MATDAT18: Materials and Data Science Hackathon

Team Composition (2 people max.)

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Project Title

Unsupervised Classification of Domains in Nanostructured Thin-films

Project Synopsis (approx. 100 words)

This project will create a tool to identify and group different nanometer-scale domains in thin-films that are comprised of one or more optoelectronic materials. Machine learning algorithms, such as knn classification, can take in Atomic Force Microscopy (AFM) scans of material properties (e.g. stiffness, conductivity, etc.) and identify different phases in the thin-film by evaluating differences in one or more of these material properties. The tool will determine the likely number of different phases within the thin-film along with the properties of each phase. This data can be used for quantitative morphological studies, as well as quantitative structure-property relationships, all with spatial resolution that is limited only by the tip radius of the AFM probe.

Identified Data-Science Collaborative Need (approx. 100 words)

Atomic Force Microscopy (AFM) is a simple and informative technique that is used in many different fields and is growing in use, especially in the field of thin-film electronics. Currently, information and analyses on thin-film morphologies portrayed in AFM micrographs is largely qualitative. By using data-science techniques, the spatially resolved composition of these micrographs can be determined and further correlated to material properties through quantitative structure-property relationships. To this end, there is a need to develop an easily interfaced tool that takes in micrograph(s), uses unsupervised Data-Science techniques to classify the phase composition of those micrographs, and outputs an easily interpretable file for further detailed analyses.

Data Origin and Access (*data must be available and sharable with data science teams* – please address: data source/origin, access privileges, sharing privileges)

Data will be stored in a sharable Google Drive folder owned by the Luscombe Lab, where data can be remotely accessed and modified by all team members. Saved in that folder will be micrographs of mechanical and electrical properties of thin-films (50-300 nm thick) as well as the material composition and deposition procedures that produced the features of each micrograph. The bulk of the micrographs will be mechanical property scans of semiconducting polymer thin-films, particularly poly(3-hexylthiophene). Some micrographs will be conductive AFM scans. To ensure generalizability of the algorithm, there will also be scans of other electrically conductive polymers and 2 component blends of organic semiconductors.

Project Description (approx. 1.5 pages, plus figures and references; please describe data size, form, dimensionality, uncertainties, number of examples, etc.)

Flexible electronic devices are enabled by the unique mechanical properties of thin-film semiconductors such as π-conjugated polymers, perovskites, and other solution-processable materials.[1-4] In order to better understand and scale-up these materials and devices made from them, it is important to understand the nanometer-scale crystallinity, composition, and other crucial material properties as well as what influences their development. Current techniques with the required resolution to distinguish between different phases in these nano-structured films, such as cryo-TEM[5] and neutron scattering[6], are costly and slow. Additionally, the information obtained by these means are not spatially resolved to large enough areas to be practical for any large scale devices. Atomic Force Microscopy (AFM) offers techniques to quickly and relatively cheaply characterize thin-films. A ten minute scan can map out five different mechanical properties with resolution around 5-10 nm, the radius of the tip of the AFM probe. A different 10 minute

Fig. 1: Image from http://futuristicnews.com

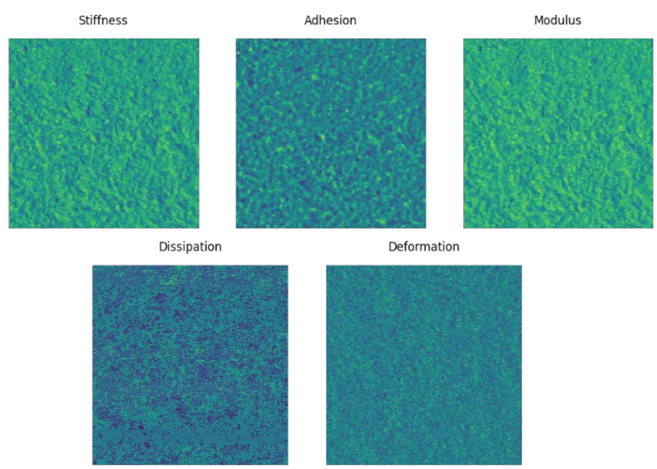

Fig 2: The five mechanical property scans of a P3HT thin-film. Grains of crystalline and amorphous P3HT are clearly visible. Each scan is 500 nm x 500 nm.

scan with a conductive AFM (c-AFM) can similarly map out the conductivity. In prior work, a threshold-based classification was developed to distinguish between amorphous and crystalline poly(3-hexylthiophene) (P3HT). This classifier chooses one class for each pixel based on its

