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Beam and Plasma Technology FEP

Barth, S.; Bartzsch, H.; Glauer, M.; Kupsch, C.; Käpplinger, C.; Leipner, E.; Neidhardt, J.; Nestler, M.; Neuhaus, F.; Perschewski, J.-O.; Schütte, T.; Urbach, J.-P.

# Project DigiMatUS:
# Digitalization of materials research on thin-film materials using the example of high-resolution piezoelectric ultrasonic sensors

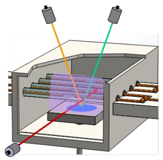
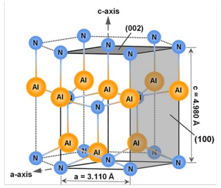
# Introduction

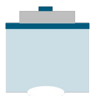
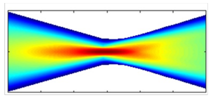
- Project overview and Background
- Thin film ontology „CoatO“
- Experimental results and machine learning
- Conclusion

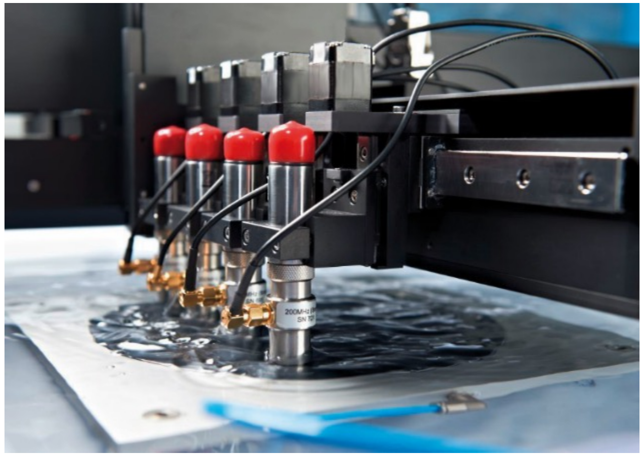
 

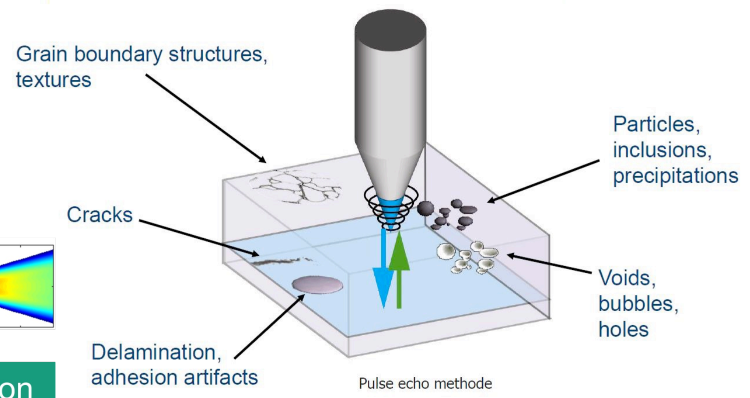
# Project Overview
## DigiMatUS

- Ultrasonic microscopy for non-destructive examination of microelectronic structures
- Use of piezoelectric $AlN/Al_XSc_{1-X}N$ thin films for generation of ultrasound waves
- Film deposition by reactive magnetron sputtering
- DigiMatUS focused on value chain:


