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Crystals and molecules in carbon nanotubes - investigating crystallography and associated physical properties on the smallest possible scale by HRTEM, MD and DFT

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Science Lecture Theatre S11, Bldg 25

Abstract

A wide variety of materials, including both low dimensional crystals and molecules, can form inclusions in both single and multiple walled carbon nanotubes [1]. From the point of view of both materials formation and electron microscopy these encapsulates are both interesting and challenging because the inclusions so formed are on the molecular scale and, in microscopy terms, correspond to weak phase objects of 'known' thickness. In terms of our understanding of the relationships between structure and properties, these materials are valuable because their small scale also makes them comparatively tractable to theoretical calculations such as Molecular Dynamics (MD) and Density Functional Theory (DFT) simulations. As a result, we have been able to obtain detailed crystal structure information from HRTEM of low dimensional crystal growth from High Resolution Transmission Electron Microscopy (HRTEM) and then cross-correlate the obtained crystallography with DFT calculations. For low dimensional semiconductors grown within nanotubes, HgTe for example, we show both modified crystal growth behaviour and modified electronic structure as a result of nanotube encapsulation [2]. For molecules formed within carbon nanotubes, it has been comparatively difficult to obtain such detailed correlation between structure and properties to the relative difficulty of obtaining precise structural data from these species due to their not being rigidly bound within the interior of the nanotubes. For the asymmetric polyoxometalate

anion $[W_6O_{19}]^{2-}$, steric locking of this species within nanotubes permits direct observation of structural distortions, permitting detailed correlation with theoretical calculations for the first time.

References

1. J. Sloan, D.E. Luzzi, A.I. Kirkland, J. L. Hutchison, and M.L.H. Green, MRS Bull. 2004, 29, 265.
2 R. Carter, J. Sloan, A. Vlandas, M. L. H. Green A. I. Kirkland, R. R. Meyer, J. L. Hutchison P. J. D. Lindan, G. Lin, J. Harding, *Phys. Rev. Lett.*, 2006, 96, 215501.
3 J. Sloan G. Matthewman, C. Dyer-Smith, A-Y. Sung, Z. Liu, K. Suenaga, A. I. Kirkland, and E. Flahaut, submitted.

Visitors are most welcome: Please note the parking arrangements. There is a designated Visitors Car Park (N1) clearly ground-marked by white paint and tickets, at a cost of $1.4/hour for up to 3 hours, are available from a dispensing machine.

Convenor: Dr. Joanne Etheridge

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