The Optical Properties of Various Polytypes of sp^2-bonded Boron Nitride.

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Hexagonal boron nitride (h-BN), an insulating two-dimensional layered material, has attracted great attention due to its fascinating properties and promising applications across the fields of photonics, quantum optics, and electronics. Given the layered structure of h-BN, various polytypes exist with high-symmetry stacking sequences where successive layers are rotated or translated, leading to a variety of physical properties. Similarly to silicon carbide, polytypism in sp^2-bonded boron nitride is to lead to a wealth of variations in the opto-electronic properties. I will report on the optical properties of a variety BN polytypes including bulk crystals grown by precipitation out of molten metallic solutions and epilayers by produced by metal-organic chemical vapor deposition on sapphire substrates [1,2]. The sp^2-bonded layered compound BN exists in more than a handful of different polytypes (i.e. different layer stacking sequences) with similar formation energies, which makes obtaining a pure monotype single crystals extremely tricky. Co-existence of polytypes in a similar crystal leads to formation of many interfaces and structural defects having deleterious influence on the internal quantum efficiency of the light-emission and on the mobility of carriers. Light emission, when recorded in standard experimental illumination conditions, is in general inhomogeneous and its yield is dominated to radiative recombination to localized stacking faults [3], even for crystals with state-of-the-art, high structural quality [4]. However, despite of this, lasing operation was reported at 215 nm [5], which has shifted the interest of sp^2-bonded BN from the laboratories of basic sciences to the fields of optoelectronic and electrical device applications. Here I present X-ray diffraction, electron microscopy and Raman light scattering experiments that were performed on a large variety of samples grown using the complementary techniques alluded to above and that we interpret with the help of group theory arguments and calculations of the phonon dispersion relations (in the context of quantum espresso). They revealed the three ordered AA' (normal), AB (Bernal), and ABC (Rhombohedral) stackings, and the disordered turbostratic (tBN) one. Characterization of the different structural polytypes are completed by micro-photoluminescence experiment measurements that furnish a one-by-one, unambiguous relationship between the sp^2-stacking and its photoluminescence spectrum [6,7]. These, together with reflectance experiment disentangle the nature of the light-matter interaction processes in sp^2- bonded BN. All polytypes studied here display an indirect configuration of their fundamental bandgap.

References:

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