INCREASING THE PRODUCTIVITY OF THE CZOCHRALSKI PROCESS APPLYING MACHINE LEARNING

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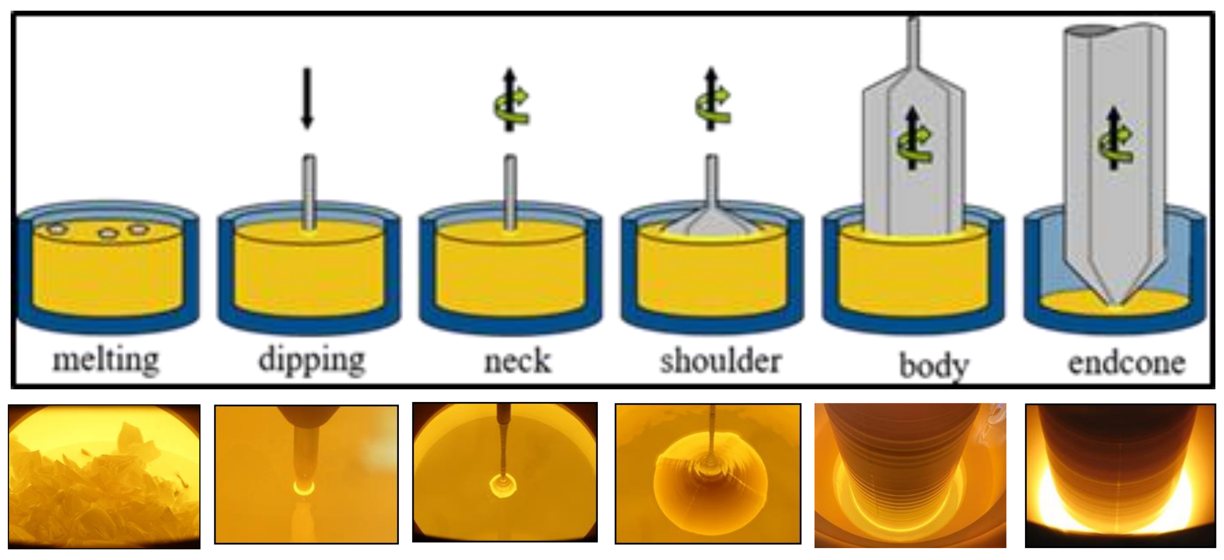
Introduction

Monocrystalline silicon for the production of solar cells has to be provided cost-effectively in large quantities. The Czochralski (Cz) technique is currently the only manufacturing method that can ensure the availability of high-quality material in sufficient quantities. Even if the crystal growth technology is highly developed, the loss of the monocrystalline structure of the growing crystal remains still a yield limiting problem. If a structure loss has occurred during crystal growth, the following options are available: The growth process can be continued, the crystal can be removed or the crystal can be melted back and a new crystallization process can be restarted. Even though productivity in the Cz process for solar silicon has reached a very high technological level, two challenges still remain. These two topics are the subject of our ongoing project work:

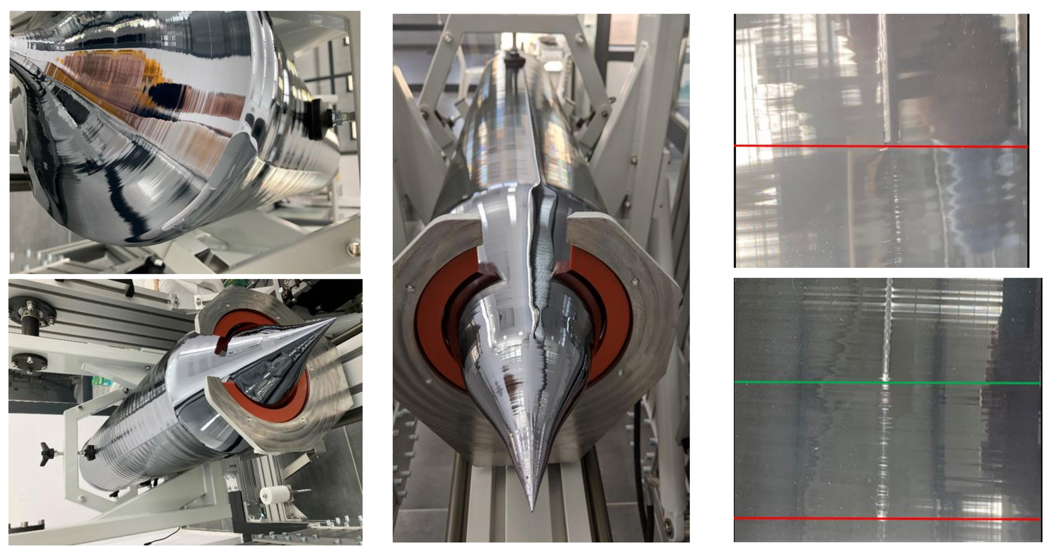
- Timely and automatable detection of a structural loss or an other anomaly in crystal growth
- Further analysis of the root causes that can trigger a structure loss.

