Stable Defects in Semiconductor Nanowires

Sanchez, A.M.[1], Gott, J.[1], Fonseka, A.[1], Zhang, Y.[2], Liu, H.[2] and Beanland, R.[1]

[1] University of Warwick, United Kingdom, [2] University College London, United Kingdom

Lattice parameter and thermal expansion mismatch constrains limit the growth of a wide range of epitaxial layers on Silicon substrates, since they cause dislocations and cracks, making the devices unviable. Nanowires (NWs) are a solution to these problems, since they are only attached to the substrate at their base. Another NW advantage is the high surface to volume ratio, making one-dimensional nanostructures of interest for next-generation of photovoltaics, sensors and optoelectronic devices.[1,2]

In principle, dislocations and defects with long-range strain field are unstable and are expelled from the NW by surface image forces. This work demonstrates the stability of steps on twin boundaries and shows that they act as non-radiative recombination centres in the NWs, captured with atomic resolution Annular Dark Field Scanning Transmission Electron Microscopy (ADF-STEM) imaging.

It was found that $\Sigma 3$ ($11\bar{2}$) boundaries have properties similar to dislocations, but no long-range strain field. The NW polarity is maintained across the (111) boundaries on either side of the step forming a para-twin. Density functional theory calculations demonstrate that these $\Sigma 3$ ($11\bar{2}$) facets produce a shift in the band edge and a closing of the band gap, acting as non-radiative recombination centres, affecting the properties of the nanowires. Additional defect interactions, producing sessile and stable dislocations have also been observed.

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