Generalisation of a novel routine for band gap mapping at sub-nanometric resolution

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Germanium and silicon-based devices for quantum computing are experiencing a huge rise in popularity over the last few years. They have proven to be magnificent candidates for efficient qubit generation, and are flexible enough to hold different quantum computing paradigms. Based on the morphology and dimensionality of the devices they may act as either spin qubits or (topological) superconducting qubits. For this purpose, heterostructures contacting combinations of pure Ge, pure Si, and alloyed SiGe with varying Si/Ge ratios are successful candidates towards the obtention of qubits [1].

Interestingly, the low effective mass and the electrically tuneable g factors that are key for the qubit performance closely correlate with the strained interface that rules the energy splitting. This constitutes an interesting materials science problem that is worth tackling at the high spatial resolutions the transmission electron microscope can offer, in search of local effects. Therefore, in the present contribution we present a new methodology that can sub-nanometrically map the band structure of semiconductor devices, and the novelty towards making it accessible, reproducible and fast for any material, specially for quantum materials.

The proposed new methodology is based on the correlation of high-resolution low-loss electron energy loss spectroscopy (EELS) and strain mapping to link the accumulations of strain with bandgap shifts [2]. The novelty lies in being able to address the limitations this kind of spectroscopy implicitly have, and semi-automate the routine to enable generalising the methodology to new materials and systems. This semi-automation is based on spectral unmixing techniques, and the possibility to produce tailored simulations to retrieve the optical response of the materials. Therefore, we present a path from the generation of the model till is extrapolation to make it more general and applicable to any system.

References

[1] Jirovec, D. et al. *Nature Materials*, (2021) doi.org/10.1038/s41563-021-01022-2
[2] Martí-sánchez, S. et al, Nat. Commun. 13, 4089 (2022).

Figures

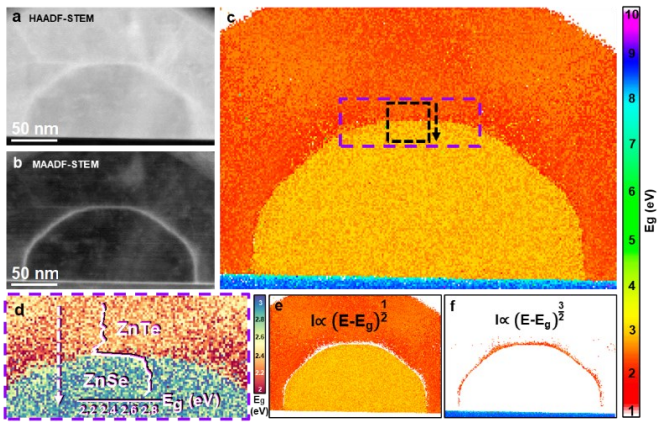

Figure 1: Bandgap maps obtained from applying the proposed methodology to a ZnSe/ZnTe nanowire.