Bismuth tri-iodide – Graphene 2D material

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A plethora of 2D materials has been studied during the last years, composed by one or a few layers of the same element, the same compound or more than one compound. Although several of them are in a well developed stage, new 2D materials emerge. Among them, Bismuth tri-iodide–Graphene have been reported a few times (theoretical and experimental results). and exhibits interesting properties. Although it has been applied as radiation detector, these predictions and results foresee photovoltaic applications for BiI_3 layers and van der Waals superstructures. Also, theoretical studies predict stable BiI_3–graphene heterostructures, with higher absorption for visible light photons related to BiI_3 monolayers. Within this framework, this work investigates the growth of van der Waals superstructures BiI_3–graphene.

BiI_3-Graphene 2D layers were obtained by physical vapor transport from BiI_3 (Aldrich 99,999%) nucleation and further growth, onto graphene covered TEM grids (single layer graphene film on a 2,5 µm holey silicon nitride film, Ted Pella), and onto 1 layer graphene film/200nm SiO_2 film on a 675 µm ultra-flat silicon substrates, 5×5 mm, Ted Pella. The growth was performed in an especially built equipment, varying initial pressure (10^{-6}–10^{-7} mBar), BiI_3 mass (6-80 mg), source (260.2 °C) and substrate (40±1 °C) temperature (and then supersaturation), and deposition time (10-120 s), with a source-substrate distance of 15.0±0.5 mm), under high purity Ar atmosphere. Layers were characterized by High Resolution Transmission Electron Microscopy (HR-TEM), Fast Fourier Transform (FFT), Energy Dispersive Spectroscopy (EDS), Scanning Electron Microscopy - Field Emission Gun (SEM-FEG), Atomic Force Microscopy (AFM) and Gracing Incidence X-Ray Diffraction (GIXRD) and X-ray Reflectometry (XRR).

Twisted BiI_3 layers which determine Moiré interference were obtained, indicating BiI_3-graphene van der Waals superstructures with two or more BiI_3 layers. It was not possible by now to obtain an uniform coverage of the substrate, but this kind of superstructure cover all the grid. In our knowledge, this is the first report of Moiré interference for BiI_3 layers, and it is similar to the interference reported for graphene and for other van der Waals superstructures (WS_2-gr, MoS_2-gr). Furthermore, Moiré diagrams indicate that the angle between layers is not constant. EDS measurements show BiI_3 as the layer composition, and FFTs show that the orientation of the layers was always with c axis perpendicular to the substrate, while BiI_3 is always present in its rhombohedral phase R-3.

GIXRD confirms layer composition as BiI_3 in agreement with EDS results, the rhombohedral phase R-3 (data correlated with file 00-048-1795 PDF4+ 2021 database and with powdered BiI_3, in agreement with HR-TEM results, and the orientation of the BiI_3 layers with the *c* axis perpendicular to the substrate, which agrees with HR-TEM results as well. According to XRR, the BiI_3 layer exhibits a density of 6.0 g/cm^3 (BiI_3 bulk 5.8 g/cm^3), a thickness of 34.6 nm, which gives approximately 16 BiI_3 layers (c= 20.72 Å), and a roughness of 6.0 nm, approximately 3-4 BiI_3 layers.

The obtained BiI_3-graphene superstructure is similar to structures of TMDs-graphene (as MoS_2-graphene), and is stable, as was theoretically predicted.