Spectroscopic insight into single step growth of atomically thin h-BN-graphene heterostuctures on top of curved crystals

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Two-dimensional materials lately attract increasing attention due to their excellent physicochemical properties. Current innovations based on 2D materials are focused on the design of hybrid layers and heterostructures, which allow obtaining new, emerging properties. Simply when considering the advantages offered by each of the 2D materials used, the functional needs in a variety of fields (electrical, photoelectric, biosensing, etc.) can be satisfied. The combination of hexagonal boron nitride (h-BN) and graphene (Gr) is among the most attractive alternatives. On the one hand, the hybrid h-BNC material enables the development of bandgap-engineered applications in electronics and optics, and generally leads to properties that are distinct from those of Gr and h-BN [1]. On the other hand, the interface between Gr and h-BN domains exhibits promising properties, e.g., its unique catalytic behaviour that drives the electrochemical production of H2O2 [2]. Finally, in-plane h-BN-Gr heterostructures, consisting of alternating strips of h-BN and Gr, may provide a feasible material platform to realize electrocatalytically switchable high-capacity CO2 capture [3].

Effective growth of h-BN-Gr in-plane heterostructures can be achieved via chemical vapor deposition (CVD) on transition metal substrates by either using a mixture of chemicals [4], or single molecular precursors [5]. The substrate plays a crucial role in determining the morphology, crystal orientation, domain size, wrinkles etc., thereby defining the physicochemical properties of the emerging material. Real surfaces or nanoparticles contain not only low-index planes, but also steps, defects or additional facets. Therefore, for technological applications it is of high importance to study surfaces containing non-trivial topography. The simplest realization of a non-trivial substrate is a curved crystal, namely a cylindrical section cut and polished around a high-symmetry plane. This geometry allows one to span a full set of vicinal planes featuring arrays of atomic steps. Taking advantage of the smooth variation of the density of steps, one can systematically study their influence on the growth and properties of the resulting 2D material.

Within present study, we have investigated the influence of the density of steps on the number and type of h-BN-Gr boundaries, as well as on the dopant density and character in the h-BN-C monolayer. Moreover, here we compare different substrates: those characterising by weak and strong bonding with h-BN-Gr layers, e.g. c-Ni(111), c-Pt(111) and c-Pd(111).

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