Optimized quality control through microstructural data mining and machine learning

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The purpose of this presentation is to guide programs benefiting the copper industry and to provide attendees with information to make independent business decisions.
The microstructure „knows“ **everything!**
→ **remembers** complex processing + **controls** complex property portfolio

Process

Microstructure

Properties

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**Microstructure** stores processing history

**Microstructure** determines properties
Quality control? - How can we **reliably classify** the microstructure?

Experts are unintentionally biased due to different subjective experiences.

Problems occur if high-performance materials with well tailored microstructures allow only minor differences ... are locally very complex ...
Data Science & Artificial Intelligence → does it really open attractive options?

Everything with much and high-dimensional data

Everything with images

→ tedious, labor-intensive work
Can't make any more progress with analytics/modeling?
Data Science & Artificial Intelligence – *manifold Possibilities!*

**General advantages of ML approaches**
- **Reproducibility**
- **Efficiency**
- **Automation**

- Key aspects in microstructure quantification and quality control!
Data Science & Artificial Intelligence – tailored approaches

General advantages of ML approaches

- Reproducibility
- Efficiency
- Automation

➤ Key aspects in microstructure quantification and quality control!
Machine Learning opens new ways for Image Processing

Microstructure analysis

Semantic Segmentation

Classification

Classification + localization

Object detection

Instance segmentation

CAT GRASS TREE

No object
Just pixels

Single object

CAT DOG DUCK

Multiple objects
Machine Learning in Microstructures – more than just „some code“

Modified after Sculley et al. Hidden technical debt in machine learning systems.
Essential approach: **reproducibility in every step**

1. Step: Sample acquisition/data selection
2. Step: **Reproducible** contrasting
3. Step: Suitable imaging
4. Step: Data preparation (registration)
5. Step: Ground truth assignment
6. Step: Selection of a suitable approach
7. Step: Feature extraction
8. Step: Training
9. Step: Interpretability?
Reproducible contrasting – **reproducible etching with monitoring**

How can we contrast the microstructure reproducibly? → **Time, Temp, Concentration...**

**in situ observation**

- Microscope
- Flow cell
- Sample
- In-/return flow

**controlled etching**

- Measuring probe
- Dropping funnel
- Cooler
- Pump
- Measuring device

*patent pending*

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Reproducible contrasting – **reproducible etching with monitoring**

EXAMPLE: Steel ➔ Contrasting with modified Beraha etching – In situ observation

*patent pending*
Reproducibility in every step

1. Step: Sample acquisition/data selection
2. Step: Reproducible contrasting
3. Step: Suitable imaging
4. Step: Data preparation (registration)
5. Step: Ground Truth assignment
6. Step: Selection of a suitable approach
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8. Step: Training
9. Step: Interpretability?
Supervised Machine Learning – establishing the **Ground Truth**

https://tinyurl.com/y4mkpzup
Supervised Machine Learning – how do we get **reliable** Ground Truth

**Supervisor + Training Data set**

→ potentially subjective influences
  - affect the **entire classification**
  - **dangerous** for complex structures

https://tinyurl.com/y4mkpzup
1. Step: **Sample acquisition/data selection**

2. Step: Reproducible contrasting

3. Step: **Suitable imaging (correlative if necessary)**

4. Step: Data preparation (registration)

5. Step: **Ground truth assignment**

6. Step: Selection of a suitable approach

7. Step: Feature extraction

8. Step: Training

9. Step: Interpretability?

Reproducibility in every step → establish reference states → simplify Ground Truth investigation
Use Correlative Microscopy: LiMi + SEM + EBSD

- Large areas
- Simple & fast
- Limited resolution

- High resolution
- Different contrasting mechanisms

- Local lattice orientation
  + crystallographic phase
- Ideal complement to LiMi/SEM
- Limited resolution
- Relatively slow
Combine local Information → Correlative Microscopy: LiMi + SEM + EBSD


Correlative Microscopy: LiMi + SEM + EBSD

Visualize comprehensive information \rightarrow from all 3 microscopy levels
Combined **Quantification** from LiMi + SEM + EBSD ➔ extract reliable data from microstructure features in all 3 levels

Combined Quantification from LiMi + SEM + EBSD

- **Which accuracies** can be achieved with
  - LiMi?
  - SEM?
  - EBSD?

