Nanoscale Physics

Near-surface electric field of nanoparticles of binary compounds with layered structure

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The theoretical studies show (see e.g. [1]) that, surface reconstruction in a binary compound with a layered structure is to split the surface atomic layer into two: upper and lower sublayers consist of atoms with negative and positive effective charges, respectively. Their values can be evaluated semiempirically based on measurable parameters [2]. It was also demonstrated that, particles of a powdered binary compound with a layered structure are almost disk-shaped [3].

We have calculated the potential distribution function $\varphi = \varphi(z)$, z is the distance from the surface, for the near-surface electric field induced by such dipole layer at the surface of a disc-shaped particle of a layered binary compound:

$$\varphi(z) = -\varphi_0\left(1 - \frac{z}{\sqrt{R^2 + z^2}}\right), \quad \varphi_0 = -\varphi(0) = \frac{NeqH}{2\varepsilon_0 S},$$

where N is the number of atomic pairs in the surface elemental unit cell, S is the 2D-cell area, q is the effective charge number of constituent atoms (i.e. their effective charges are $\pm qe$), H is the dipole layer thickness, φ_0 is the depth of the near-surface potential well, and R is the particle radius. It is clear that due to the existence of near-surface electric field, a powder of a layered binary compound can easily adsorb positive ions from the environment, as well as polarize it.

Suggested mechanism of inducing the near-surface electric field is true nano-scale effect because at the limit of infinite surface, $R \to \infty$, potential function tend to the constant, $\varphi(z) \to -\varphi_0$, i.e. electric field strength vanishes.

1. *Slotman G. J., Fasolino A.* Structure, stability and defects of single layer hexagonal BN in comparison to graphene // J Phys Condensed Matter, – 2013. **– 25**, – N 045009.
2. *Chkhartishvili L. S., Dekanosidze Sh. V., Naisuradze N.I.* Estimation of atomic charges in polar crystals // Trends Mod Sci. – 2014, **– 23**, – P. 51-54.
3. *Chkhartishvili L.* Correlation between surface specific area and particles average size: Hexagonal boron nitride nano-powders // Nano Studies. – 2012, **– 6**, – P. 65-76.