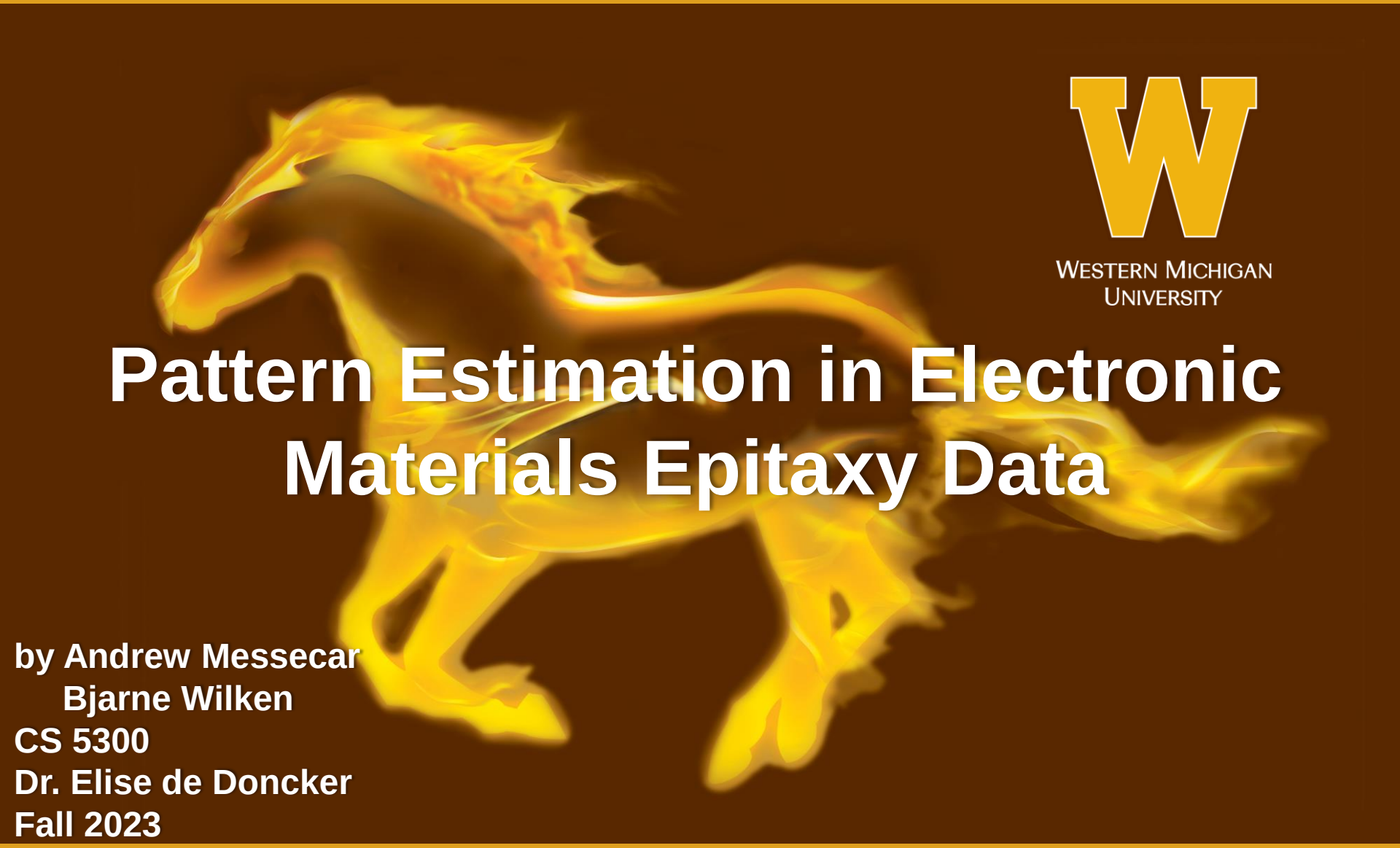

WESTERN MICHIGAN UNIVERSITY

Pattern Estimation in Electronic Materials Epitaxy Data

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CS 5300
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Outline

- Motivation
- Background
  - Parameter Tuning & Selection Strategies
  - Molecular Beam Epitaxy
  - Epitaxy & Characterization of III–Nitride Materials
  - Metal–Organic Chemical Vapor Deposition (MOCVD) of Transition Metal Dichalcogenides
  - Optical Emission Spectra of N_2 Plasma
- Strategy

Motivation

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- Machine learning technologies, including but not limited to artificial neural systems, can aid with pattern recognition and estimation.
- The universal approximation theorem is nice.
- Well – designed and optimized neural network algorithms can help us to learn the real relationship between operating parameters and experimental outcomes.

