Contribution ID: **95** Type: **Oral Presentation**

Understanding the role of the subtstrate in off-lattice simulations of graphene growth on copper

Monday, 11 July 2016 12:40 (20 minutes)

Abstract content
   (Max 300 words)
Formatting &
Special chars

Chemical vapour deposition (CVD) growth of graphene on copper has been identified as the most promising route for scalable synthesis of graphene. It is important to understand the fundamental surface growth mechanisms in order to optimise material quality, but detailed in situ imaging of growth in CVD is extremely difficult. Comparison of post-growth experimental data with dynamic simulations of growth can overcome this problem.

Experimental observations of partial-coverage graphene grown on copper foils with well-defined crystallographic microstructure [e.g. (111), (100) and (210) grains] indicate clearly that the surface orientation affects the growth rate, island size distribution (ISD) and orientation of graphene islands [NR Wilson, Nano Research 6.2 (2013): 99-112]. Ab inito simulation cannot reach length scales relevant to these phenomena, and it would be challenging to use such methods even to address interaction of growing graphene with the local symmetry of the crystalline substrate.

In this work we introduce a minimal off-lattice model which captures variations in growth rate, island orientation and ISD between different low index copper faces. We compare our simulation data to available experimental results, in particular finding similar graphene orientations for the different low index Cu faces. Our model is also capable of exploring the effect of mismatch, thermal expansion and surface disorder.

Primary author: Mr ENSTONE, Gwilym (University of Warwick)

Presenter: Mr ENSTONE, Gwilym (University of Warwick)

Session Classification: Parallel Track B