Switching of Magnetocrystalline Anisotropy of a Single Layer Cobalt Film by Graphene

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Abstract
Two-dimensional graphene has demonstrated outstanding physical properties such as exceptional electrical, thermal, and mechanical properties [1,2], but also very long spin diffusion lengths at room temperature [3–7]. This offers an unprecedented platform for the advent of lateral spintronics. For instance, graphene interfaced with insulators/semiconductors (SiC, SiO_2, Al_2O_3), magnetic insulator EuO [8,9], and magnetic metals have been intensively studied in recent years. Among many interesting phenomena which have been recently proposed for graphene/magnetic metal interfaces, perpendicular magnetic anisotropy (PMA) has been attracting much attention in a view of its general interest for spintronics. In particular, PMA has been reported in Co/graphene interface [10]. However, a single layer of Co film, either free standing or on substrates (e.g. Pt, Au, etc.), persists in-plane anisotropy and switching it to the out-of-plane one is a big challenge. In this work, we report graphene proximity induced switching of magnetocrystalline anisotropy of single layer Co film from the in-plane to out-of-plane orientation with a large PMA value comparable to thicker Co films.

The calculations were performed in two steps using Vienna Ab-Initio Simulation Package (VASP), which is based on density functional theory with generalized gradient approximation (PBE), for the exchange correlation potential and projector augmented wave based pseudopotentials [11]. First, the structures are relaxed with no spin-orbit interaction taken into account for determining the most favorable adsorption geometry of graphene on Co. Then the spin-orbit coupling was included and the total energy of the system was determined as a function of the orientation of the magnetic moments. The 19×19×1 *k*-point mesh was used in all calculations and the energy cutoff was set to 520 eV. The atomic structures were relaxed until the forces were smaller than 1 meV/Å. For the anisotropy calculations, the total energies were converged to with precision of 10^{-7} eV.

First, the magnetocrystalline anisotropy of a free standing Co layer was calculated and found to be about -2.17 mJ/m^2 favoring in-plane anisotropy. Next, we optimized one Co single layer on graphene sheet. Two high symmetric structures are considered: BC stacking (Co sitting on the center of hexagonal cell of graphene) and AB stacking (Co is placed on top of carbon atoms). We found that BC stacking is a semi-stable phase and it preserves the in-plane anisotropy with a bit larger absolute value of 2.23 mJ/m^2. Interestingly, for the stable phase of AB stacking the anisotropy switches to out-of-plane direction with a value of 1.43 mJ/m^2, which is comparable to thicker Co films. We find that the hybridization between C-p_z and Co-d_Z2 plays the crucial role in switching the anisotropy of Co film. At the same time, the Dirac point of graphene is also modified by Co presence.

This work is supported by EU Future Emerging Technology Flagship "Graphene" and ANR NMGEM.

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