IOCM 2025 Conference
The 4th International Online Conference on Materials
3–6 November 2025 | Online
MDPI

Machine Learning-Driven Insight into Crystallization Kinetics in Liquid Crystals

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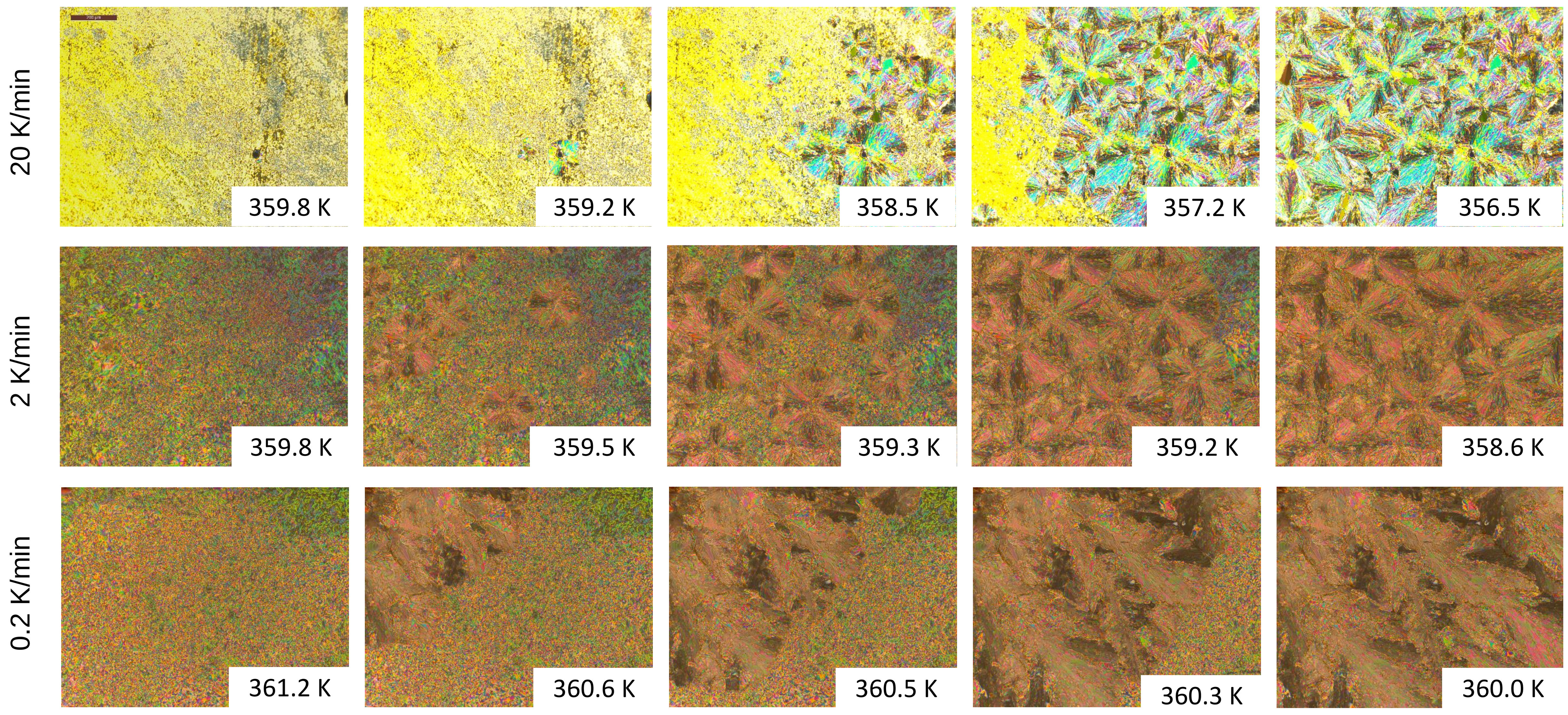
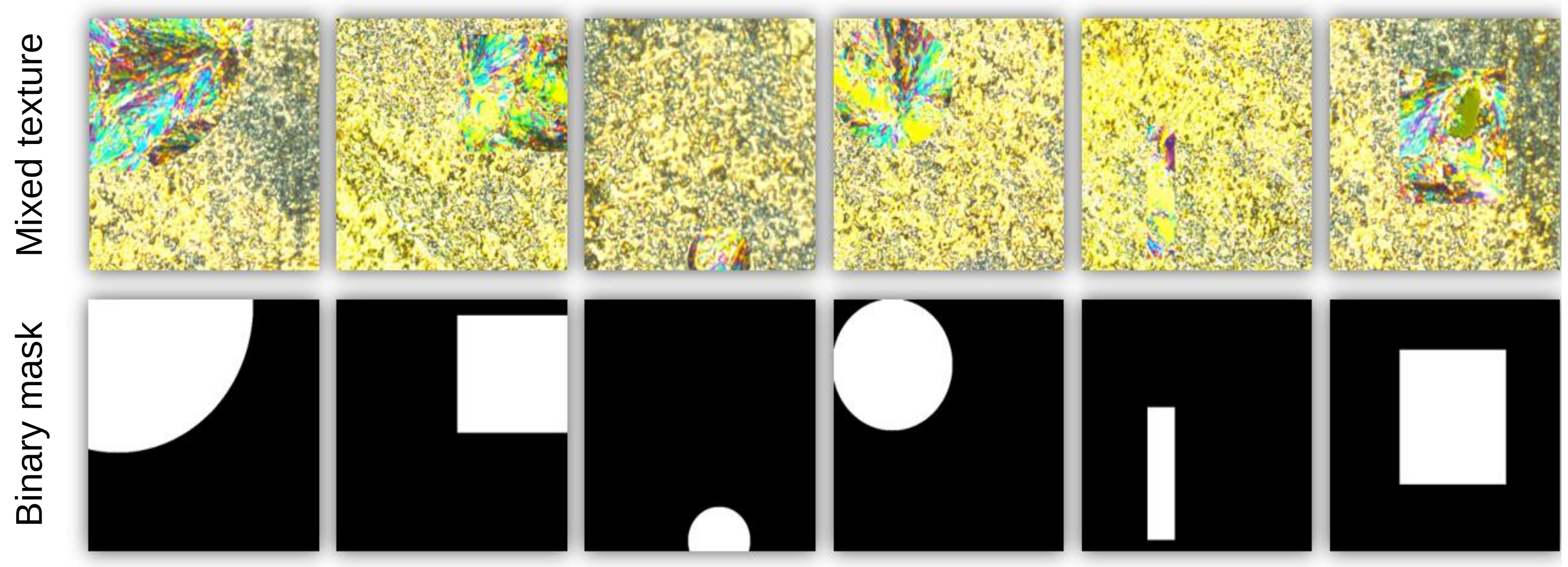
INTRODUCTION & AIM

