Monte Carlo modelling of nanocluster growth on graphene

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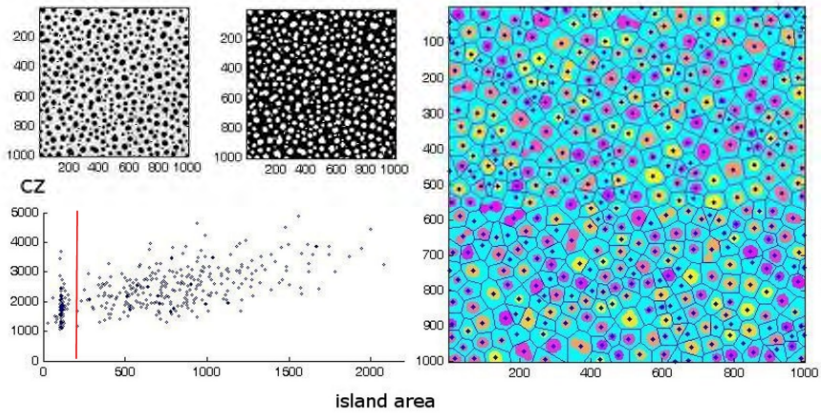
Background

Graphene and chemically modified graphene (CMG) are remarkable materials and the subject of intense research activity. One can gain insight into the interaction of CMG with other materials by using CMG as a substrate for vapour deposition. We have just published a paper [Small **7** (2011) 3202] where various metals (Au, Ti, etc.) were deposited to a few nm thickness on to CMG in transmission electron microscopy (TEM) supports. The high electron transparency of the CMG allows very high quality TEM images of the metal film to be *rapidly* obtained, giving much greater statistical robustness than, say, by scanned probe imaging. We claim that the whole range of growth morphologies observed can be qualitatively explained with just two parameters: the miniproject will allow us to refine this simple energetic model by better understanding the kinetics. Understanding the size and spatial distributions of Au nanoclusters on CMG will form the focus of the miniproject and give insights into the basic growth mechanisms. We want to develop a kinetic Monte Carlo (kMC) model to explain the bimodal size distribution and peculiar capture zone (CZ) – island area relationship. This model should include migration of clusters as well as adatoms and is the key deliverable of the project. The kMC model will be developed in collaboration with Dr. Paul Mulheran at the University of Strathclyde [Europhys. Lett. **49** (2000) 617].



Top left: raw and thresholded TEM image section of 7.5 nm Au on CMG.
Right: Voronoi polygons (the CZs) around Au islands.
Bottom left: island area vs. CZ area – the red line separates "small" islands. We think these (2D?) islands are less mobile than larger clusters.

Project objectives

1. Re-analyse an *existing* series of TEM images of Au on CMG: extend preliminary analysis done by Gavin Bell (using MATLAB), particularly to improve "small island" extraction.
2. Develop a simple kMC model for Au deposition on CMG, incorporating cluster diffusion.
3. Optionally (more likely PhD work) – extend the kMC model to incorporate explicitly the structures of CMG, randomly functionalised at the atomic scale plus micron-scale layer number-dependence.

Practical aspects

The student will need to assimilate some background in thin film / cluster growth. No new data collection is required for the miniproject. Skills in image analysis and kMC modelling will be developed. Objective 1 should be a straightforward but valuable extension of existing work. The kMC model could be implemented by adapting existing codes (FORTRAN), or developing codes from scratch; the starting point will be simple point island models, suitable for modelling the growth of small clusters.

Potential PhD work

There is great scope for continuing and extending this work, which would benefit all the graphene research in Physics and Chemistry. For example, our recent "AMIGO" Physics Day highlighted the need for better understanding graphene growth itself – there is no accepted model for the elementary steps in graphene growth! Our TEMs and deposition systems will continue to produce state-of-the-art data, so a PhD could focus entirely on modelling (though an interested student could certainly learn and perform some microscopy). Extensions to the modelling beyond option 3 above might include scaling analysis and theory development for the scale-invariance that emerges in these non-equilibrium growth systems, as well as understanding in atomistic detail the growth mechanisms that drive the larger-scale organisational behaviour observed in the experiments.