Machine →

Process →


Film →

Transducer →

Application



# Project Overview

## DigiMatUS consortium

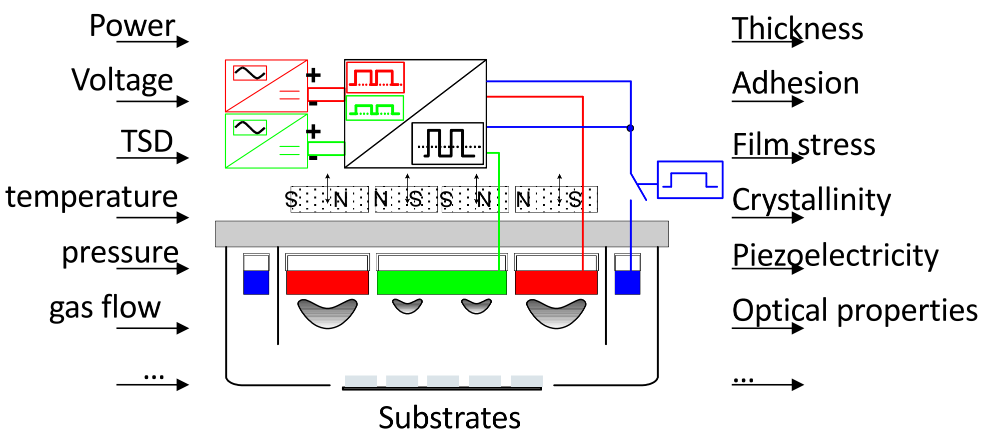
- 3 industrial partners:

- 3 academic partners:

# Challenges

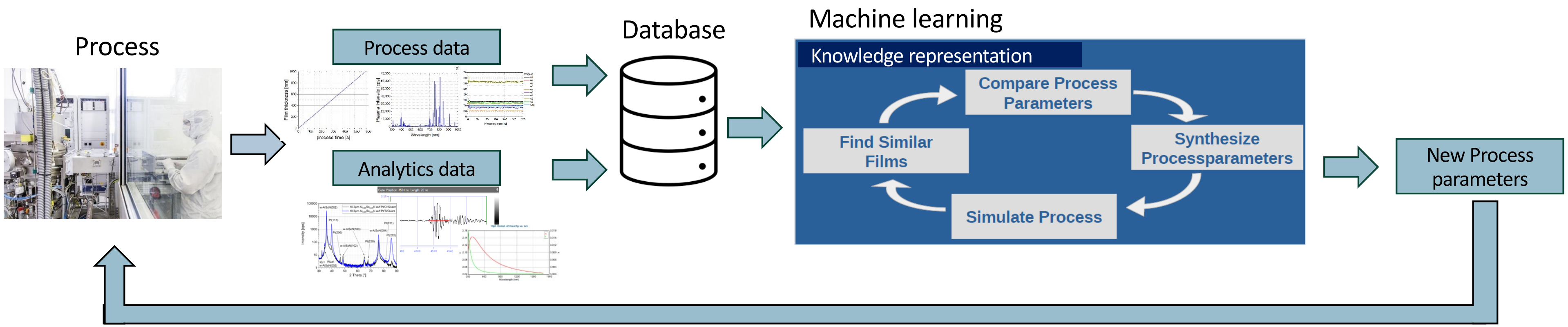
- Developing new processes/ materials or optimizing process-material-device value chain often costly and time-consuming
- Few datapoints for machine learning approach
- Complex interrelationships of mutually influencing process parameters
- Not all relevant machine and process parameters can be recorded



# Project Approach

- Development of an ontology for thin-film processes, properties and materials
- Combination of extensive in-situ measurement of process and plasma properties, in-situ film growth with ex-situ film and transducer characterization
- Training of machine learning algorithm with available experimental data and expert knowledge



