**SPM–(S)TEM correlative studies for nanoscale characterisation and data curation for implied transfer learning.**

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## Abstract

The use of machine learning has driven major advances in scientific progress, enabled by large, standardised, and well-labelled datasets. In particular with Alexnet in 2012 for image recognition, AlphaFold in 2020 for protein prediction and ChatGPT-3 in 2022 with Large language models.[1,2,3] In both electron microscopy and Scanning probe microscopy however, the scarcity of curated training data and the low throughput of atomic-resolution techniques often limits the adoption of supervised learning methods.[4,5] Although automation is improving through manufacturer-provided software interfaces, e.g. 'Autoscript' from Thermofisher scientific in electron microscopy, and digital twin software, human oversight remains essential during operation.[6] An approach that would enable a combinatorial approach to generating sufficient labelled data could be through transfer learning. Here we present a framework for correlative SPM–(S)TEM studies based on physics-informed digital twins. By simulating TEM and AFM images from shared atomic structures, paired and aligned datasets can be generated across modalities.[7,8] This approach enables cross-modal correlation and the potential for transfer learning between microscopy techniques, providing a scalable route to data curation, automation, and improved feature detection using supervised based approaches in nanoscale characterisation. This helps pave the way for correlative experimental studies for training algorithms and AI agents for improved automation.

## Methodology:

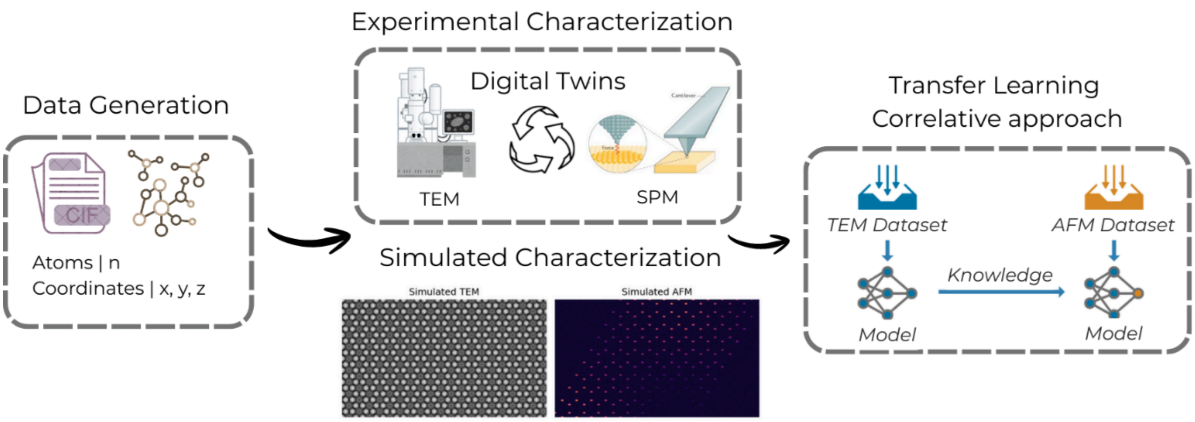
The proposed framework is based on physics-informed digital twins of SPM and (S)TEM. Atomic structures, imported from crystallographic information files (CIFs) or atomistic simulations, serve as a common ground truth. Structures can be modified to include realistic features such as ripples, strain, or defects. Due to simulation constraints, only a few units cells are simulated. TEM images are generated using multislice electron scattering simulations from the abTEM python package, which accurately capture phase contrast, defocus dependence, and aberration effects. Imaging parameters such as accelerating voltage, convergence angle, and defocus are explicitly controlled, enabling standardised datasets with known imaging conditions.[7]

AFM images are simulated by constructing a surface height map from atomic coordinates, followed by convolution with a model tip geometry. This approach reproduces key features of experimental AFM, including finite tip radius effects and smoothing.[8] Noise can be added to emulate realistic experimental conditions. While the contrast mechanisms in TEM and AFM are different, they are intrinsically linked to the resultant underlying structure. Correlative microscopy approaches typically relies on fiducial markers and specialised workflows for alignment, in practice however, as AFM is only mapping the surface and height topology, compared to TEM imaging with signal from the whole depth of the sample, care is needed to be taken into account with correlation. As such, only 2-d materials are considered, with the example in figure 1 shown from simulated 1 layer graphene.

Pixel-wise correlation and feature-level comparisons can therefore be performed. The resulting paired datasets provide labelled training data suitable for supervised and transfer learning across modalities. Such paired datasets are particularly valuable for transfer learning. Models trained on abundant, high-throughput SPM data could be adapted to interpret lower-throughput TEM images, or vice versa. This approach may reduce the need for large experimental TEM datasets and accelerate automation and feature detection, and further allow for wider training needed to power feature segmentation for the improvement of AI microscopy agents. See Figure 1.

By combining correlative microscopy with physics-based digital twins, the proposed framework addresses a central bottleneck in applying machine learning to electron microscopy: the lack of labelled, standardised data. While experimental validation remains essential, simulated datasets offer scalability, reproducibility, and perfect ground truth.

In the longer term, Combined with digital twins, it would allow the generation of a combined labelled dataset with this approach could enable unified multimodal datasets spanning SPM, TEM, STEM, SEM, and X-ray techniques, supporting data-driven discovery and automated analysis in nanoscale characterisation, for the training of AI microscopy agents.

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