Crystallography, Electron Microscopy and Functional Evolution of Atomically Thin Confined Nanowires

Sloan, J.[1], Vasylenko, A.[1], Slade, C.[1], Marks, S.[1], Kashtiban, R.[1], Burdanova, M.[1], Medeiros, P.[2], Wynn, J.[2], Kret, S.[3], Dłużewski, P.[3], Faulques, E.[4], Smith, D.[5], Lloyd-Hughes, J.[1], Quigley, D.[1] and Morris, A.[6]

[1] Department of Physics, University of Warwick, United Kingdom, [2] Cavendish Laboratory, University of Cambridge, United Kingdom, [3] Institute of Physics, Polish Academy of Sciences, Poland, [4] Institut des Matériaux Jean Rouxel, University of Nantes, France, [5] School of Physics and Astronomy, University of Southampton, United Kingdom, [6] School of Metallurgy and Materials, University of Birmingham, United Kingdom

A logical extension to fabrication of monolayer 2D materials such as graphene and the 2D layered Transition Metal Dichalcogenides (TMDCs) is creation of atomically regulated nanowires as thin as a single atom column in width.[1,2] In close concert with increasing nanotube diameter, the number of columns of atoms per nanowire accommodated in cross section changes along with symmetry and functionality.[1-7] We have created atomically regulated nanowires by confining them within the smallest diameter carbon nanotubes (Fig. 1(a)), and are investigating their structural and electronic properties (Fig. 1(b)). In terms of their experimental characterisation, these materials provide the ultimate benchmark for testing the highest resolution imaging methodologies, in particular aberration-corrected Transmission Electron Microscopy and Scanning Transmission Electron Microscopy and also spectroscopic imaging.[2,4-7]

A wide variety of different types of materials can be inserted into SWNTs, including halides,[1,2] metals,[1,3] semi-metals,[6,7] semi-conductors (Fig. 2(a) and (b)),[7] ferro-magnetic materials,[1] and Phase Change Materials.[5,8] Imposition of low-dimensional symmetry induces novel phonon characteristics in several of these materials, making them accessible to Raman spectroscopy.[3,6,7] All of these aspects, and many more, can be modelled either *ab initio* or *a posteriori* by Density Functional Theory methods[3-5] which allow for both predictive modelling and diagnostic interpretation of existing and novel low-dimensional systems, allowing for the creation of an effectively unlimited palette of atomically regulated crystals whose structures can be synthesized, predicted, synthesized, their properties modelled and measured, their phase-change characteristics mapped on an atom-column by atom column basis. The extraordinary collective potential that these nanomaterials represent, and in particular the electron imaging techniques we have used to investigate them and the recent progress made will be introduced in this presentation.

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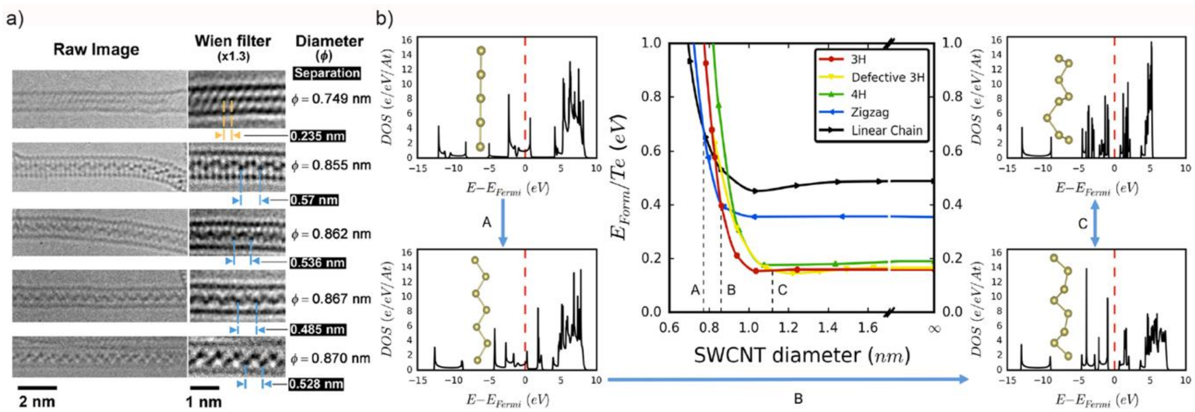

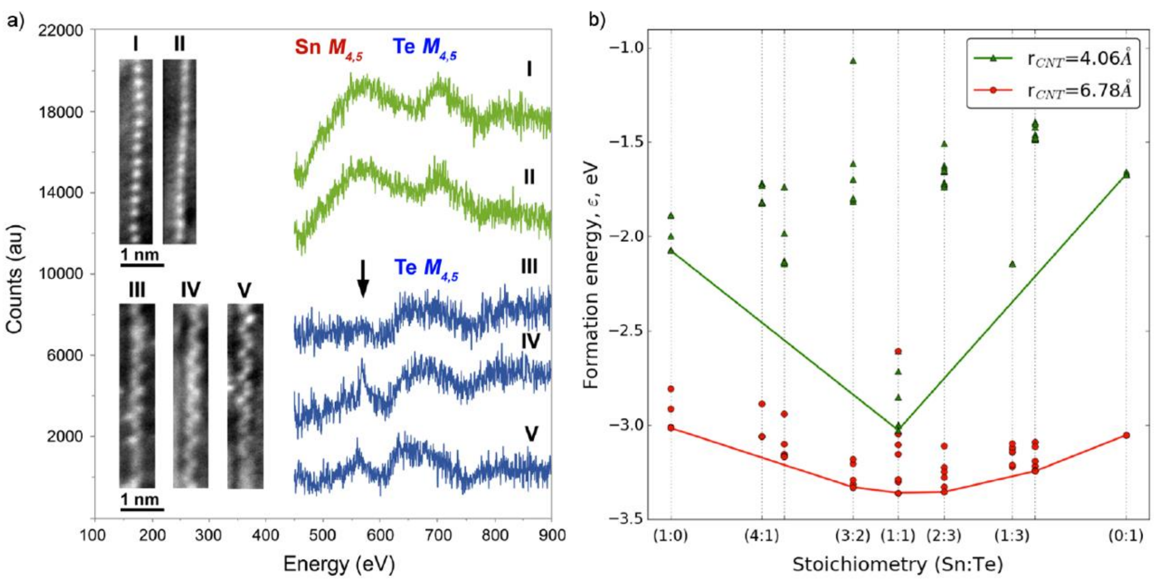

FIG. 1. (a) AC-TEM images of SWNTs with 1D Te extreme nanowires. (b) Central panel: Formation energy/encapsulated atom as a function of the encapsulating diameter. A–C diameters at which we predict structural transitions to occur. L/R panels: Geometries of the structures involved in the transitions A–C, along with the corresponding densities of states (DOS) [4].

FIG. 2. (a) EELS at the outmost electron shells (M-edge) in SnTe 1D atomic chains and Te coils encapsulated within SWCNTs. Note that Te coils are only obtained in nanowires depleted in Sn as indicated with an arrow. (b) Convex hull construction for SnTe nanowires with different stoichiometries embedded in CNT(6,6), r=4.06 Å and CNT(10,10), r=6.78 Å [9].