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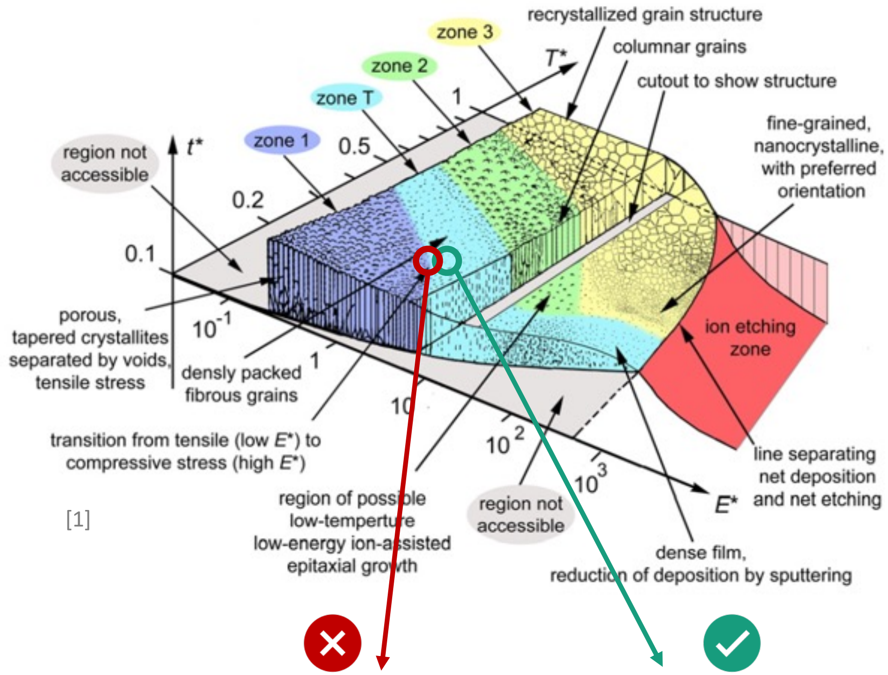
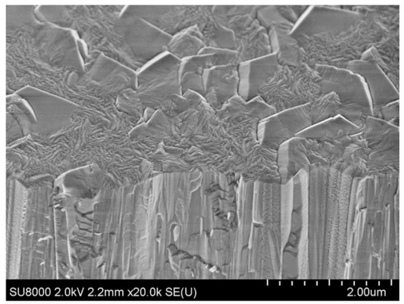
# Background

## Thin film deposition

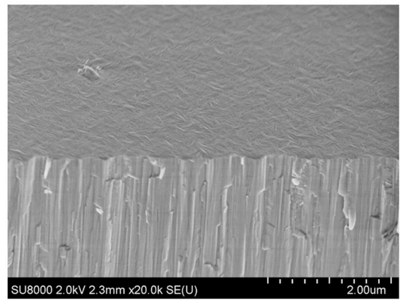
- Film deposition by vacuum-based reactive magnetron sputtering
- Film properties strongly depending on process conditions




[1]




AlN on Si




AlN on Si


[1] A. Anders. “A structure zone diagram including plasma-based deposition and ion etching”. Thin Solid Films 518.15 (2010), pp. 4087–4090. https://doi.org/10.1016/j.tsf.2009.10.145.

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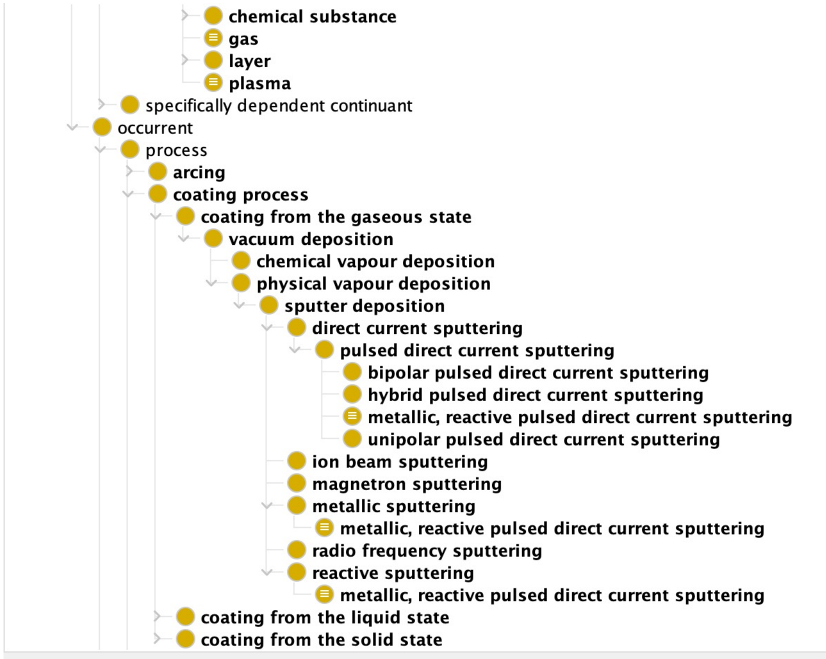
# Ontology CoatO

