Near-band edge optical properties of exfoliated h-BN layers.

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Abstract

Hexagonal boron nitride is a wide band gap semiconductor (~ 6.5 eV), which meets a growing interest for graphene engineering [1]. In particular electron mobility of graphene is shown to be preserved when it is supported by a h-BN film, in particular when mechanically exfoliated from h-BN crystallites. Nevertheless the use of BN sheets grown by CVD techniques remains an open issue as this material might present structural defects degrading graphene properties. It is therefore highly desirable to better know optical and electronic properties of thin BN layers, in correlation with their structural properties and the impact of the underlying BN layer on electronic properties of graphene.
Until recently, these properties were poorly known due to both the scarcity of crystals and suitable investigation tools. This situation has changed thanks, first, to the development of dedicated photoluminescence (PL) and cathodoluminescence (CL) experiments running at 4K and adapted to the detection in the far UV range [2, 3, 4], and second to the availability of high quality single crystals [5]. H-BN has been shown to display original optical properties, governed by strong Frenkel-type excitonic effects, in the 5.5 – 6 eV energy range [2, 3, 6]. The existence of these high energy excitons has been confirmed by reliable theoretical calculations [7, 8]. Furthermore, since excitons are highly sensitive to their environment, they are easily trapped on defects such as dislocations, as revealed by combined cathodoluminescence measurements and transmission electron microscopy (TEM) observations [4].
In this work, we examine how these properties can be further exploited for the characterization of BN layers to be used as support for graphene. We carry out optical and structural characterizations of this material by combining CL at 4K in the UV range (up to 6eV) and electron microscopy. Thin layers have been obtained by mechanically exfoliating small crystallites. Exfoliated flakes were reported on SiO_2 substrates for AFM thickness measurements, as described in [9].
Results are illustrated in Figure 1 and detailed in [10]. As for the bulk, excitonic emission consists of two series of lines called S and D. In the bulk, S excitons have been found to be self-trapped, due to a Jahn-Teller effect [3]. Emission related to D lines is found to be localized on defects such as grain boundaries, whereas in defect free areas, D lines completely vanish and only S lines are observed. D/S ratio can therefore be used as a qualification parameter of the defect densities present in the layers. Furthermore, when film thickness stands below 5-6 atomic layers, energies of S and D lines are shifted towards higher energies. This shift can be due to a perturbation in the strain environment of the exciton induced by the reduction in thickness or by the exciton confinement. Ongoing investigation of single and double atomic layers will permit to further investigate this effect and understand its exact origin. This shift in energy could be used for the determination of the number of layers, complementary to AFM measurements.

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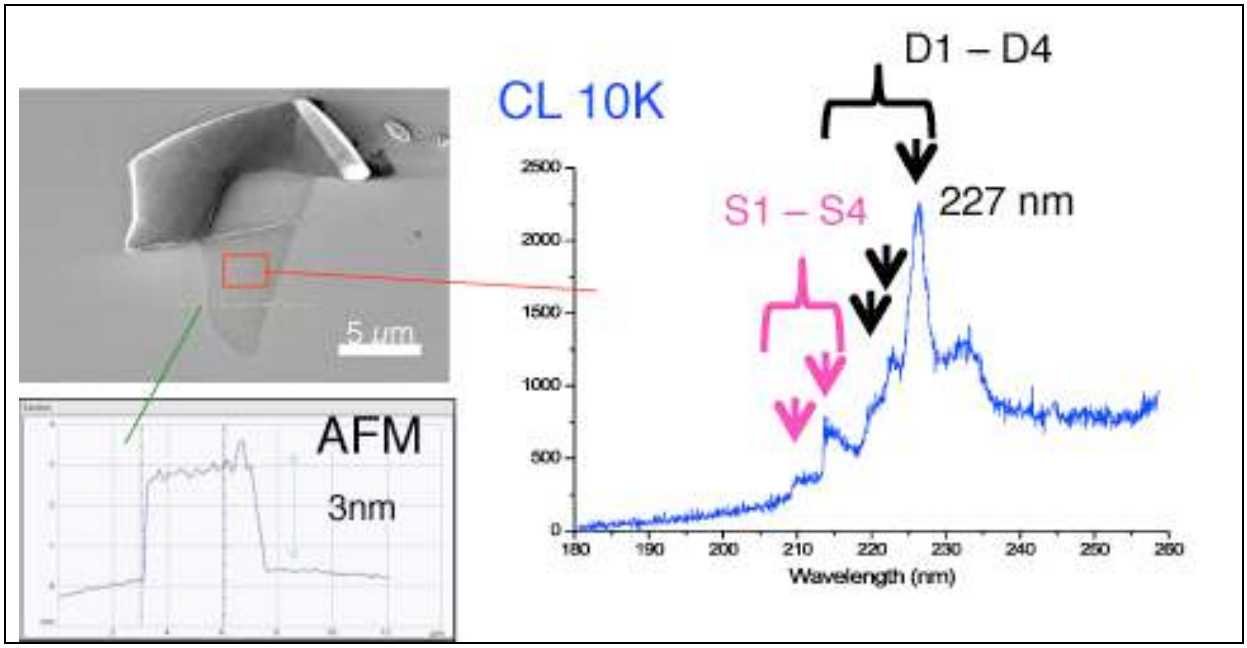

Figure 1: Left: AFM image of an exfoliated h-BN flake. Thickness measurement by AFM along the cross section indicated by the dashed green line, indicates that the flake is composed up to 9 atomic sheets. Right: CL spectrum recorded at 4K on the area of the flake indicated by the red square. The near band edge emission is composed of S and D lines.