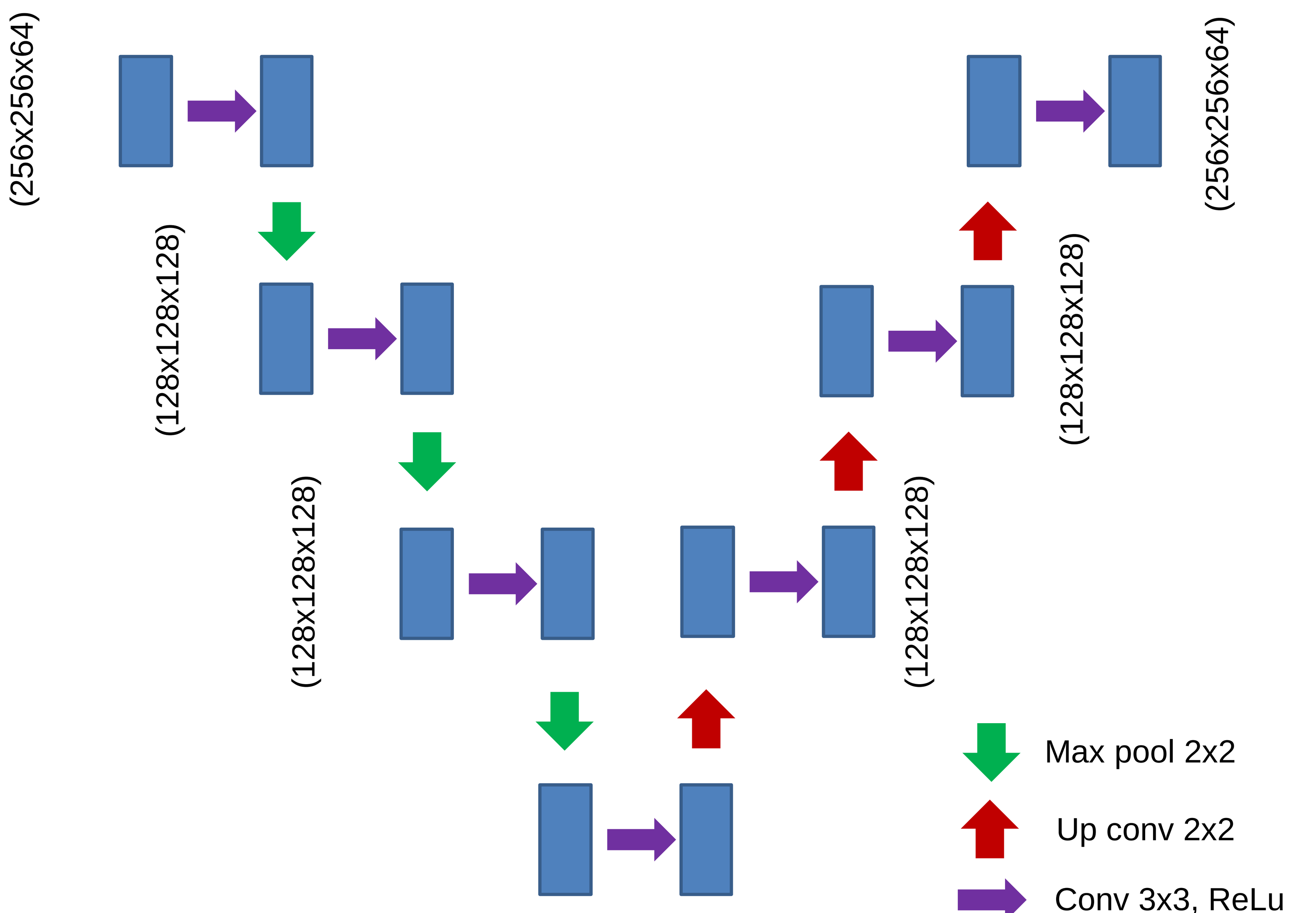


$$D(T) = \frac{S_{Cr}(T)}{S}$$

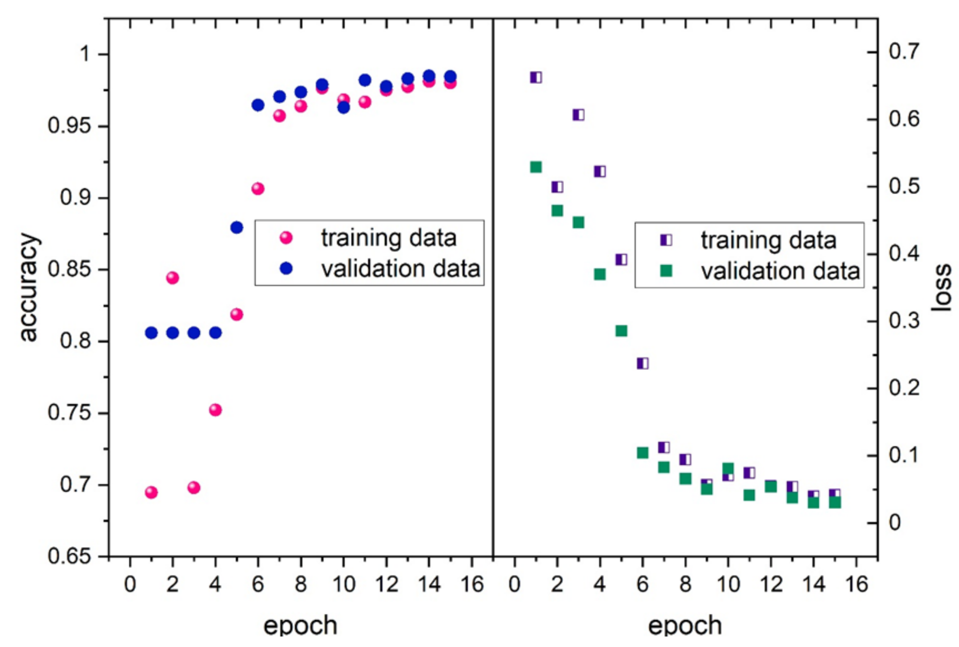
The main objective of this work is to develop and demonstrate an automated method for determining the degree of crystallization based on polarized optical microscopy images. To achieve this, an image segmentation approach using the U-Net convolutional neural network architecture is proposed for the automatic identification of crystalline and non-crystalline regions in polarizing microscopy textures. The method is applied to a model liquid crystal compound, 4-nonyloxybenzylidene-4′-propylaniline (9BA4), which exhibits nematic, smectic C, and crystalline phases upon cooling. By employing automated image analysis, the degree of crystallization D(T) is accurately determined as a function of temperature, significantly reducing the need for manual and time-consuming texture classification. Furthermore, the U-Net segmentation is used to identify phase transition regions and track the crystallization process with high spatial precision. Finally, the effectiveness of the proposed approach is evaluated by comparing the automated segmentation results with conventional manual analysis.