- CoatO is BFO based, between mid- and application-level ontology
- PMDCo V3 alignment planned after its release
- Vocabulary for machine and process parameter as well as film properties (e.g. optical and electrical)



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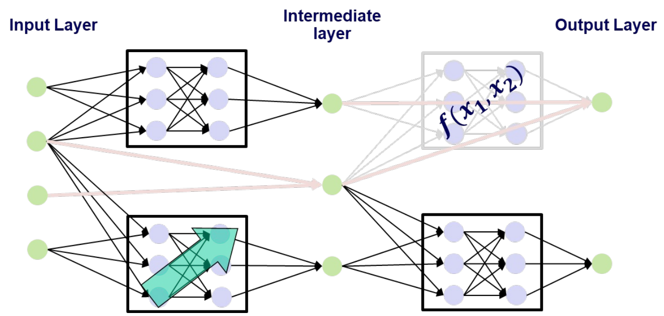
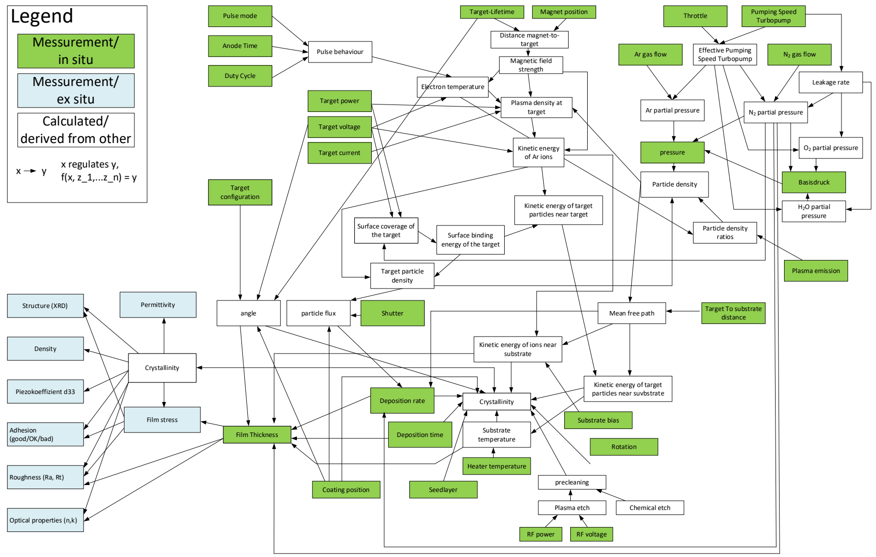
# Expert knowledge and Machine learning

## Approach

- Ontological model to represent dependencies of coating machine and process parameters, plasma properties and film (growth + properties)
- Dependencies and expert knowledge are cast into hybrid machine learning model with symbolic rules
- Reduced parameter space reduces data hunger

