Two-Dimensional Boron-Nitride Layers as Flexoelectric Nanogenerators

I. NAUMOV, A. BRATKOVSKY, Hewlett-Packard Labs, Palo Alto, V. RANJAN, North Carolina State U, Raleigh — The direct conversion of ambient motion into electrical energy, especially at nanoscale, is fundamental and technological challenge. Boron-Nitride non-centrosymmetric monolayers are piezoelectrics that can sustain much larger structural and produce very large (a few Volts) voltage drop across flexed nanostrips. We show, with the use of ab-initio calculations, the existence of giant nonlinear flexoelectric effect in BN 2D strips. The induced polarization is quadratic in amplitude of atomic displacements \( A \), yet the dipole moment per unit cell is about four times larger compared to PbZrTiO3 [1]. The resulting voltage drop across the BN nanostrip is set by bandgap in material \( E_g/q \sim 5 \text{ Volts} \) and nearly independent of the strip width. The large voltage produced by this inert bio-compatible material may find a variety of applications and, in particular, as nanogenerators and sensors powered by an ambient motion or agitation. Prior alternatives, like ZnO, GaN and CdS, are leaky, generate much smaller voltage, and impractical [2]. [1] I.Naumov, A.Bratkovsky, V.Ranjan, arXiv:0810.1775 (2008). [2] Y. Qin, X. Wang, Z.L. Wang, Nature 451, 809 (2008); M.A. Schubert et al, Appl. Phys. Lett. 316, 122904 (2008)