AI for Materials Science: Tuning Laser-Induced Graphene Production

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

Data Science meets Optimization Workshop, 11 August 2019
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
Experimental Setup
Evaluation of Irradiated Material

\[ \frac{I_G}{I_D} = 1.2 \]

\[ \frac{I_G}{I_D} = 6.8 \]
Morphology of Irradiated Material
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

Predictions work even with small training dataset (19 points) and AI Model achieved IG/ID ratio (>6) after 1st prediction.

During Training:
- After 1st prediction:
  - Prediction:
  - Actual:

50 um

50 um