

Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Extreme Tellurium nanowires encapsulated within narrow-diameter single-walled carbon nanotubes: Theory and experiments. PAULO V C MEDEIROS, University of Cambridge, SAMUEL MARKS, University of Warwick, JAMIE WYNN, University of Cambridge, ANDRIJ VASYLENKO, University of Warwick, QUANTIN RAMASSE3, SuperSTEM Laboratory, DAVID QUIGLEY, JEREMY SLOAN, University of Warwick, ANDREW MORRIS, University of Cambridge — Extreme nanowires are the ultimate class of crystalline materials: They are the smallest possible periodic materials. With atom-wide motifs repeated along one single dimension, they offer a unique perspective into the Physics and Chemistry of low-dimensional systems. The interior of narrow single-walled carbon nanotubes (NSWCNTs), on the other hand, provides an ideal environment for the creation of such materials. We report the observation of extreme Te nanowires grown inside NSWCNTs. We start by discussing how implicit single-walled carbon nanotubes SWCNTs can be introduced to speed up the structural searches on SWCNT-encapsulated structures. Then, using high-precision, high-throughput *ab initio* calculations, along with state-of-the-art imaging techniques, we unambiguously determine the phase evolution of encapsulated Te as a function of the diameters of the encapsulating NSWCNTs. From 1-atom-wide linear chains – the ultimate extreme nanowires, elemental Te evolves into zigzag chains and, still within very narrow SWCNTs, forms helical structures that are the one-dimensional analogues of bulk Tellurium.

Paulo V C Medeiros
University of Cambridge

Date submitted: 11 Nov 2016

Electronic form version 1.4