### Neuro-symbolic learning & reasoning

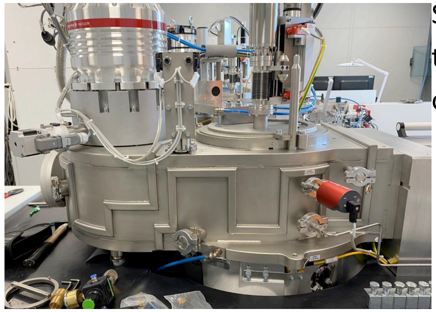


# Experimental Results

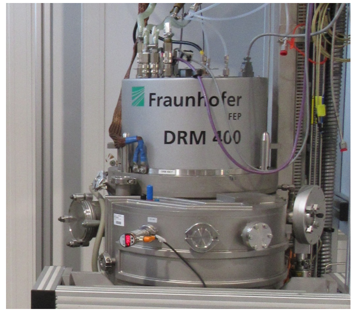
## Depositions – in situ

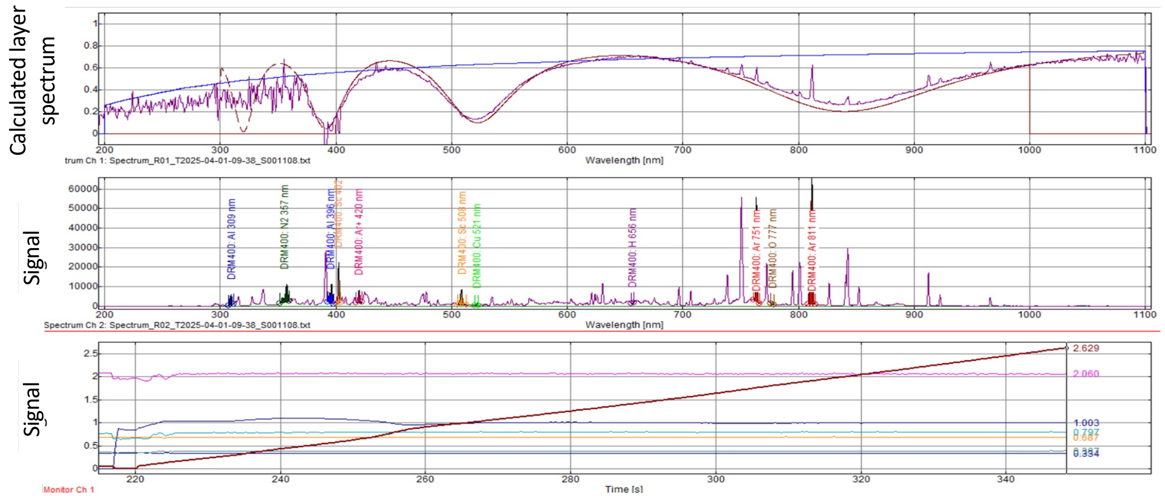
- Use of two different machine configurations for deposition
- In-situ monitoring of:
- machine parameters,
- plasma emission spectra,
- film growth



Sputter-up, confocal two magnetron configuration

Sputter down, double ring magn. configuration



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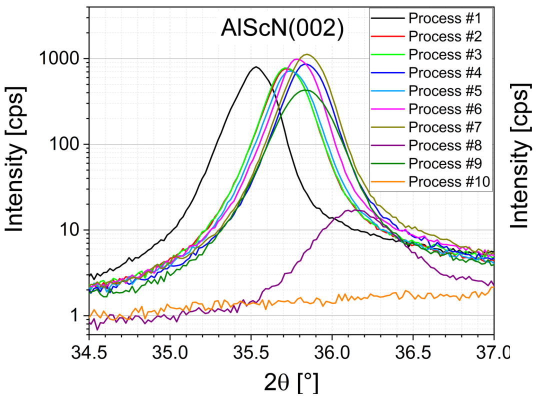
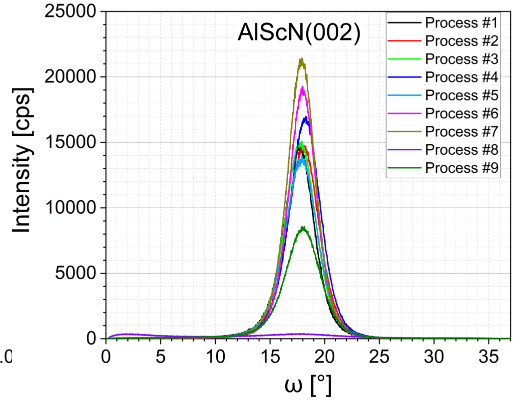
# Experimental Results