Crystal Growth

Crystal Growing Process Sequence

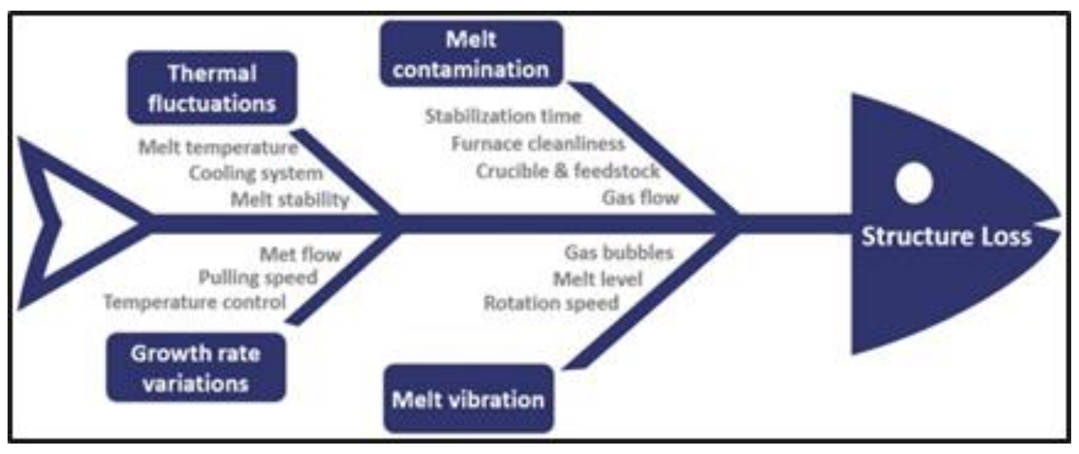


Appearance of Growth Lines



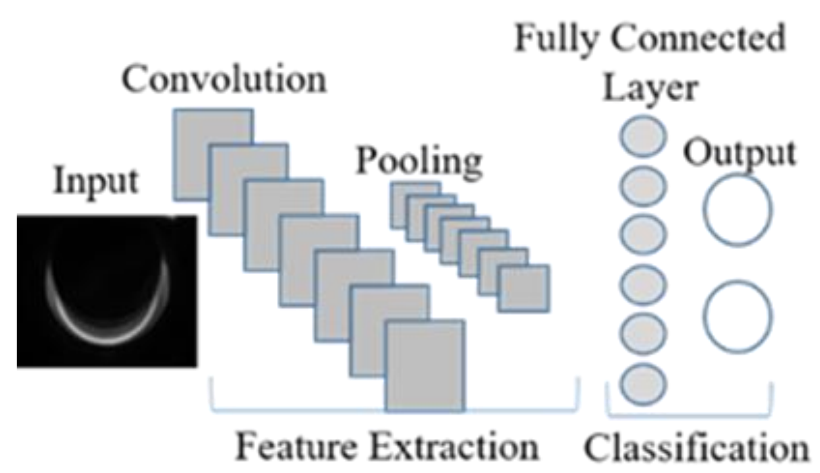
In the case of <100> crystal orientation, a monocrystal exhibits four growth lines. As long as the growing crystal shows continuous growth lines, it has a monocrystalline structure. The disappearance of these growth lines during the growth process is an indication of a loss of monocrystalline structure.