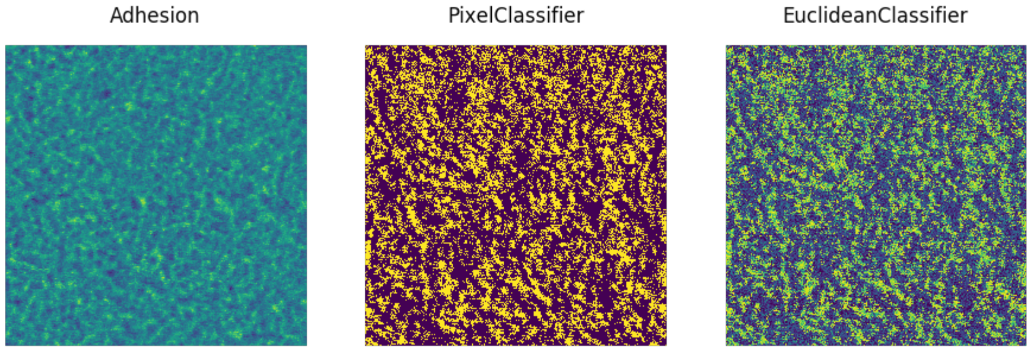

Fig. 3: The results of two different classifiers based on using user in-put thresholds. On the far left, a representative scan of adhesive properties for each pixel is included for reference. Each scan is 500 x 500 nm.

properties and those of the 8 pixels sorrounding it. The threshold is easily changed and based on a brief literature search on the mechanical properties of amorphous and crystalline P3HT. An unsupervised classification method, rather than user inputted thresholds, would allow this tool and the analyses based on it to be far more generalizable. The interconnection between mechanical and optoelectronic properties is prevalent in both organic and inorganic materials and their hybrids. This means that the more generalizable and robust the tool is, the more useful it will be.

Data for this project will be provided by the Luscombe lab and will contain a few different categories of micrographs. All data will be saved as .txt files and will primarily comprise of background subtracted and processed micrographs (raw data available). The .txt files will describe a 3D matrix of the stacked property scans, so each pixel is a vector of its properties. Each of these .txt files will pertain to a scan from a thin-film with specific processing conditions. In the main category of data (approximately 400 files) , the processing conditions of each P3HT thin-film are varied, particularly annealing duration and temperature. These scans will be associated with a hole mobility measurement as found through Organic Field-Effect Transistor (OFET) measurements. In addition to the mechanical property scans of the P3HT thin-films, there will also be a number of mechanical property scans of different blends or materials, such as P3HT:PCBM or PEDOT:PSS (approximately 30 files). Finally, there will also be c-AFM scans of a few representative samples from each of the previously mentioned materials (approximately 30 files).

This project is part of an existing effort to create scalable and generalizable tools to analyze thin-film electronic materials in a quantitative and meaningful way. It is the hope of our team to use this “hackathon” as a means to establish connections and collaborations with rigorous data scientists so that we may improve the tools we are developing and accelerate their development. The end-goal is to create open-source tools for the materials science community, hopefully integrating our efforts with current efforts, such as Pycroscopy[7], to the benefit of all.

References:

1. Dimitrakopoulos, C.D.; Malenfant, P.R.L. Organic Thin Film Transistors for Large Area Electronics. *Adv. Mater.,* **2002**, 14, 99-117.

2. Choi, Ji-Hyuk *et al.* Bandlike Transport in Strongly Coupled and Doped Quantum Dot Solids: A Route to High-Performance Thin-Film Electronics. *Nano Lett.*, **2012**, 12, 5, 2631-2638.
3. Nomura, Kenji *et al.* Room-temperature fabrication of transparentflexible thin-film transistors using amorphous oxide semiconductors. *Nature*, **2004**, 432, 488-492.
4. Brivio, Federico; Walker, Alison B.; Walsh, Aron. Structural and electronic properties of hybrid perovskites for high-efficiency thin-film photovoltaics from first-principles. *APL Mat.*, **2013**, 1, 042111.
5. Wirix, Maarten J.M., *et al.* Three-Dimensional Structure of P3HT Assemblies in Organic Solvents Revealed by Cryo-TEM. *Nano Lett.*, **2014**, 14, 4, 2033-2038.
6. Yin, Wen; Dadmun, Mark. A New Model for the Morphology of P3HT/PCBM Organic Photovoltaics from Small-Angle Neutron Scattering: Rivers and Streams. *ACS Nano*, **2011**, 5, 6, 4756-4768.
7. Github.com/pycroscopy/pycroscopy.