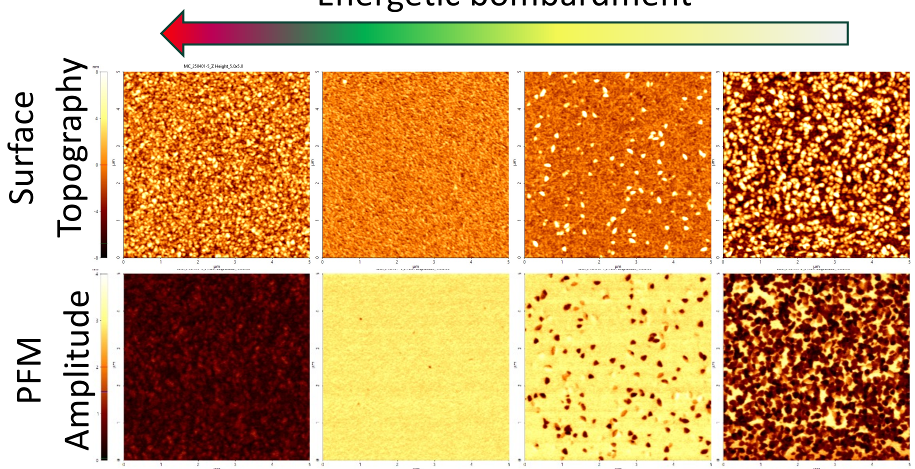
## Analytics – ex situ

- Ex-situ measurement of coated transducers
- Structural, electrical, optical and piezoelectric properties

Coated transducer

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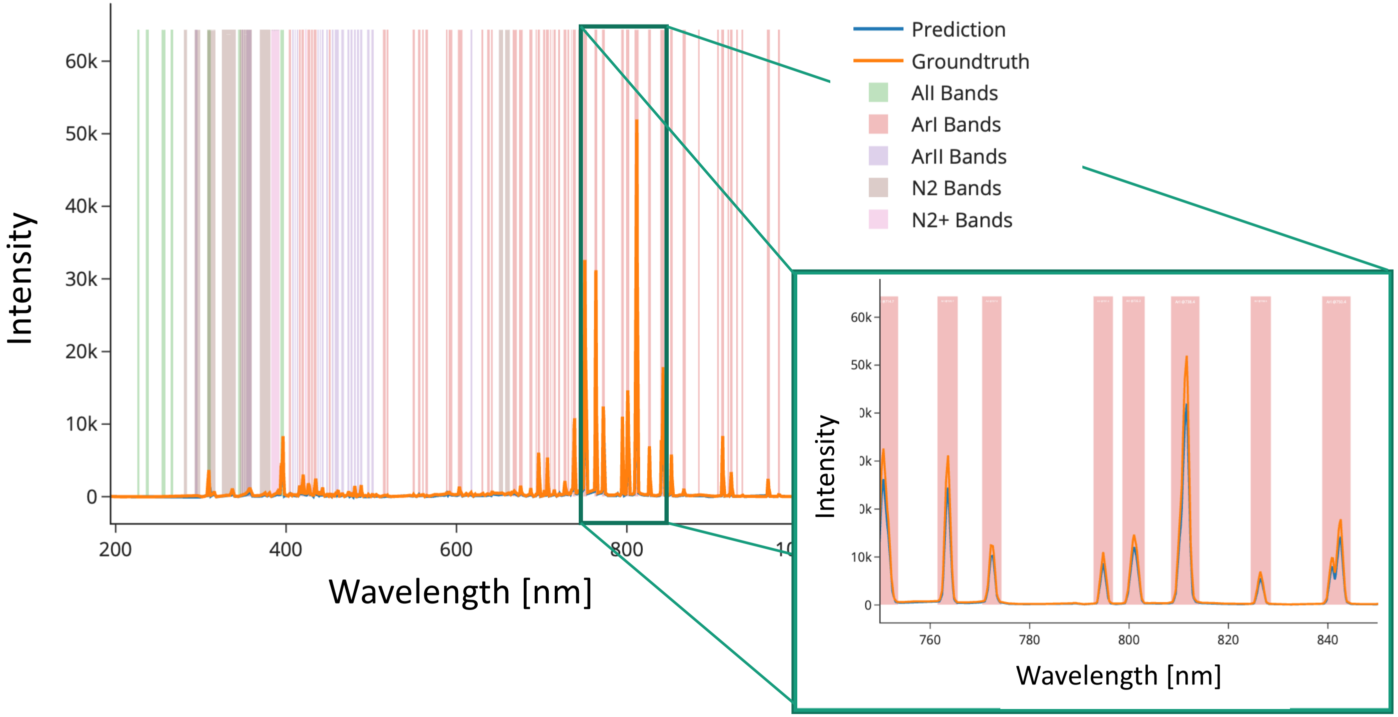
# Machine Learning / Demonstrator

