Experimental and computational studies of Si and Ge layers on diamond for enhanced NEA applications

Natural or labgrown diamond has the unusual property, that when terminated with hydrogen, its surface exhibits negative electron affinity (NEA). This means that electrons can be extracted from the surface of diamond easily and efficiently, and this has led to a number of potential applications for diamond devices as electron sources in vacuum.

Recent experimental work (Bristol, Arizona State Uni) and theoretical work (Bristol & Newcastle) have shown that diamond terminated with suitable metal-oxides can have NEA values that are significantly higher than those from hydrogen, and that these surfaces can be stable up to 1000 K. Such surface terminations include LiO, MgO, TiO, AlO, VO, and a range of others yet to be tested. Diamond with a suitable surface termination therefore is an excellent candidate for use in thermionic heat converters for use in solar power generators. In these, solar heat is captured by a parabolic reflector and focused onto such a diamond surface, causing electrons to be thermionically emitted. These are captured by a cooler counter electrode, and used to drive an external circuit, i.e. solar heat is converted into electric power. Such thermionic converters could be used in parallel with current photovoltaic cells to capture both the visible and IR (heat) portions of the solar spectrum, greatly increasing the efficiency of solar power generation.

Recent reports from Australian groups suggest that sub-monolayers of Si or Ge on diamond may also improve the NEA significantly, whilst remaining air and temperature stable. In this PhD, the student will use the new nanoESCA facility at UoB, equipped with an evaporation/deposition chamber, to deposit sub-monolayers of first, Si and later, Ge, onto single-crystal diamond surfaces. The effectiveness of these surfaces as electron emission sources will then be tested both in situ in the nanoESCA facility (without breaking vacuum), and also in a bespoke thermionic test rig.
The experimental work will be guided by theoretical modelling (initially as a miniproject at Newcastle, but continuing as a major part of the PhD at Bristol) and by surface analysis such as SIMS or XPS (initially at Aberystwyth but also continuing at Bristol throughout the project). The modelling at Bristol will be performed by bespoke computer packages (CASTEP and CRYSTAL) which have been extensively used by the theory group at Bristol for the past decade to model diamond surfaces. The models can predict the geometries of the adsorbate atoms, and the likely electron affinities of different configurations and coverages of the Si or Ge on the surface.

The ultimate aim would be identify and study in detail an adsorbate (Si or Ge) that would greatly enhance the NEA of a diamond surface, be stable at high temperatures (1000 K), give a high electron yield at low temperatures (600 K), not degrade with use, and be suitable for use in a commercial thermionic heat convertor.

For the computational side, the aims would be to simulate addition of Si atoms to a (100) diamond surface, varying the coverage from sub-monolayers to 1 ML, and by minimising the energy, predict the optimal geometries for the adsorbed species, their thermal stability, and investigate the factors that determine the resulting electron affinity. We will also simulate the effects of partial and full oxidation of the added Si. Ideally, an optimal coverage and configuration would be identified which can be used to guide the experimental work. Following Si, we would move on to modelling Ge addition and compare thermodynamics, structure and electronic behaviour with those of the Group I and II elements and Al.

For further details please contact:

Prof Paul May: paul.may@bristol.ac.uk
Prof Neil Allan: neil.allan@bristol.ac.uk