Magnetic Anisotropy of FeCo Thin Films with B, C and N

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Modern science has reached the ultimate level of monoatomic layers in the race for miniaturization of electronic devices, and the limit of about twenty atomic monolayers for magnetic tunnel junctions with perpendicular magnetic anisotropy [1, 2]. Layered systems are particularly interesting for their ability to tune effective material parameters such as the magnetic anisotropy energy (MAE). Among such systems, iron-based layered systems are of considerable interest. An intriguing and important topic from the point of view of applications is the influence of the crystallographic structure of Fe, its thickness, and the presence of other layers above and below the Fe layer on magnetic parameters such as the MAE of the studied system.

Here we present a theoretical investigation of the magnetic anisotropy of FeCo thin films with B, C and N dopants located in octahedral interstitial positions. The theoretical study is based on calculations using the full-potential local-orbital electronic structure code FPLO [3] and the generalized gradient approximation. The chemical disorder in FeCo layers was modeled using the virtual crystal approximation. The layer structures were subjected to geometry optimization of interlayer distances and vicinity region of the dopant sites. We determined the local magnetic moments and excess charge at each position in the films. We identified the effect of dopant atoms on the magnetic properties of the FeCo films such as magnetization and magnetic anisotropy.

References:

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