Automated Atomic Scale Data Analysis and Modelling for (Scanning) Transmission Electron Microscopy

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The process of discovering and refining new materials, as well as enhancing existing ones for a variety of uses, including quantum applications, is a complex and multifaceted endeavor. This involves identifying needs, reviewing existing literature, proposing materials, engineering devices, characterizing materials, and testing applications. However, the process can be hindered by its time-intensive and costly nature, especially when precision at the atomic level is necessary to comprehend the functionality of materials and heterostructured devices.

In this digital age and with quantum supremacy in the horizon, semiconductor heterostructures within a chip have become indispensable and ubiquitous, propelling significant industrial value chains. They facilitate progress in both emerging sectors like quantum applications and established ones. For that, the trend of miniaturization, which is now reaching nanoscale dimensions and nearing the atomic limit, is a key driver of progress which demands special characterization needs. [1,2] To answer these needs, we present different solutions relying on AI-enhanced analytical frameworks based on ML/DL, which automates TEM data analysis,[3] aimed at the comprehensive characterization of materials and device structures, with a particular focus on materials for energy and environmental applications, as well as quantum devices and their related heterostructures.

The characterization that must answer these demands is Transmission Electron Microscopy (TEM), as the most optimal way to access structural information at the atomic level. We propose a workflow capable of processing both parallel illumination TEM and Scanning TEM (STEM) data, although it is specially designed for the latter. In addition, it can extract compositional information from Electron Energy Loss Spectroscopy (EELS), which is used to make the characterization an exhaustive and complete process. Importantly, the workflow we suggest combines traditional algorithmic, with unsupervised and supervised machine learning algorithms. This way, we ensure that model-based computing and artificial intelligence work hand by hand to provide the comprehensive and material-independent solution we seek for. [3]

Our pioneering workflow autonomously determines material composition, crystallographic phase, and spatial orientation across various regions of (S)TEM-based images or image datasets through detailed model comparison. It is completed with automated strain analysis, enabling a comprehensive characterization of the device's structural properties. Eventually, we incorporate the extracted knowledge to automate the creation of models that could facilitate theoretical simulations and would provide vital physical and chemical insights necessary for understanding the device's performance in practical applications. [3]

Although the method is highly versatile, we focus on quantum computing devices to autonomously optimize their functional properties. In particular, we have proved it with SiGe quantum well heterostructures that demonstrated outstanding quantum performance for spin qubits generation. [1,2] However, the main advantage of placing our workflow beyond state of the art is its generalization capabilities. It works for any material configuration and not only does it answer the pressing automation needs but unlocks getting physical models and simulations of complex devices with unprecedented accuracy.[4]

References

[1] Jirovec, D. et al. Nature Materials, (2021)
[2] Paquelet, B. et al Nat. Commun. 14, 1385 (2023).
[3] Botifoll M., Pinto-Huguet I., et. al, Nanoscale Horizons, 7, 1427 (2022)
[4] Botifoll M., Pinto-Huguet I., et. al, submitted (2025)

Figures

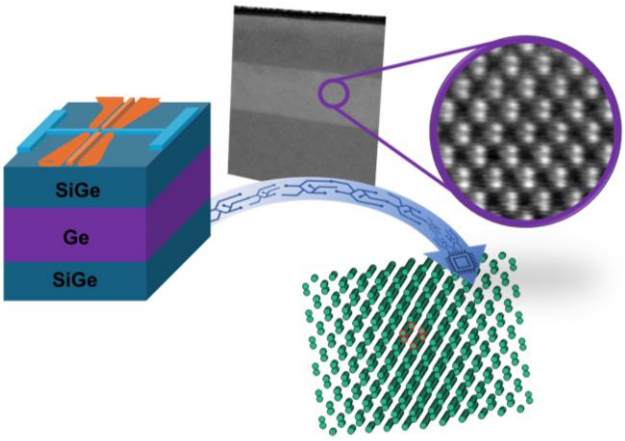

Figure 1. Global workflow of our methodology applied to the study of Ge/Si devices.