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, SiO2, Al2O3), 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 10⁻⁵ eV.

First, the magnetocrystalline anisotropy of a free standing Co layer was calculated and found to be about -2.17 mJ/m² 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/m². Interestingly, for the stable phase of AB stacking the anisotropy switches to out-of-plane direction with a value of 1.43 mJ/m², which is comparable to thicker Co films. We find that the hybridization between C-p and Co-d₂ 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.

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References