NDnano
Notre Dame Nanoscience and Technology

NDnano Summer Undergraduate Research
2024 Project Summary

1. Student name & home university:

Anna Skoropad; University of Notre Dame

2. ND faculty name & department:

Prof. Gabriel R. Burks, Department of Chemical & Biomolecular Engineering
Prof. Yamil Colon, Department of Chemical & Biomolecular Engineering

3. Summer project title:

Polymer Crystallization for Automated Materials

4. Briefly describe new skills you acquired during your summer research:

This summer I learned how to: 1) grow polymer single crystals using self-seeding crystallization and isothermal filtration; 2) prep samples for thermal analysis using differential scanning calorimetry (DSC) and thermogravimetric analysis (TGA); 3) analyze polymer samples with various microscopy techniques, like Scanning Electron Microscopy (SEM), Atomic Force Microscopy (AFM), and Transmission Electron Microscopy (TEM); and 4) how to write code for a Convolutional Neural Network (CNN). This was the first step in a process to develop correlations between my sample images and their respective processing conditions. In addition to newly acquired research skills, I also learned how to collaborate with my teammates and to present my work to others.

5. Briefly share a practical application/end use of your research:

With Machine Learning, my group will be able to characterize polymer materials based on their properties and processing conditions. This will allow us to design plastics to minimize their negative impact on pollution, global warming, and marine life. The analysis of the polymer structure with CNN will be much faster, which means that we will be able to find the right procedure to produce plastic that is stronger, cheaper, and also more environmentally sustainable.

6. 50- to 75-word abstract of your project:

With machine learning, there has appeared a new opportunity to study plastic. The team grew single crystals of polyethylene dissolved in xylene, with a self-seeding method. Having captured the images of the crystals, a Convolutional Neural Network will help characterize the material.

The network will correlate the procedure of manufacturing with the desired material. Further particle trapping using microfluidics will be used to analyze the crystals and feed the network with more data.

7. References for papers, posters, or presentations of your research:

[1] Blundell et al., 2006, "Nature of Self-Seeding Polyethylene Crystal Nuclei", Journal of Macromolecular Science, Part B: Physics, 2:2, 301-336, DOI: 10.1080/00222346808212454

[2] A. Shenoy et al., 2016, "Stokes Trap for Multiplexed Particle Manipulation and Assembly using Fluidics", PNAS,,113(15)39

[3] A. Keller, 1959, "The Morphology of Crystalline Polymers", From the H.H. Wills Physics Laboratory, University of Bristol, England.

[4] D. J. Blundell et al., 1996, "A New Self-Nucleation Phenomenon and Its Application to the Growing of Polymer Crystals from Solution", Polymer Letters, Vol. 4, PP. 481-486

[5] M. Tanyeri et al., 2010, "Hydrodynamic trap for single particles and cells", Applied Physics Letters 96, 224101

Plastic plays an important role in our lives, but more than half of the produced plastic ends up in a landfill or ocean. Biodegradable plastic seems to be a better option, but it is more expensive and lacks qualities, like strength or durability. It became much easier to study polymer materials with the rise of Machine Learning, and this project aims to classify plastic with Convolutional Neural Network in order to optimize the material properties that better suit our demands.

In the lab, we grew single crystals of polymer-xylene solutions using a self-seeding method. The samples were heated up and cooled down to the desired temperatures with oil baths, like silicon oil bath, which was helpful in reaching high dissolution temperatures. The samples were filtered, to eliminate any excess free polymer. To grow the most optimal crystal, different parameters were changed, like concentration, dissolution temperature or dissolution time. Usually, 0.01% concentrations of Polyethylene in p-Xylene were used. Afterwards, they were analyzed with an Optical Microscope that had Phase Shifts and Polarizer attached to it. This made it possible to see any birefringent surfaces that are transparent under regular lenses. SEM helped get a better resolution and analyze the sample population in a better detail. Those images were then studied to see the size distribution.