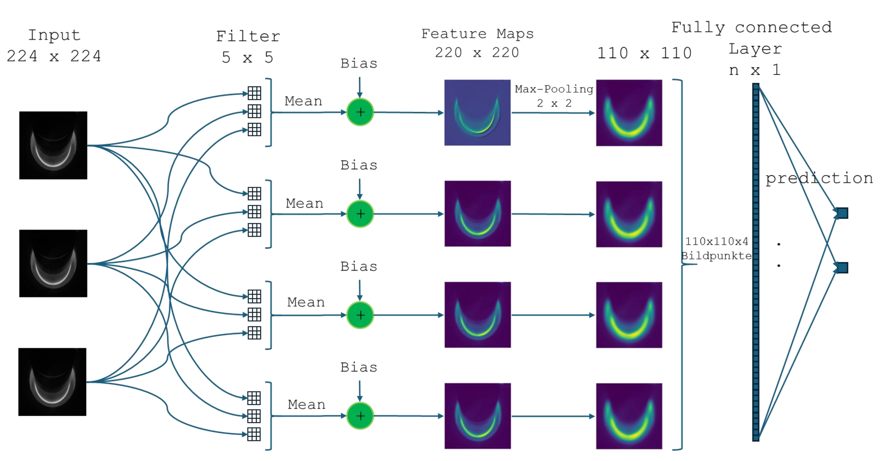
Loss of Monocrystalline Structure

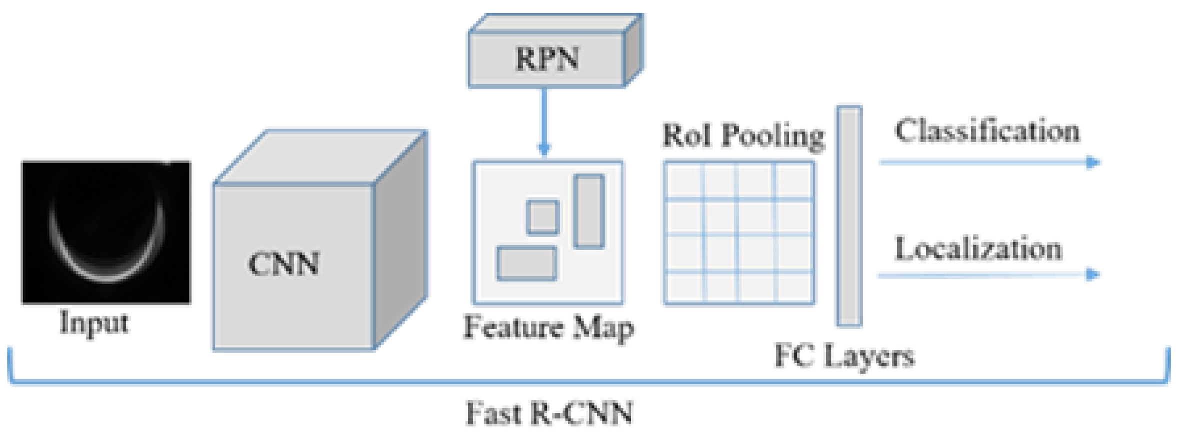


The distribution and level of the thermal stresses in the growing crystal, process parameters, the quality of the starting materials and consumables as well as process conditions that are difficult to quantify have to be taken into account. Hendawi's diagram provides an overview of some of the possible triggers for the occurrence of a structure loss [1].

Methodological Approach to Structure Loss Detection Applying Deep Neural Networks

