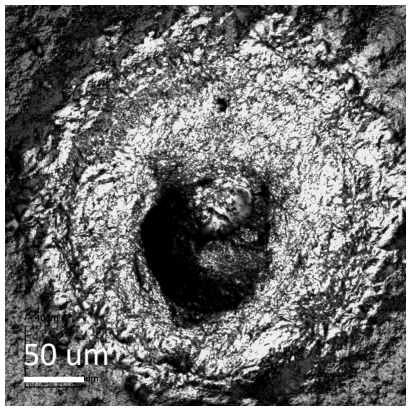
Explored Parameter Space

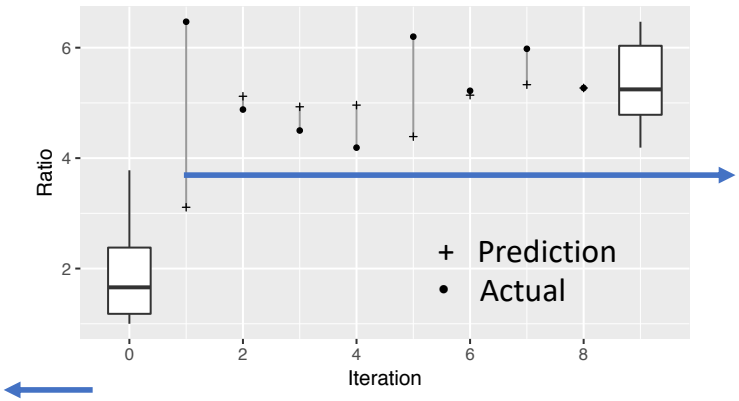


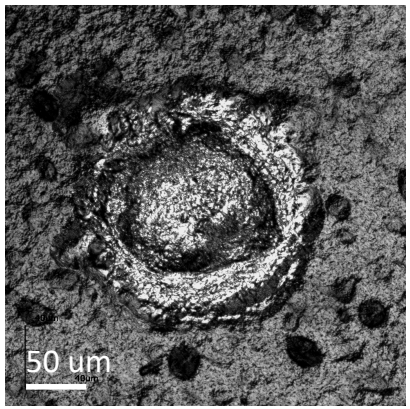
Outlook

- ▷ application to other materials
- ▷ more in-depth investigation of Bayesian Optimization performance
- ▷ inform understanding of process by what surrogate model has learned

Summary







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