Features of voltage-driven magnetic anisotropy in tunnel magnetic tunnel junctions

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1. Introduction

Magnetic tunnel junctions (MTJs) represent a key building block of modern spintronic devices, with their performance critically determined by the inter-play between interfacial properties and magnetic anisotropy. A promising route toward low-power control of magnetization is the utilization of voltage-tcontrolled magnetic anisotropy (VCMA), where an applied electric field modifies the orbital hybridization at the ferromagnet/insulator interface. In this twork, we investigate VCMA effects in MTJs based on 3d transition metals, with particular attention to CoFeB/MgO and related systems. The study combines experimental observations with theoretical modeling of spin-dependent charge redistribution at the metal–oxide interface. Applying a gate voltage across the junction modifies the occupancy of 3d orbitals, thereby tuning perpendicular magnetic anisotropy (PMA). The mechanism is linked to the modulation of Fe and Co d-states hybridized with oxygen p-orbitals in the MgO barrier. As a result, voltage control provides a reversible and ener-gy-efficient method of manipulating the easy axis of magnetization without the need for large spin-polarized currents. Our results reveal a significant anisotropy change, on the order of tens of μJ/m² per volt, which is comparable to or larger than spin-transfer torque switching thresholds in nanoscale devices. We further show that the effect strongly depends on interface quality, crystalline ordering of the oxide barrier, and the choice of the 3d ferro-magnet. First-principles calculations support the experimental findings and indicate that the interfacial electronic structure plays a dominant role in de-termining the voltage response. This study highlights the potential of voltage-controlled anisotropy as a scalable pathway for spintronic applications, including non-volatile magnetic memory and logic architectures. By reducing energy consumption while maintaining fast switching speeds, VCMA in 3d-metal-based MTJs offers a viable approach toward next-generation low-power spintronic devices.

2. The crystalline spin-orbit-induced magnetic anisotropy energy

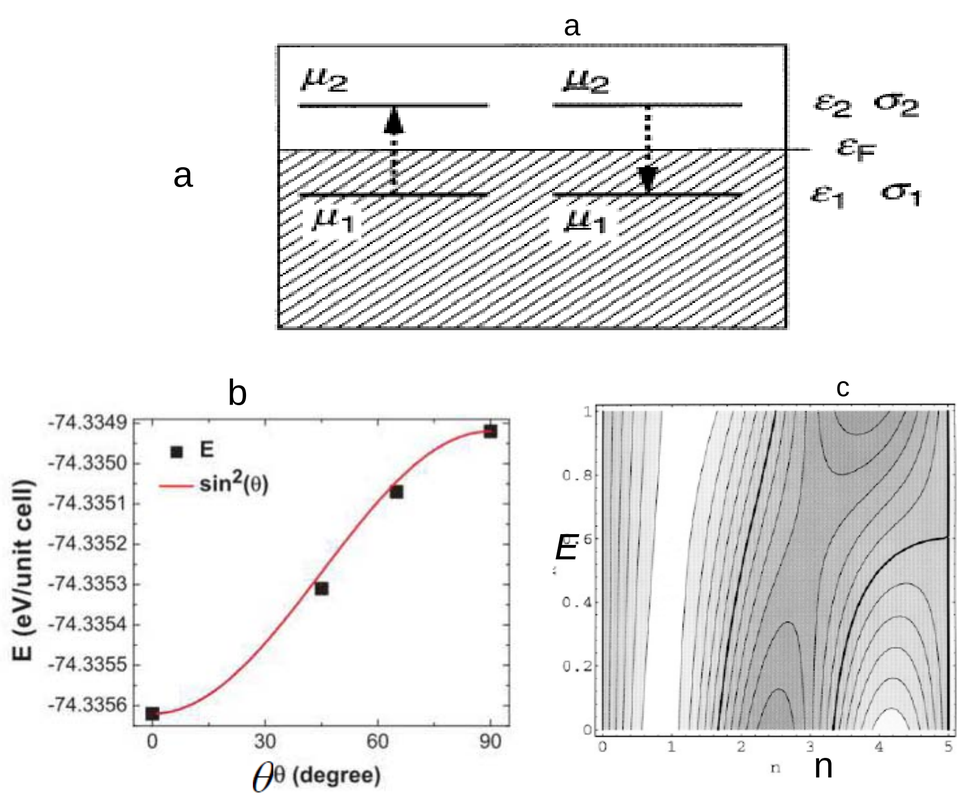

Figure 1. (a) Graphical representation of the second-order contribution to the MAE due to virtual excitations from a degenerate occupied level with spin σ_1 and orbital characters μ_1 and μ_1 to an unoccupied level with spin σ_2 and orbital characters μ_2 μ_2. (b) Angular dependence of the magnetic energy. (c) The dependence of MAE as function of the *d*-band filling, *n* .

The magnetocrystalline anisotropy of ferromagnetic nanolayers is related to the relativistic spin-orbit coupling, in which the spin moment of the electron interacts with the magnetic field of the orbital motion of the electron around atomic nuclei. This on the scale of the crystal lattice, leads to the effect of dominant directions of magne-tization, which correspond to stable states with minimum energy. Spin-orbit coupling acts as a “link” between the spin orientation and the spatial orientation of the orbital wave function. If a *d*-orbital is partially occupied, the electron energy depends on the direction of its spin relative to the crystal axes. This creates an energy difference between different magnetization directions that is exactly the origin of magnetic anisotropy. In the studied magnetic tunnel junctions based on 3-*d* transition metals, the magnetic properties are determined by the electronic structure of 3-*d* orbital for-med by the splitting in the crystal field of the five-fold degenerate electron *d*- state. Taking into account the determined influence of such magnetic orbital within the framework of the microscopic tight-binding model it is possible to analytically des-cribe the features of the magneto-crystalline energy anisotropy.

