

Structural Studies of Defects and Defect Dynamics in Graphene

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To usefully deploy Graphene and related materials in electronic applications [1-3] it is essential to understand the behavior of point defects, which have been the subject of extensive research over decades for silicon devices. High resolution Transmission Electron Microscopy is the ideal characterization tool for studying the formation and evolution of defects in Graphene in real space. Moreover, recent instrumental advances make it possible to image these defects at primary energies below those that cause significant specimen damage whilst retaining sufficient spatial resolution to resolve the local atomic configuration in the Graphene lattice around the defect site [4].

In this paper we will discuss the controlled formation of several defect types in Graphene, including mono- and di-vacancies and will demonstrate that the evolution of these into more complex extended defects can be controlled by electron beam irradiation [5]. Density functional theory (DFT) calculations have been used to evaluate the energetics of several defect configurations which indicate possible pathways by which these can evolve.

We will also report dynamic studies of small defect structures in Graphene, which enable reaction pathways between different structural forms to be evaluated.

- [1] Novoselov, K. S et al. *Nature* **2012**, 490, 192.
[2] Schwierz, F. Graphene Transistors. *Nature Nanotech.* **2010**, 5, 487.
[3] Britnell, L et al. *Science* **2012**, 335, 947.
[4] Robertson, A.W. et al. *Nature Communications* **2012**, 3, 1144.
[5] Robertson, A.W. et al. *ACS Nano* 2013, **7** (5), 4495.

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