

Examination of the Corrugation in Hydrogenated Graphene on Ir(111) by Standing Wave XPS

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The X-ray Standing Wave (XSW)-technique is an experimental method which exploits the standing wave generated by interference between the incident and reflected waves of X-rays that arise at the Bragg condition to provide a direct experimental measurement of adsorption height [1], see Figure 1a. Specifically, small changes in the photon energy will vary the phase of the standing wave, moving anti-nodes between the Bragg planes.

This results in a variation of photon intensity as a function of position, which can be monitored by photoemission yield from XPS. This allows us to locate the source of different components spatially with sub-Angstrom resolution [2], and therefore the position of adsorbates can be measured directly with very high accuracy.

It has previously been reported by our group [3] that hydrogenation of graphene on Ir(111) at high temperatures (630 K) forms an ordered pattern of hydrogen clusters, and hence sp^3 -hybridised carbon, in FCC areas of the graphene/Ir(111) moiré superstructure. This periodic pattern is particularly interesting, since it leads to a band gap opening in graphene [3].

For the mentioned system, this method has enabled us to determine the average distance to the Ir(111) surface of sp^2 and sp^3 carbon related to pristine and hydrogenated parts of graphene, respectively. The measurement indicates that upon hydrogenation, graphene is pinned to the Iridium substrate in the hydrogenated regions, see Figure 1.b.

References:

- [1] Zegenhagen, J. (1993). Surface structure determination with X-ray standing waves. *Surface Science Reports*, 18(7-8), 202-271.
- [2] Busse, C., Lazić, P., Djemour, R., Coraux, J., Gerber, T., Atodiresei, N., ... & Michely, T. (2011). Graphene on Ir (111): physisorption with chemical modulation. *Physical review letters*, 107(3), 036101.
- [3] Jørgensen, J. H., Čabo, A. G., Balog, R., Kyhl, L., Groves, M. N., Cassidy, A. M., ... & Lammich, L. (2016). Symmetry-driven band gap engineering in hydrogen functionalized graphene. *ACS nano*, 10(12), 10798-10807.

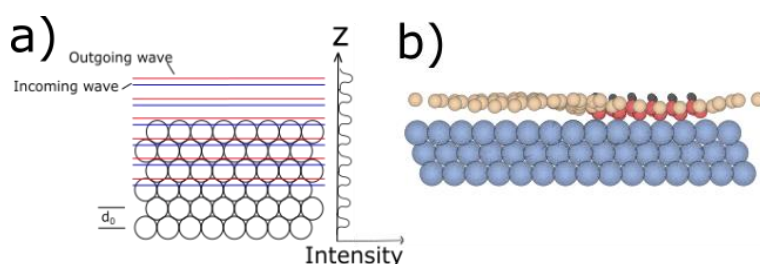


Fig 1: a) An illustration of the principle behind the XSW with the incoming (blue) and outgoing waves (red) in a crystal lattice with inter-layer spacing d_0 as well as the intensity of the resulting wave. b) The system at hand with a sheet of graphene (brown sp^2 , red sp^3) and clusters of hydrogen (black) on an Iridium crystal (blue). The graphene corrugates visibly.