$$E = -\xi^2 \sum_{\sigma^i,\sigma^j} \sum_{\nu;i,j=1,2} A(\nu,\sigma^i,\sigma^j) \left\langle \mu'_1,\sigma^i \left| \boldsymbol{L}\cdot\boldsymbol{S} \right| \mu'_2,\sigma^j \right\rangle \left\langle \mu_2,\sigma^j \left| \boldsymbol{L}\cdot\boldsymbol{S} \right| \mu_1,\sigma^i \right\rangle \qquad (1)$$

$\nu = \mu_1,\mu_2,\mu'_1,\mu'_2$ $\sigma^{1(2)} = \uparrow(\downarrow)$, coefficient $A(\nu,\sigma^i,\sigma^j)$i *i*s the electron density functional, where

$$A(\nu,\sigma^i,\sigma^j) = (-1)^{i-j} \int_{\varepsilon_1<\varepsilon_F<\varepsilon_2} \frac{d\varepsilon_1 d\varepsilon_2}{\varepsilon_2-\varepsilon_1} \sum_{\boldsymbol{k}} n_{\mu_1,\mu'_1,\sigma_1}(\boldsymbol{k},\varepsilon) n_{\mu_2,\mu'_2,\sigma_2}(\boldsymbol{k},\varepsilon)$$

Here $L\cdot S$ is the operator of spin-orbit interaction. Here the spatial orbital states de-dermines the magnetocrystalline anisotropy energy the investigated nanostructures..

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3. Influence of electric field on magnetic anisotropy

The influence of the electric field on the perpendicular magnetic anisotropy energy (MAE) and consequently on the magnetization anisotropy is associated with the redis-tribution of electric change among the *3d* orbitals, in particular, related to the spin de-pendent electric field-induced screen effect and the hybridization *d*-orbital with the 2*p*-orbital of the tunnel metallooxcide barrier (in particular, MgO). This is qualitatively is detemined by the spin-orbit interaction,

$$E_{\mathrm{MAE}} = \xi^2 \sum_{i,j;\sigma,\sigma'} \frac{\left|\left\langle j \mid L_Z \mid i \right\rangle\right|^2 - \left|\left\langle j \mid L_x \mid i \right\rangle\right|^2}{\varepsilon_j^{\sigma'} - \varepsilon_i^{o}} \qquad (2)$$

where $|i>$ and $|j>$ are unperturbed wave functions for occupied and unoccupied tates ,ε_i^{σ} and $\varepsilon_j^{\sigma'}$ are corresponding energies.of for σ and σ' spin states. The magni-tude of the perpendicular magnetic anisotropy is determined by the energy zones formed by 3*d* orbitals and depends on their filling . The electron band structure of a ferromagnetic nanolayer in a crystal field undergoes splitting in a tetragonal crystal field at the interface, FeCo|MgO (Fig. 2a, left). In the framework of this simple model, non-monotonic dependence of MAE on the orbital filling has been demonstrated (Fig. 2b left). An estimate of the MAE on the electric field applied to the magnetic tun-nel junction also been obtained (Fig. 2a,b right).

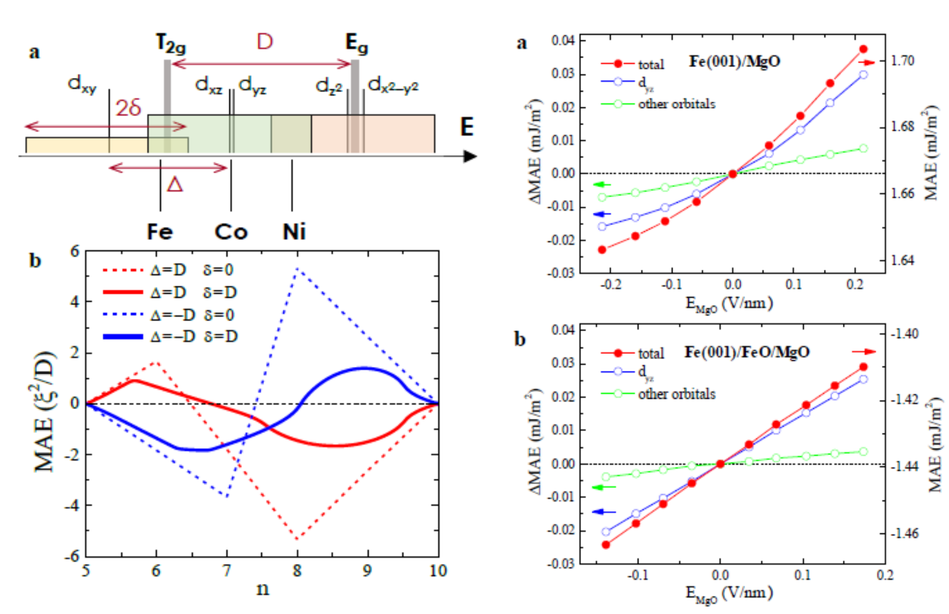

Figure. 2. left (a) Schematic of the minority 3*d* orbital splitting by the crystal field of tetragonal symmetry. Broadening of the orbital levels mimics the energy bands. The vertical black dotted lines represent the Fermi energies of Fe, Co and Ni. (b) MAE as a function of orbital band filling n, for different values of the T2g level splitting Δ and broadening δ,. Right, voltage dependences of MAE: (a) Fe(001)/MgO and (b) Fe(001)/FeO/MgO *in* MgO (red curves) and E-field induced changes in the orbital contribution to MAE (green and blue curves). .