Exchange Bias(EB): II.FM Partial Wall Models

Detian Yang

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Outline

1. **Semiclassical Justification of the phenomenological free energy formula**

   R L Stamps 2000 J. Phys. D: Appl. Phys. ***33*** *R247*

2. **FM Partial (Incomplete) Domain Wall Model**

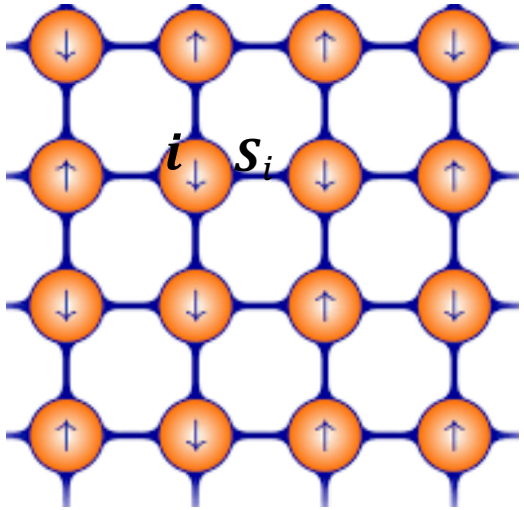
   M. Kiwi, J. Mejia-Lopez, R. D. Portugal and R. Ramirez, Europhys. Lett., 48 (5), pp. 573-579 (1999)
   M. Kiwi et al. / Solid State Communications 116 (2000) 315–319
   M.Kiwi et al. Appl. Phys. Lett. ***75****, 3995 (1999)*
   J. Mejia-Lopez et al. Journal of Magnetism and Magnetic Materials 241 (2002) 364–370

Spin Vector Array Model(SVAM) $E_{\text{inter}} = -\boldsymbol{H}Mt_{\text{f}}\cdot\boldsymbol{f}+J_1\boldsymbol{f}\cdot\boldsymbol{a}+J_2(\boldsymbol{f}\cdot\boldsymbol{a})^2+\sigma(1-\boldsymbol{a}\cdot\boldsymbol{n}_{\text{af}})$

(1) Magnetic moments are represented by an array of classical spin vectors $\boldsymbol{S}_i$

(2) *Lattice structure is taken as simple cubic*

(3) Equilibrium configurations are found by numerically integrating torque equations using a relaxation method: find **zero torque configurations** by numerically integrating the ***Landau–Lifshitz equations*** of motion for each spin



Landau–Lifshitz equations

$$\frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{S}_i = -\gamma\boldsymbol{S}_i\times\nabla_{\boldsymbol{S}_i}\mathcal{H}+\lambda\boldsymbol{S}_i\times\boldsymbol{S}_i\times\nabla_{\boldsymbol{S}_i}\mathcal{H}$$

$$\mathcal{H} = \sum_{i,j}^{N} J_{i,j}\boldsymbol{S}_i\cdot\boldsymbol{S}_j + \sum_{i}^{N}\left[-g\mu_{\text{B}}\boldsymbol{H}\cdot\boldsymbol{S}_i + K_i\left(\boldsymbol{S}_i\cdot\hat{\boldsymbol{n}}_{\text{af}}\right)^2\right]$$

Kim J-V, Wee L, Stamps R L and Street R 1999 *IEEE Trans. Magn.* **35** 2994–7

L. Wee, R. L. Stamps, and R. E. Camley ,Journal of Applied Physics **89**, 6913 (2001)

Semiclassical Justification of the Phenomenological Model

Goal: **Under a series of acceptable assumptions, SVAM is equivalent to phenomenological model**

(1) Justify the existence of biquadratic term, i.e. $J_2 \neq 0$

(2) Uncompensated interface: $J_1 \gg J_2$, while compensated interface: $J_1 = 0, J_2 \neq 0$

(3) Suggest the potential existence of FM partial wall

$$E_{\text{inter}} = -\boldsymbol{H} M t_{\text{f}} \cdot \boldsymbol{f} + J_1 \boldsymbol{f} \cdot \boldsymbol{a} + J_2 (\boldsymbol{f} \cdot \boldsymbol{a})^2 + \sigma (1 - \boldsymbol{a} \cdot \boldsymbol{n}_{\text{af}})$$

