Spin-Current Control by Induced Electric-Polarization Reversal in Ni/hBN/Ni Magnetic Tunnel Junction: A Cross-Correlation Materials

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In a typical magnetic tunnel junction (MTJ), resistance is controlled by the magnetic alignment of upper and lower ferromagnetic materials. Anti-parallel (parallel) configuration of upper and lower ferromagnetic materials gives high (low) resistance. Here, we propose additional degree of freedom on MTJ. Within anti-parallel configuration (APC), spin-filtering effect occurs depending on the polarization of the insulator layer.

We considered an ab-initio study of MTJ consisting of hexagonal boron nitride (hBN) sandwiched between Ni(111) layers. A maximum of two pd-hybridization bonds stabilized the structure, with APC proving to be the most favorable magnetic alignment, in line with the results of previous experimental studies [1]. Within two pd-hybridizations structure, there are asymmetric and symmetric stacking arrangement with total energy difference ≈ 33 meV where the former has lower energy. In the case of symmetric stacking arrangement, our transmission probability result shows a typical functionality of magnetic tunnel junction. Meanwhile, in the asymmetric stacking arrangement, a structural deformation from a flat hBN plane to a rugged hBN plane occurs. The buckling direction is two-fold and can be tuned by applying an external electric field. When the buckling direction is switched, the induced dipole moment in the hBN layer is also switched to have a reversed dipole. On the other hand, an induced magnetic moment at an N site appears when the structural deformation leading N to move closer to one of the Ni atoms. Interestingly, the magnetic moment direction is switched by the position of the N layer in the resulting bi-stable state with electrical polarization when APC is chosen. The transmission probability calculation of asymmetric stacking arrangement exhibits a spin-filtering effect where the spin-polarized current is controlled by the electric field when a field-induced reversal of the polarization is realized.

![Figure 1: Transmission probability for symmetric stacking arrangement (a), asymmetric stacking arrangement (b,c,d) (right)](image)

References:
