Using machine learning to analyse X-ray data and understand thin film growth

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Artificial intelligence / machine learning is playing an increasing role in the discovery of new materials and analysis of experiments. In a first example we show that machine learning can speed up X-ray experiments through smarter analysis. Multiple XRR curves from a real-time thin film deposition experiment (see Figure) can be co-refined with a convolutional neural network (CNN). The CNN takes 80 XRR curves as input and predicts parameters of a time-dependent growth model as output. The flexibility of a CNN means that a time-dependent model with only few parameters and including prior knowledge can be directly fitted to the data, instead of having to predict 240 thicknesses, SLDs, and roughnesses for each of the 80 scans individually. The co-refinement of multiple curves also means that there is redundancy in the dataset. Indeed the CNN can still predict accurate parameters when the number of measured data-points are reduced by an order of magnitude enabling faster experiments with sparse sampling in the future.

In a second example we show how machine learning enables novel analysis strategies of microscopy images that have not existed before. We use kinetic Monte-Carlo simulations to obtain images of nucleation and sub-monolayer thin film growth. Traditionally features such as the island density would have been extracted from images at various temperatures and fundamental growth parameters such as the binding energy or the diffusion barrier would have been estimated using an Arrhenius law. Here we use a CNN to extract this information from a single image at a single temperature. This theoretical study shows that CNNs can extract more information from images than current analysis methods. CNNs therefore will be useful for fundamental studies of growth kinetics and growth optimization through better knowledge of microscopic parameters.