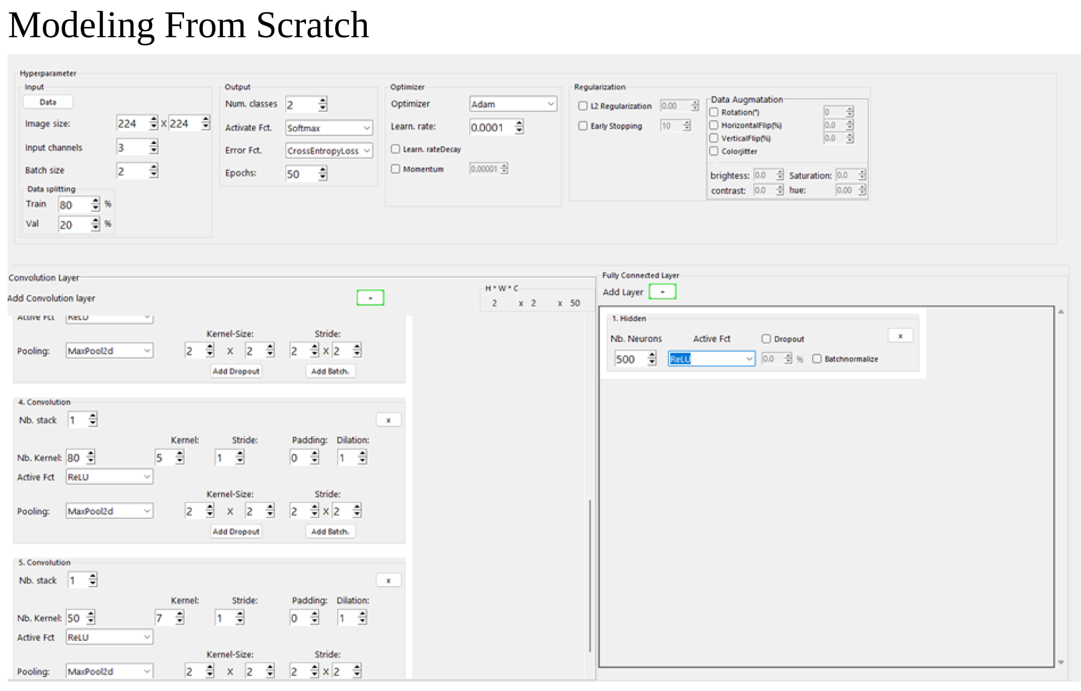




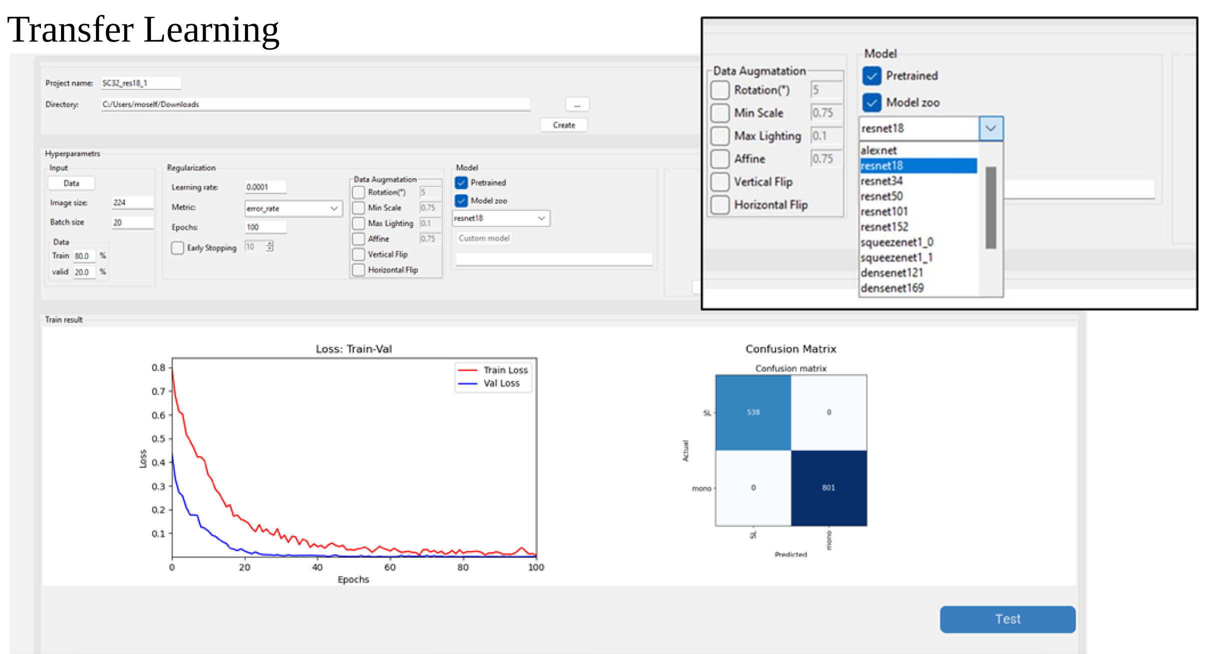


Software for Implementing Convolutional Neural Networks for Image Classification [2]

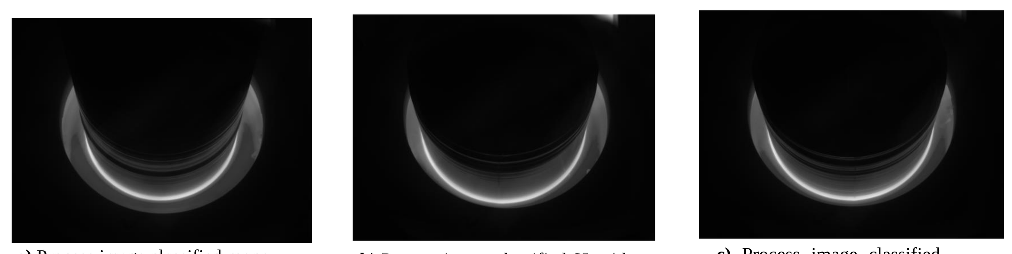
Modeling From Scratch



Transfer Learning



An Accurately Labeled Dataset of Process Images is Essential for Training CNN Models

