Computer Vision Applied to Polymer Particles in Liquid Crystal (LC) to Enable On-the-Fly Characterization of their Morphology and Size Distribution, Among Other Properties

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MATERIALS

Abstract:

Monitoring polymerization reactions in-situ provides many advantages like real-time feedback for tuning conditions and viewing undisturbed growth. However, image quality can be reduced due to difficulties in viewing the reaction such as vibrations and long working distances with a microscope. This project explores approaches to enhance lower quality in-situ microscope images of polymers in liquid crystal from an initiated chemical vapor deposition (iCVD) reactor by using an enhanced super resolution generative adversarial network (ESRGAN). To train ESRGAN, polymer test systems were set up in an iCVD reactor, and low-quality in-situ images of the polymers were taken along with corresponding high-quality ex-situ images. We cropped matching single-cluster images and applied different pre-processing techniques while varying hyperparameters such as learning rate and weight decay. The accuracy of these methods was evaluated with the Structural Similarity Index Measure (SSIM) and visually compared to the reference high-quality images. We found that overall, ESRGAN has strong potential for polymer image enhancement, and changeable hyperparameters gives it versatility for different images. However, further model optimization is needed before it is adapted for real polymerization images. The adaptability of ESRGAN makes this approach applicable for more varied use like new types of polymers or different microscope setups.

Summary of Research:

Initiated chemical vapor deposition (iCVD) in liquid crystal (LC) has the capability to produce tunable polymer growths like nanospheres with potential for use in drug delivery or separations for chromatography1. In-situ monitoring of the reaction is possible through a window with a long-distance focal length lens Keyence VHX 970F microscope. However, issues with vibrations and external noise are compounded by the viewing distance, so the images from the microscope are blurry and low-quality. The samples can be high-quality ex-situ imaged by an Olympus BX41 microscope although this requires stopping the reaction to remove samples, which can also disturb polymers.

With the assistance of a machine learning-based approach, we can enhance the in-situ images to more closely match the quality of the high-quality ex-situ images. Previous preliminary research has found that the enhanced super-resolution generative adversarial networks (ESRGAN) model outperforms other models for this purpose.

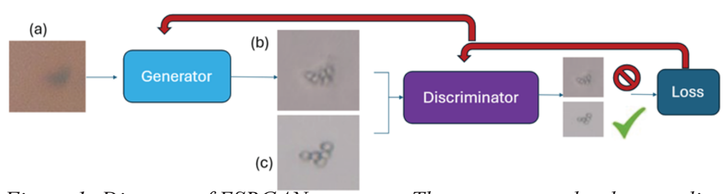

Figure 1: Diagram of ESRGAN structure. The generator takes low-quality images (a) and enhances them (b). The discriminator detects real (c) from fake images and then model updates from loss functions.

ESRGAN has two key components: the generator and the discriminator (Figure 1). For training, the generator takes a low-quality image and tries to enhance it to look like a high-quality image. The discriminator is then given that enhanced image along with the actual high-quality image and tries to determine which is the real one. Then the model calculates loss functions for how poorly the generator and discriminator performed so that the generator and discriminator can improve their weights. This process is iterative, with the generator and discriminator improving each other thousands of steps. In addition to the images used for training, many are set aside solely for testing the performance of the model to limit overfitting.

We tried multiple configurations of ESRGAN by varying hyperparameters, which are parameters in ESRGAN that can be adjusted to change how the model learns. We mainly looked at learning rate (.0001-.001), weight decay (0 or .0001), and number of epochs(10-300).

A test system was created using commercially available 5µ polystyrene spheres dispersed in the liquid crystal, allowing for fixed particle sizes and faster data collection compared to growing polymers.

Training the model with images of the entire LC grid causes complications with identifying the same polymer across low and high-quality images, therefore we used 64x64 pixel cropped patches, 32x32 pixel downscaled cropped patches, and 64x64 images where the contour of the particle was cropped and the background was replaced with white (Figure 2).

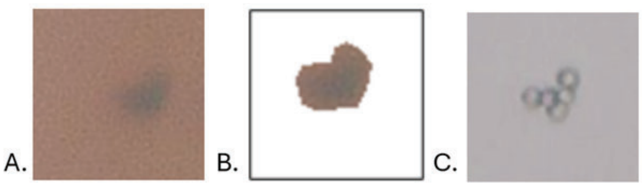

Figure 2: A. Low quality cropped polymer cluster, with B. its contour cropped and C. their high-quality reference. These images were used as three different training inputs for ESRGAN.

Conclusions and Future Steps:

As an exploratory project, a main goal of this project was to explore the feasibility of different approaches. Weight decay stabilized training of the 64x64 images and produced best overall results. Conversely, with 32x32 images, removing weight decay allowed the model to make riskier, but successful, improvements. While contour cropping the particles was not effective, ESRGAN was generally robust against noise. The main limitation was particle size estimation accuracy (Figure 3), likely due to inconsistent scaling during preprocessing. Remaking the dataset may resolve this issue. Overall, these findings establish a strong foundation for adapting ESRGAN for polymerization imaging.

For future development, ESRGAN should be adapted to work on real polymerization images, and polymers of different sizes. Training on lower magnification images would be more effective at capturing more polymers in the frame, fitting six full grids into the frame instead of one. Implementing the model with video capabilities would aid in faster and more convenient analysis during reactions. Applying a different de-noising program to the low and high quality images could also potentially increase the ground truth image quality and accelerate training.

References:

[1] Apoorva Jain et al., Single-step synthesis of shaped polymeric particles using initiated chemical vapor deposition in liquid crystals. Sci. Adv. 10,eadp5573(2024).DOI:10.1126/sciadv.adp5573