Background: Parameter Optimization

- Hold–Out Method & k–Fold Cross Validation

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- Penalty–based Regularization Techniques

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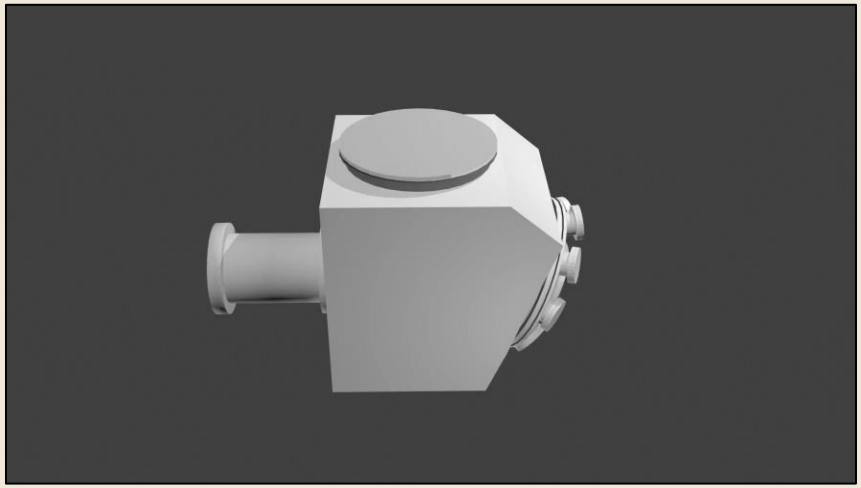
- Bayesian Optimization of Hyperparameters

Background: Molecular Beam Epitaxy

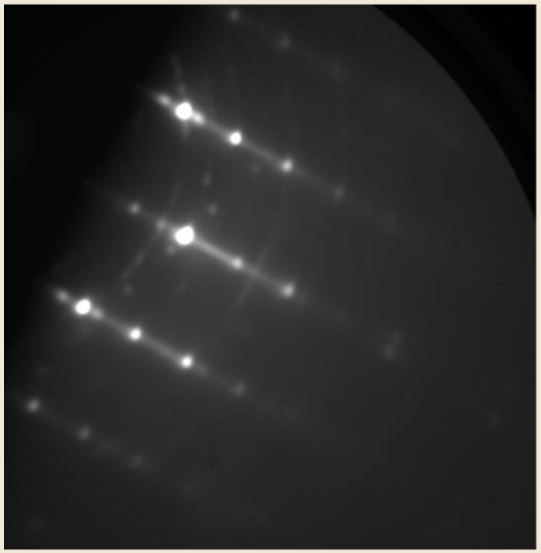
- Ultra–high vacuum synthesis technique
- Bottom–up growth of thin film crystals
- Offers high purity and atomic level control and precision during growth



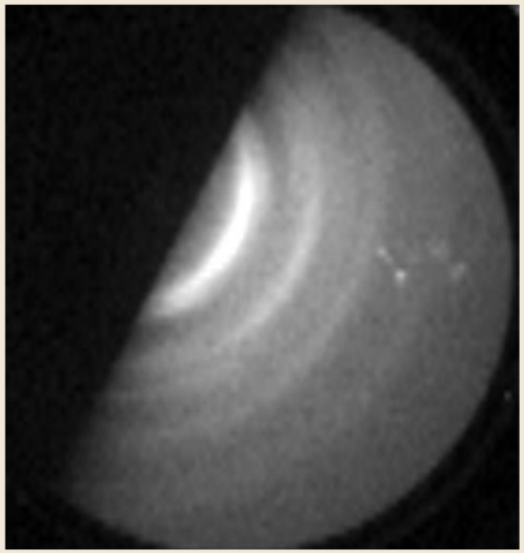
Animation Source: Nathaniel Feldberg, Ph.D.