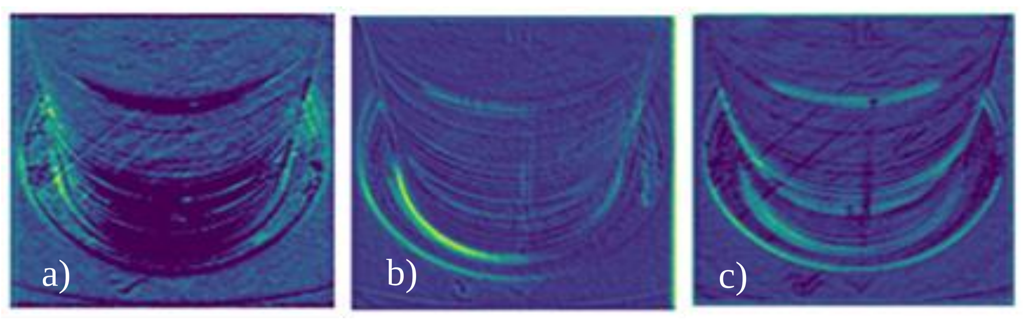


a) Process image classified mono with growth line visible in the meniscus region

b) Process image classified SL with growth line outside the meniscus region

c) Process image classified SL with absence of growth line

Corresponding Feature Maps of ResNet 18



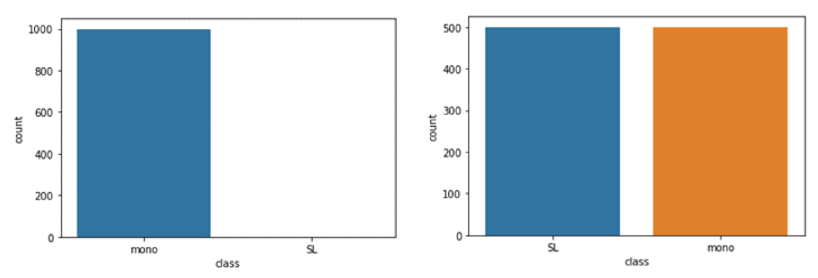
Evaluation of training performance

True label \ Predicted label		
	T_{mono}	F_{SL}
	F_{mono}	T_{SL}

$$accuracy = \frac{T_{mono}+T_{SL}}{T_{mono}+T_{SL}+F_{mono}+F_{SL}}$$

$$precision = \frac{T_{mono}}{T_{mono}+F_{mono}}$$

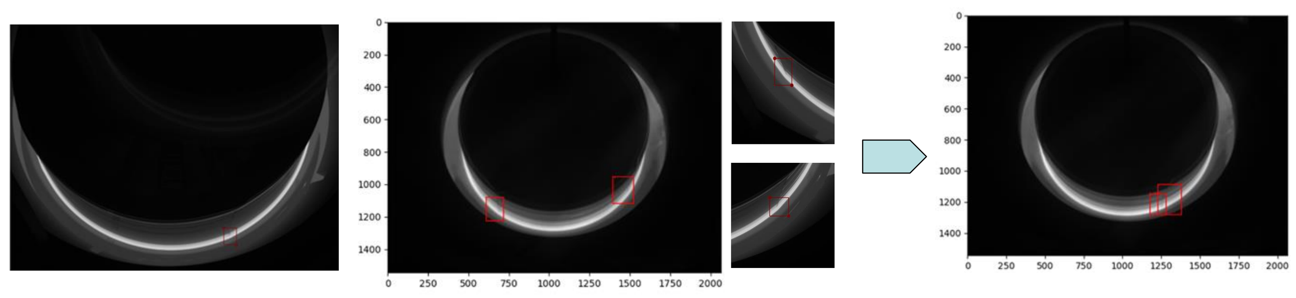
Inference of 1000 test images: 500 “mono”, 500 “sl”



