Transforming Carbon Onions into Nanodiamond

Nigel Marks

Nanochemistry Research Institute, Curtin University

Abstract:
Nanometre-sized diamond grains are commonly found in certain primitive meteorites, but their origin is puzzling. Using evidence from atomistic simulation we have identified a mechanism by which nanodiamonds form abundantly in space in a two-stage process involving condensation of vapour to form carbononions (nested fullerenes) followed by transformation to nanodiamond in an energetic impact. This non-equilibrium process is consistent with common environments in space and invokes the fewest assumptions of any proposed model.

The simulations identify an optimal energy window of 1-2 eV/atom in which carbon onions are efficiently transformed into nanodiamond within a picosecond. The process differs substantially from conventional mechanisms for accessing the diamond (sp3-bonded) phase which require high temperature and/or pressure. Recently we commenced an experimental program to test this hypothesis, commissioning a sputtering deposition system coupled to a custom-built pulsed power supply. In parallel with the experiments we have also developed new mathematical schemes to derive atomic coordinates for the carbon onions that are used as inputs for the simulations.

Biography:
A/Prof Nigel Marks is a material scientist with a major interest in atomistic computer simulation. He received his PhD in 1997 at The University of Sydney and worked at the Australian Nuclear Science Technology Organisation and the Queen's University of Belfast before returning to Sydney University on an ARC Postdoctoral Fellowship. After five years as a teaching and research academic he moved to Curtin University in 2008 to develop a program in nuclear materials simulation. In 2012 he was awarded an ARC Future Fellowship on nanodiamond synthesis from carbon onions. His other research interests include self-assembly in carbon, radiation damage in solids, semiconductor nanostructures and chemical effects due to beta-decay.