METHOD

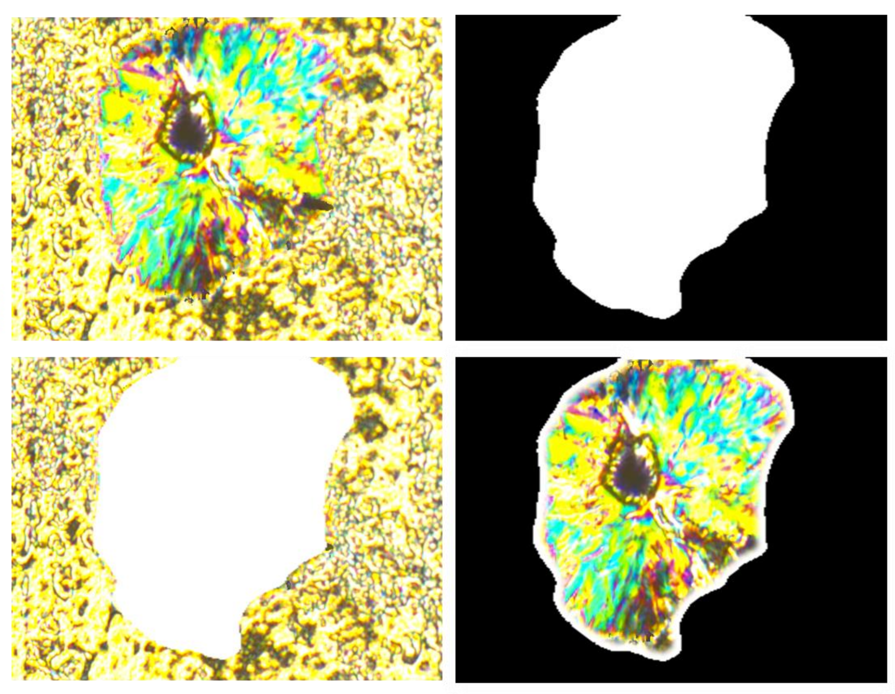


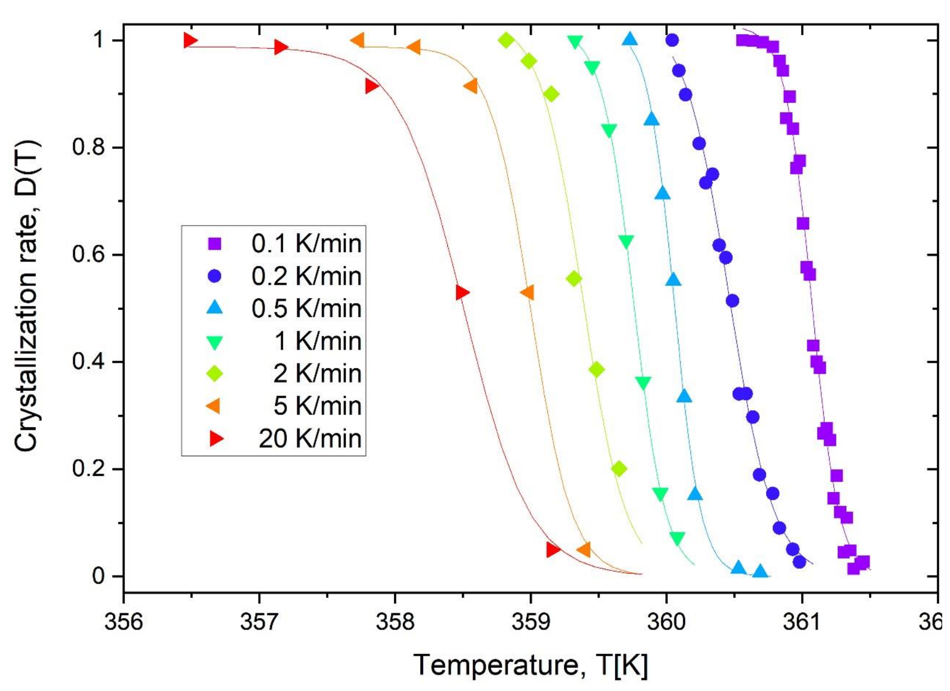


RESULTS & DISCUSSION

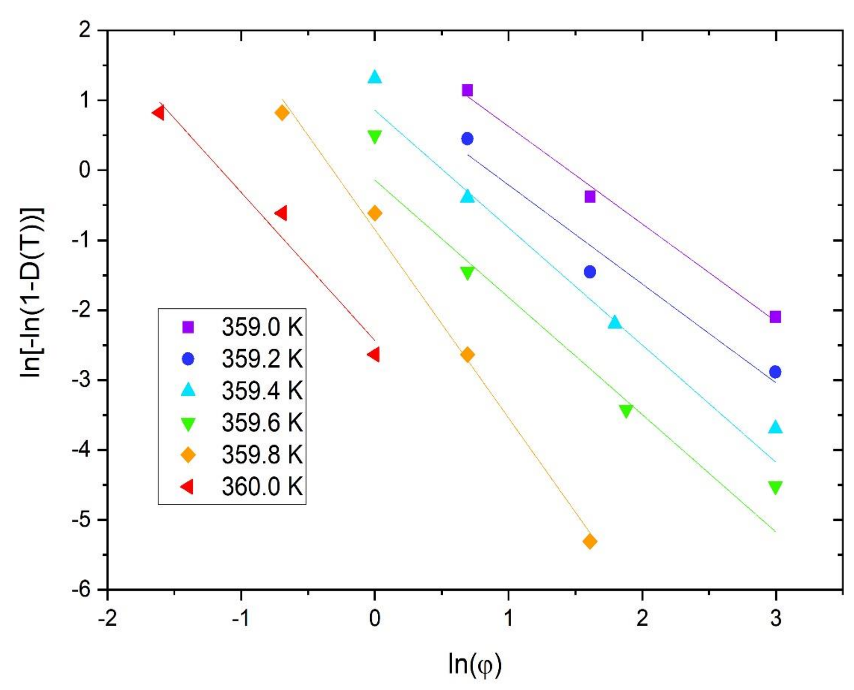


Accuracy and loss score of U-Net neural network for training and validation data. Model reach the accuracy





$$1 - D(T) = e^{\frac{-K(T)}{\varphi^m}}$$



Ozawa Model

CONCLUSION

The U-Net neural network effectively segments microscopy images and accurately identifies irregular crystalline phase boundaries, demonstrating strong generalization capabilities. Its use enables automated and rapid phase identification in polarized light microscopy images, eliminating the need for manual annotation. By binarizing the network's probability maps, the degree of crystallization was quantitatively determined based on the fraction of pixels assigned to the crystalline phase. The method was applied at different cooling rates, allowing the fitting of the Ozawa model, which revealed increasing mmm values with temperature, indicating a shift toward more synchronized two-dimensional growth. This approach can be easily extended to other liquid crystalline compounds or material classes.

REFERENCES / ACKNOWLEDGEMENT

The research results were funded by the Miniatura 8 project 2024/08/X/ST3/00769.

N. Osiecka-Drewniak, Z. Galewski, M. Piwowarczyk, E. Juszyńska-Gałązka „Deep Learning Analysis of Crystallization Using Polarized Light Microscopy and U-Net Segmentami" *J. Phys. Chem. B* **428** (2025) 127511.