

Type of presentation: Oral

IT-11-O-1669 Electrostatic potential of single-layer graphene measured using electron holography and ab-initio calculations

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Graphene, a single-layer, hexagonally-coordinated carbon material has attracted huge attention in a wide range of fields due to its unique structural properties [1]. For example, it has found applications in electronic devices, energy storage, and electrocatalysis [2]. Characterisation of graphene imposes a requirement for high sensitivity to image a thickness of one atom. High-resolution TEM and ADF-STEM have been used to study the atomic arrangements and defects in graphene (and its related materials). The electrostatic potential of a single layer of graphene, a fundamental quantity of a materials structure property, is however less explored.

Here we use electron holography and density functional theory calculations to accurately measure the electrostatic potential of a single-layer of graphene. A C_s and C_c aberration-corrected TEM (Pico), operated at 80kV, was used to take holograms of graphene. The biprism voltage was set to be 175V, giving interference fringes of spacing 0.04nm. The graphene was grown using chemical vapour deposition on a SiO_2 substrate and then transferred onto a TEM grid.

Figure 1 shows the phase of a typical area of the graphene sheet. It can be seen that there is a band near the edge of the graphene and some patches across the graphene sheet with larger phase shifts, which are typical features of silicon oxide and other hydrocarbon contamination left on graphene from TEM specimen preparation. The edges of the graphene sheet are more than a one-layer thick although patches of single-layer graphene can be found.

Figure 2 shows a region of single-layer graphene near the edge, after 2-hours of electron beam illumination to form a hole for the reference wave. The modulus of the Fourier transform of the complex wave-function (shown in the inset of figure 2) shows that high spatial resolution information is present in the phase (with the 1-210 reflection visible). The phase shift from the single layer graphene was measured to be 58 mrad (with respect to the vacuum) and the phase profile is shown in the inset of figure 2.

In order to compare the experimental measurement of the electrostatic potential with theory, both all-electron (Wien2K) and density functional theory calculations (VASP) were used. The theoretical calculation gives good agreement with the experimental measurement. Further implications from the theoretical calculations will be discussed in the presentation.

References: [1] K. S. Novoselov et. al., Science, 2004, 306, 666 [2] Y. Sun et. al., Energy Environ. Sci., 2011, 4, 1113

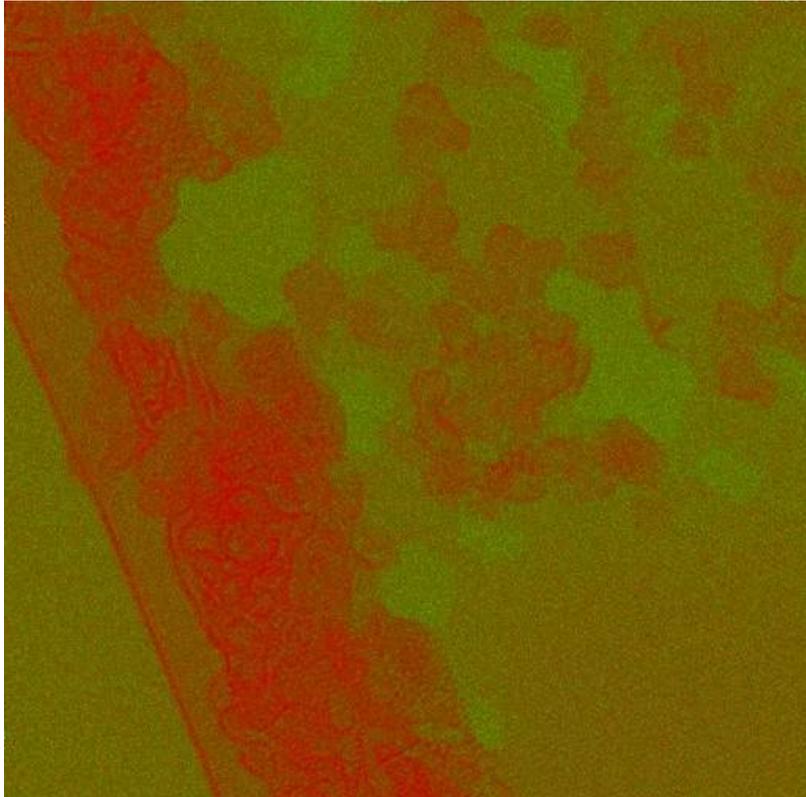


Fig. 1: Phase of the hologram of a typical region of a graphene sheet.

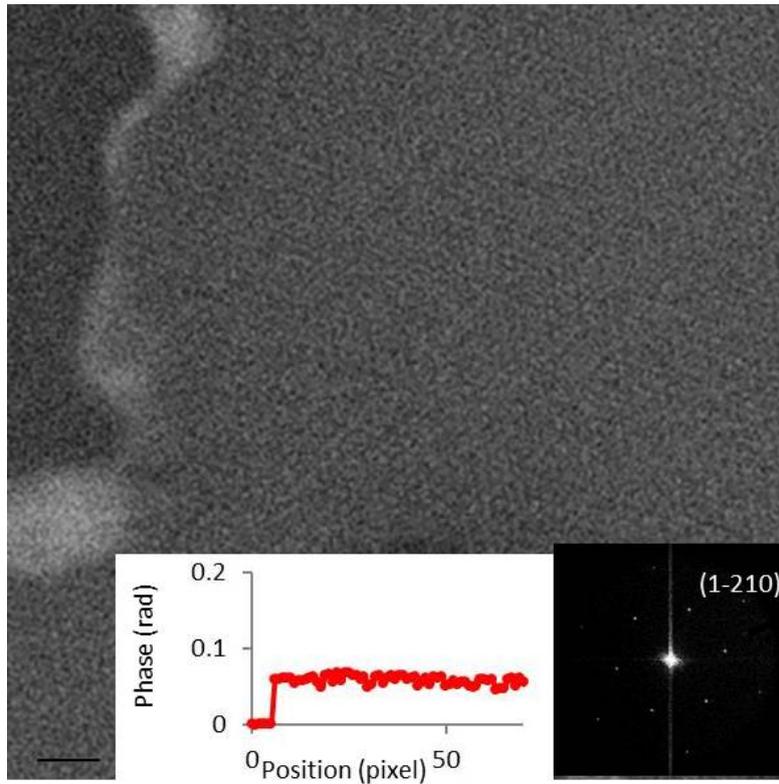


Fig. 2: Phase of the hologram of the single-layer graphene. Inset (right) shows the modulus of the fft of the complex wave, and the inset (left) shows the phase profile from the vacuum to the graphene region.