Integration of experimental images with materials models

Supervisor: Eugenie Hunsicker (E.Hunsicker@lboro.ac.uk) and Andrew Archer

Nature of work: This project involves modelling and programming to develop new methods for inverse problems in materials science, linking numerical models with experimental image data through Bayesian methods in data science.

Area: Machine Learning, Data Science, Statistics, Applied Mathematics, Materials Science

Potential implications: Over the past thirty years, mathematical modelling of materials has produced tremendous insights into the self-organisation of matter at the nano scale into complex structures. This can occur through a variety of mechanisms, including evaporation of a solution to leave behind a pattern of nanoparticles on a surface, called *evaporative deposition,* which is known experimentally to produce structures of importance in industrial applications such as thin film transistors and resonators. As yet, however, there is only a general qualitative understanding of how these models relate to experiments and how structures depend on the conditions under which they are produced. Bridging the current gap between model and experiment will require a rigorous quantitative method for fitting the models to experimental data. **The primary goal of this PhD is the first general method for assimilating experimental structure data into computational materials models**.

Brief description: Short summary (~150 words), add a picture/image to attract students.

Examples of patterns that have been experimentally created through evaporative deposition are shown in the first column of Figure 1. If we could harness these natural mechanisms, we could create new structured materials and nano-devices in a cost, time, and energy-efficient manner. Current research has produced numerical models of these processes, using Monte Carlo (MC) methods [1] as well as Dynamic Density Functional Theory (DDFT)[2], (see Figure 1ii,iii), which explain how the underlying physics generates the variety of structures observed.

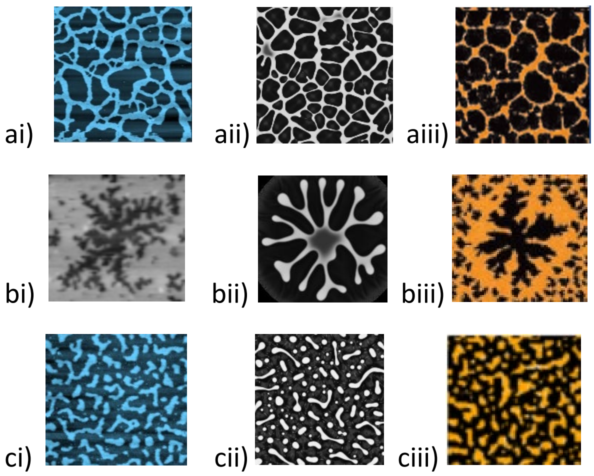

***Figure 1**: Cellular (a), branching (b) and worm-like (c) structures produced by experiment (ai-ci), DDFT model (aii-cii) and MC model (aiii-ciii).*

In this project, the student will develop a workflow using particle statistics and machine learning to derive a quantitative description of structures, and a rigorous method for comparing them. This will permit the statistical fitting of computational models to experimental data and the quantitative prediction and control of structures produced under a variety of conditions. The student will implement this in the context of evaporative deposition, and will use it to answer the three important questions: *How variable are the structures created under the same or similar experimental conditions? How tightly do conditions need to be controlled in order to repeatably produce structures that are similar enough to be interchangeable for industrial uses? How can we determine the correct laboratory conditions to produce specific structures?*