

Nanostructure makes crystalline compound physically reactive

Hexagonal boron nitride (h-BN) belongs to a class of crystalline compounds with layered structure: it consists of parallel honeycomb layers, in which hexagons vertices are alternatively occupied by boron (B) and nitrogen (N) atoms. Intra-layer bonds between neighboring atoms are strong, mostly of covalent type, while inter-layer bonds are week, mostly of van der Waals type. Correspondingly, intra-layer B–N bonds are significantly shorter than that of inter-layer B–N bonds. Bonding in h-BN is with a small ionic deal related to opposite signs of effective charges possessed by the constituent B and N atoms – positive and negative, respectively.

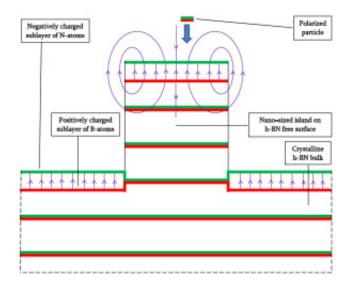


Fig. 1. Schematic view of the cross section of h-BN crystal with nano-sized islands on the free flat surface.

Character of bonding determines the reconstruction that takes place in the free surface layer – B and N atoms can be rather easily displaced in opposite directions perpendicular to the initial layer. Thus, surface reconstruction in h-BN involves splitting the surface layer into two sublayers, which consists of atoms with positive and negative effective charges. It implies the formation of an ultrathin dipole layer at the free surface.

Static dipole layer has to induce the corresponding static electric field, which in the limit of an ideally flat infinitive crystalline surface, is concentrated between sublayers. This makes flat h-BN surfaces practically non-reactive with environment. But, if the material is nanostructured – consists of nano-sized particles, grains, pores, etc. – there is also expected the emergence of a near-surface electric field of significance strength. This novel nano-effect explains high physical

1/2



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reactivity frequently revealed by the nanostructured h-BN: due to non-zero near-surface field it can polarize and attract various particles from the environment. In particular, nanoporous boron nitride fibers are found to be an effective material capturing large non-polar molecules of organic pollutants from aqueous solutions.

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2/2