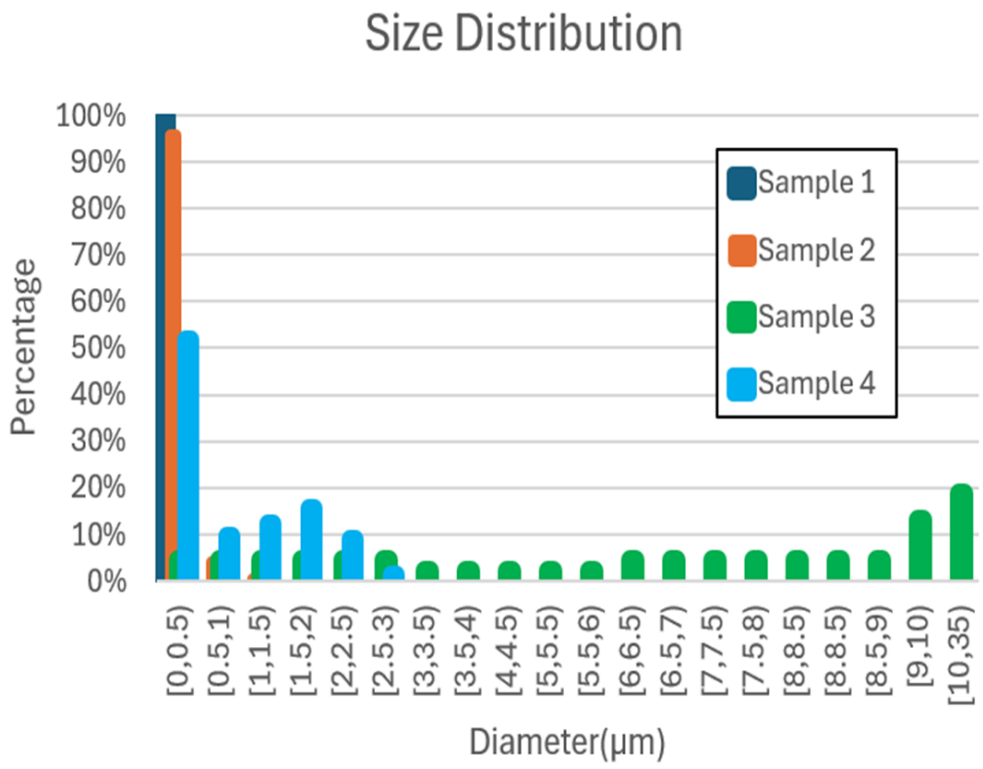


Figure 1. A graph showing the size distribution of 4 different samples. Sample 1 was self-seeded at 98℃ for 5 minutes. Sample 2 was self-seeded at 100℃ for 5 minutes. Sample 3 and Sample 4 were dissolved at 96℃ for 20 and 30 minutes respectively.

AFM helped to study the height of the lamellar sheets and confirm the uniformity of it throughout the samples. TEM was used to identify the nature of the crystalline body in the samples and confirm the dimensions of the crystal with literature values. This helped to determine whether the crystals seen under the microscope aren't noise or some other material.

In collaboration with Prof. Colon's lab, we got trained on Machine Learning code. Some of the images of the samples were fed to the Convolutional Neural Network, where the most important features were extracted. In order to increase the training dataset size, HyperSpy will be used to rotate the particles on the images. 80% of the data will be used to train the model and optimize different layers to decrease the error, and 20% of the data will be used to test the network. The Machine will correlate the images of the morphology of the samples, and properties of the material in the future, with the processing procedure.

Future research will be done to trap the polymer single crystals under a microscope using microfluidics. Stokes Trap will be used to feed the particle with different conditions, which will change the particle and open new opportunities to learn its responses to various circumstances. This will also be included in the training dataset. Finally, more work will be done to make a sample with more uniform and larger crystals. This will ensure that the images taken in the Stokes Trap will have a good enough quality.