Ultra-thin films of lead iodide on graphene: influence of the substrate on the opto-structural properties probed in real time

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Lead iodide (PbI_2) is a large bandgap 2D layered material belonging to the metal halide family. It has emerged as an excellent candidate for photodetectors and is a key component in metal halide perovskites solar cells. In the current work, we highlight the influence of the interface interaction on the crystalline and opto-structural properties of lead iodide layers deposited on graphene/SiC (0001) by Molecular Beam Epitaxy.

To achieve the best control of the growth process, the growing layer is characterized in real-time by GIFAD (Grazing Incidence Fast Atom Diffraction), QMS (Quadrupole Mass Spectrometry), and SDRS (Surface Differential Reflectance Spectroscopy). In particular, GIFAD provides fine information on the organization dynamics and the electron density profile at distances similar to those probed by local probes such as STM or AFM [1]. This electron density profile, which is directly related to the atomic positions within the lattice, can also be used to extract possible charge transfer within the lattice and/or with the substrate. GIFAD being a very soft technique, it can monitor the growth of the most fragile materials for hours without any damage [2]. SDRS yields information on the optical properties, which can then be correlated to the structural changes of the growing layer provided by GIFAD.

The GIFAD data reveal a layer-by-layer growth (fig. 1) by van der Waals epitaxy according to the armchair (PbI_2)/zigzag (graphene) stacking with non-commensurability of unit cells. We observe a 6% strain as well as specific optical features on the first monolayer that could result from an interface interaction stronger than van der Waals.

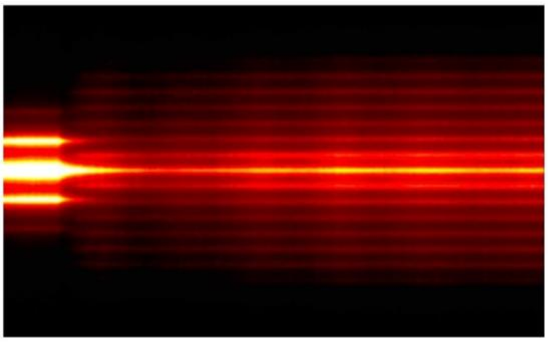

***Fig. 1**. Real-time monitoring by GIFAD of the growth of PbI_2 on graphene/SiC(0001). The intensity oscillations demonstrate a layer-by-layer growth, with a well defined alignment of the lattices.*

[1] H. Khemliche et al., Applied Physics Letters. 95, 151901, 2009
[2] A. Momeni et al., J. Phys. Chem. Lett. 9, 908, 2018