- **Which method is sufficient/necessary for which question?**

- **Is more objective class definition possible** purely via EBSD data? → too slow, time-consuming 😞
- **Automated EBSD-based ground truth assignment?** 😊

**References by correlative microscopy → GOAL for series application:** simplification to LiMi
Key advantage: we do it just once (... for each kind of material)

→ objective, reproducible ground truth through correlative EBSD data

Example: lath-like Bainit in multi phase steel

Final data set for training of reliable ground truth:

Effort only: 36 images SEM + 51 images LiMi
How good is the quality of image segmentation by Machine Learning? → pixel-by-pixel segmentation accuracy better than 90%!

Note: Pixel-by-pixel segmentation may be biased by phase fraction (also in case of manual segmentation)

Overall conclusion:
Machine Learning segmentation significantly outperforms segmentation accuracy of qualified experts in every case:

Experts: 75-78% accuracy (less complex) 70-75% (most complex)
ML: 95-98% accuracy (less complex) 90-95% (most complex)

Scientific remark* more conservative accuracy (+ fully unbiased)
is „Intersection over Union“ (IoU):

<table>
<thead>
<tr>
<th>LiMi image set (51 images)</th>
<th>SEM image set (36 images)</th>
</tr>
</thead>
<tbody>
<tr>
<td>IoU background</td>
<td>IoU foreground</td>
</tr>
<tr>
<td>88.9 ± 1.4 %</td>
<td>74.1 ± 1.5 %</td>
</tr>
<tr>
<td>IoU foreground = lath bainite</td>
<td>IoU foreground = lath bainite</td>
</tr>
<tr>
<td>77.7 ± 4.2 %</td>
<td>80.4 ± 3.9 %</td>
</tr>
</tbody>
</table>

What about Copper materials? 
→ can they also have complex, multi phase microstructures?

The cast structure of CuAl10Fe5Ni5 is used for highly stressed components, such as ship propellers.
Another example of profitable use of Machine Learning

→ **morphological classification of inclusions** - without chemical information (EDX)

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Scientific remark*

accuracy = f(precision, recall)

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Do we really find all microstructural elements of this class? = class recall

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Do we really classify all microstructural elements precise? = class precision

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### Table: Classification Results

<table>
<thead>
<tr>
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</thead>
<tbody>
<tr>
<td>true Carbonitride</td>
<td>453</td>
<td>13</td>
<td>22</td>
<td>7</td>
<td>5</td>
<td>90.6%</td>
</tr>
<tr>
<td>true Contamination</td>
<td>0</td>
<td>500</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>100.0%</td>
</tr>
<tr>
<td>true Oxide</td>
<td>14</td>
<td>10</td>
<td>339</td>
<td>2</td>
<td>135</td>
<td>67.8%</td>
</tr>
<tr>
<td>true Sulfide</td>
<td>2</td>
<td>17</td>
<td>12</td>
<td>464</td>
<td>5</td>
<td>92.8%</td>
</tr>
<tr>
<td>true Oxide-Sulfide</td>
<td>7</td>
<td>3</td>
<td>100</td>
<td>2</td>
<td>388</td>
<td>77.6%</td>
</tr>
</tbody>
</table>

class recall:

- Carbonitride: 95.2%
- Contamination: 92.1%
- Oxide: 71.7%
- Sulfide: 97.7%
- Oxide-Sulfide: 72.8%

F1 score:

- Carbonitride: 92.8%
- Contamination: 95.9%
- Oxide: 69.7%
- Sulfide: 95.2%
- Oxide-Sulfide: 75.1%

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*Scientific remark: accuracy = f(precision, recall)*

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**accuracy = 85.8%**
„Take Home Messages“

- Holistic approach: not only look at images and Machine Learning algorithms, but also consider **sample contrasting, image acquisition and ground truth assignment**
  - Advanced Quantitative Metallography plays a significant role!
  - Needed for sustained successful Machine Learning implementations

- Establish references through correlative microscopy
  - Serial application ➔ **Be efficient: apply simplest + fastest characterization method**

- Machine Learning and Deep Learning can automize simple, tedious tasks and enable **complex segmentation and reliable microstructure classification**

- High quality image set: **30-50 micrographs are sufficient to train an accurate ML model**
  - Relevant for new quality control tasks ➔ reliable + fast ➔ basis for automation