- Prediction of plasma properties (emission spectra) from process parameters
- Color coded to align spectra with species and their various excitation states



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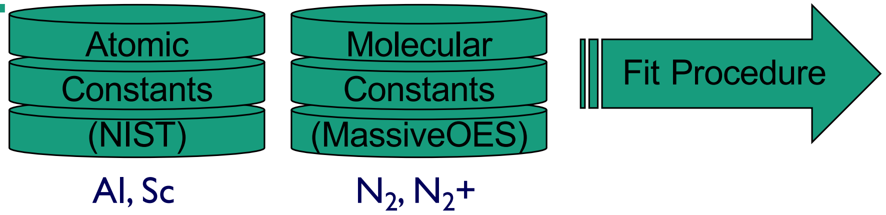
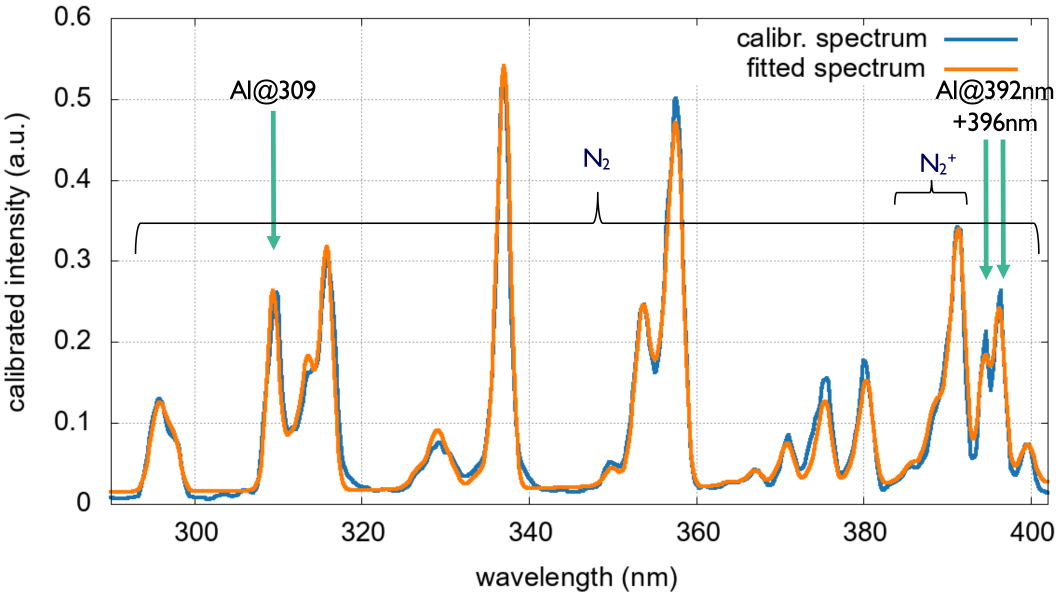
# Potential Data Analysis

## Physical models for spectroscopic data, Deriving physical quantities from emission spectra




$$I(\lambda) = f(T_{gas}, n_{N_2}, n_{N_2^+}, n_{Al}, n_{Sc})$$




- Fit by MassiveOES:
- Species considered; N2, N2+, Al, (no Sc in this experiment)
- Assumption of thermal population

Results:

$T_{rot}$ = 381 K

$n_{N2}$ = $4.8 \times 10^{-7}$

$n_{N2+}$ = $3.9 \times 10^{-6}$

MassiveOES:
Voráč, J., Kusýn, L., Synek, P. (2019) Deducing rotational quantum-state distributions from overlapping molecular spectra. *Review of Scientific Instruments* 90, 123102

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# Conclusion

- Training of machine learning algorithm with experimental data and expert data
- Demonstrator: Prediction of plasma properties from process parameters
- Ongoing:
  - Training models for predicting layer properties
  - Evaluation of neuro-symbolic model
  - Cased-based reasoning for selecting promising process parameters, prediction of properties of thin films based on process parameters
- Development of a structured experimental and simulation-based digital description of thin-film sensor materials for ultrasonic microscopy

 

# Thank you for your attention!

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