classified according b + c

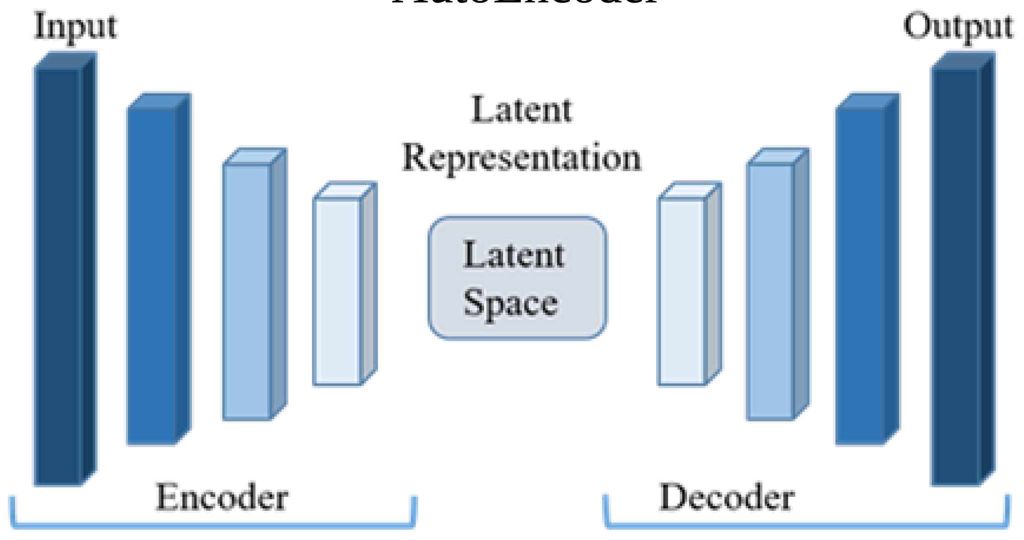
classified according a + c

First results are promising



Methodological Approach to Structure Loss Analysis Applying Deep Neural Networks

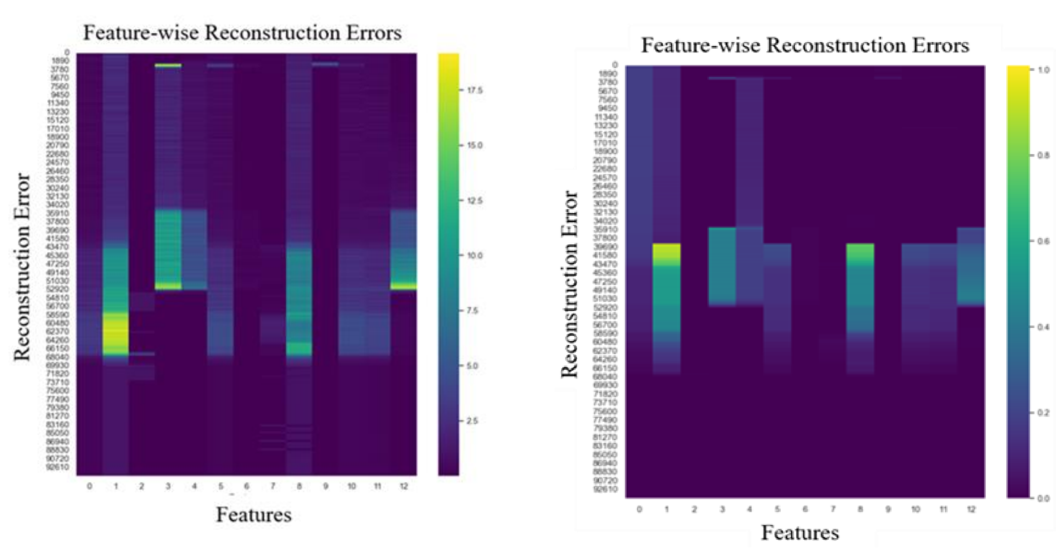
AutoEncoder



An unsupervised learning method like AutoEncoder is applied in order to find correlations to process parameters. AutoEncoders are trained exclusively with process data representing perfect process conditions.

The input data are compressed into the latent space in the neural network of the AutoEncoder. All information from the undisturbed process are available in reduced form in the latent space. Decoding the latent space trains the network to reconstruct the input data as best as possible. The aim of this procedure is to learn undisturbed process data. During inference, i.e. applying the trained model to undisturbed process data, the AutoEncoder will reconstruct the undisturbed process data as best as possible. If the process data are disturbed or show anomalies, the reconstruction will reveal anomalies.

Heat map of the reconstruction error (time scale) versus 12 process parameters (out of 150)



Objective of Ongoing Project

The ongoing project is split into two areas:

- Automated image recognition based on a Deep Neural Network to detect the loss of monocrystalline structure in an early stage of the growing crystal
- Analysis of the recorded process data based on a Deep Neural Network to find correlations to irregular crystal growth

References:

[1] R. Hendawi, Marisa Di Sabatino, Journal of Crystal Growth **629** (2024), 127564

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