Characterization Data

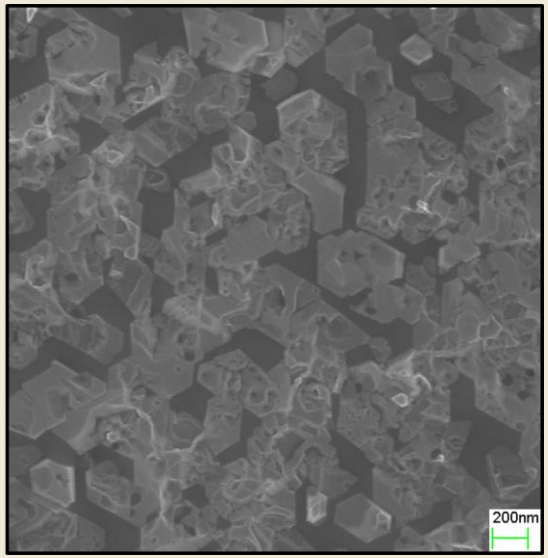
Single Crystalline



Polycrystalline

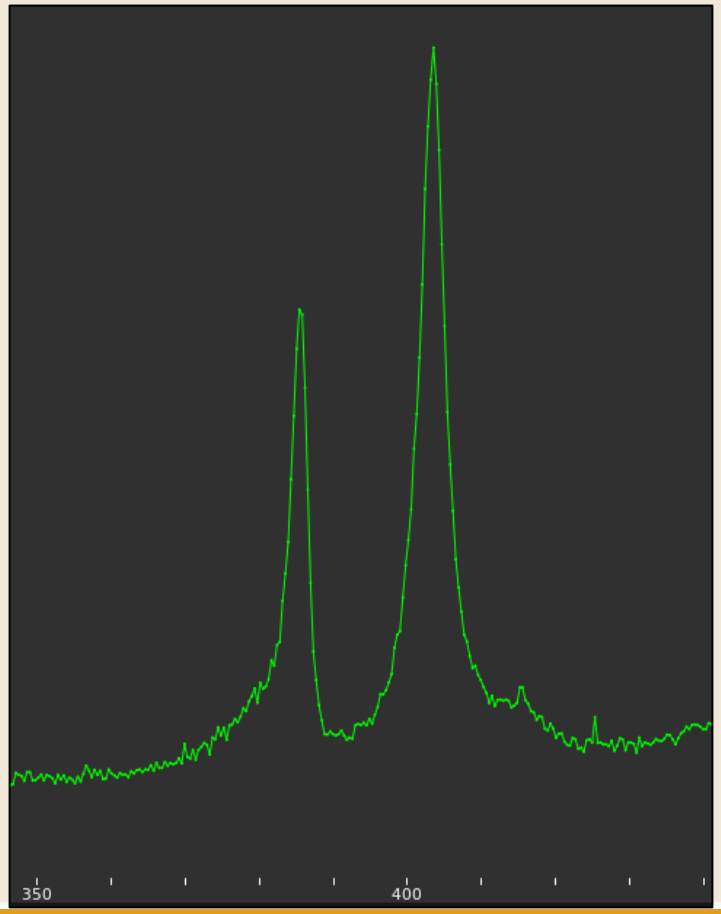


Scanning Electron Micrograph

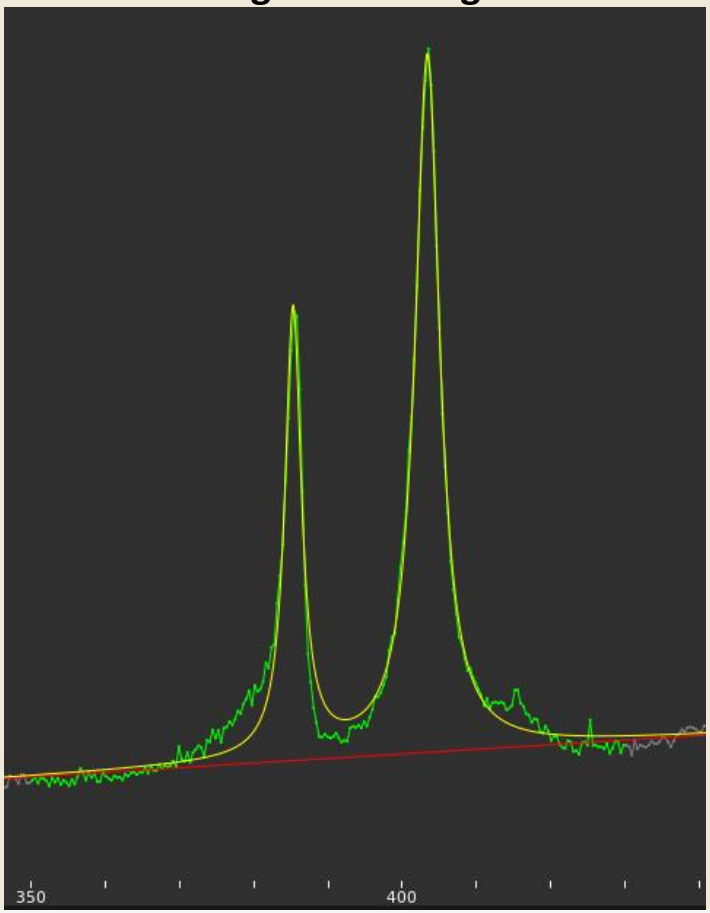


Raman Spectra of MoS_2 Thin Films

Raman Spectrum of MoS_2



Fitting E_{2g} and A_{1g} Modes

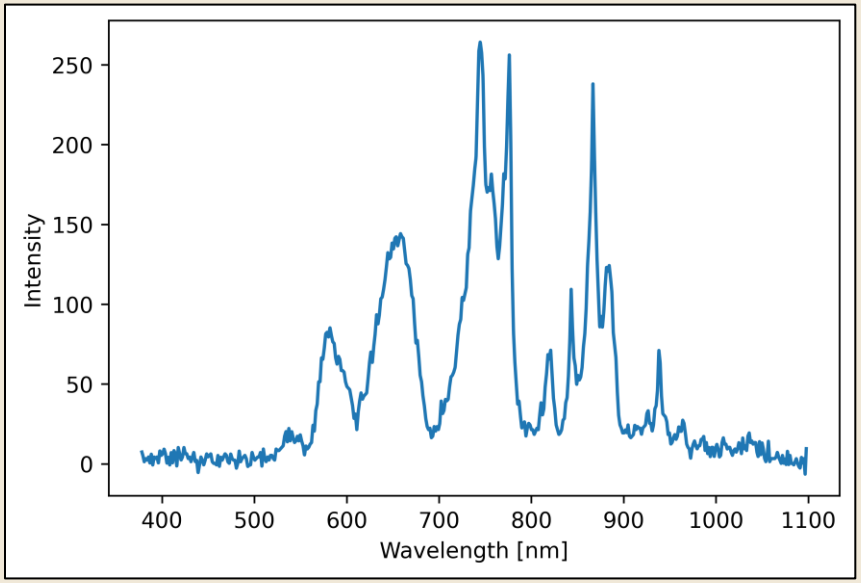


Additional Data: N_2 Plasma

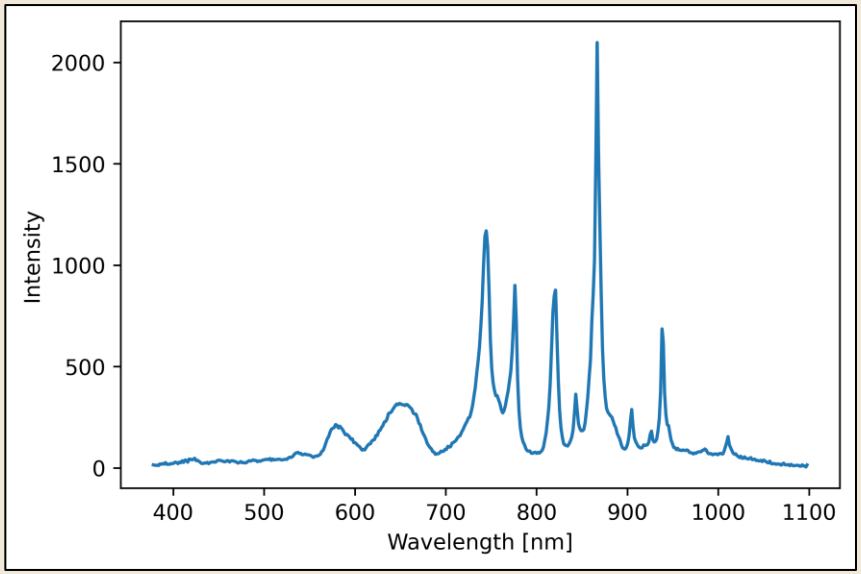
- Optical Emission Spectra (OES) data have been acquired for a radio frequency nitrogen plasma source specifically designed for the growth of electronic materials.
- OES data allows for measurements of the relative concentrations of different active nitrogen species within the plasma.
- These measurements combined with the operating parameters provide additional data.

Optical Emission Spectra of N_2 Plasma

Low Power: 100W



High Power: 500W



Python3 Implementation Strategy

- Import libraries and data
- Randomly organize data points into no less than 3 different data sets (train, test, validate).
- Implement generalization strategies for ANNs.
- Log validation performance for comparison.
- Use champion algorithm to generalize to all possible values of operating parameters.
- Compare to literature.