R.L. Stamps, J. Phys. D: Appl. Phys. 33 (2000) R247

Semiclassical Justification of the Phenomenal Model

$$E = E_{\mathrm{f}} + E_{\mathrm{af}} + E_{\mathrm{inter}}.$$

$$E_{\mathrm{f}} = \sum_{i \in \mathrm{ferro}} \left[-\boldsymbol{H} \cdot \boldsymbol{f}_i - \sum_{\langle i,j \rangle} J_{i,j} \boldsymbol{f}_i \cdot \boldsymbol{f}_j - K_i \left(\boldsymbol{f}_i \cdot \hat{\boldsymbol{n}}_{\mathrm{f}} \right)^2 \right]$$

$$E_{\mathrm{af}} = \sum_{i \in \mathrm{antiferro}} \left[-\boldsymbol{H} \cdot (\boldsymbol{a}_i + \boldsymbol{b}_i + \sum_{\langle i,j \rangle} J_{i,j} \boldsymbol{a}_i \cdot \boldsymbol{b}_j - K_i \times \left[\left(\boldsymbol{a}_i \cdot \hat{\boldsymbol{n}}_{\mathrm{af}} \right)^2 + \left(\boldsymbol{b}_i \cdot \hat{\boldsymbol{n}}_{\mathrm{af}} \right)^2 \right] \right]$$

$$E_{\mathrm{inter}} = \sum_{i,j \in \mathrm{interface}} J_{\mathrm{a}} \boldsymbol{f}_i \cdot \boldsymbol{a}_j - \sum_{\langle i,j \rangle} J_{\mathrm{b}} \boldsymbol{f}_i \cdot \boldsymbol{b}_j .$$

f_i: lattice vectors of FM; a_i, b_i: lattice vectors of AFM;
$\hat{n}_f$, $\hat{n}_{af}$: unit vectors of anisotropy easy axis of FM and AFM;

$$\boldsymbol{l}_i = \boldsymbol{a}_i + \boldsymbol{b}_i$$
$$\boldsymbol{t}_i = \boldsymbol{a}_i - \boldsymbol{b}_i .$$

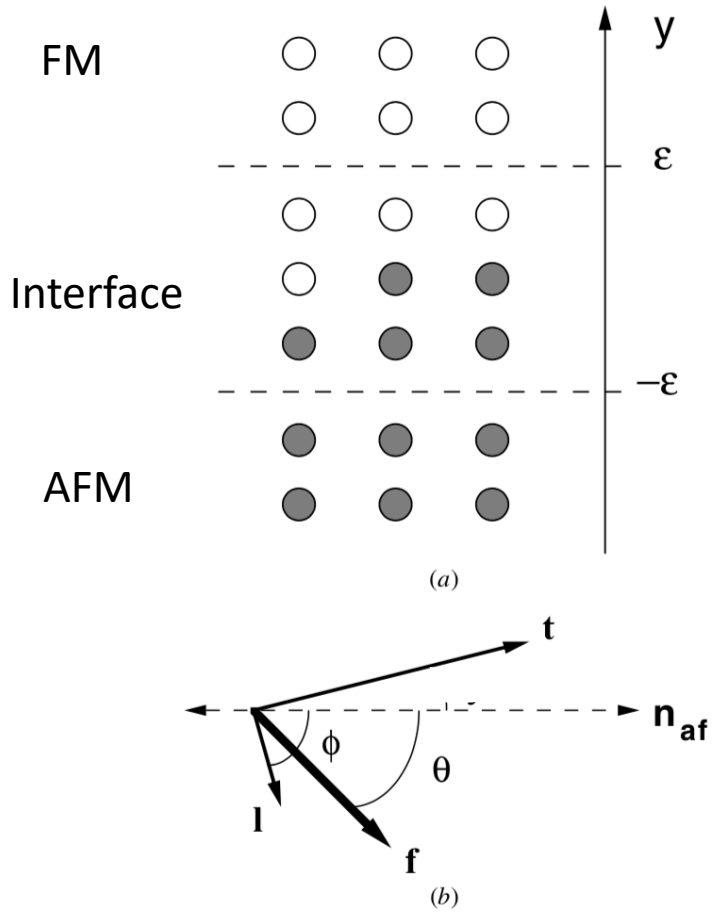
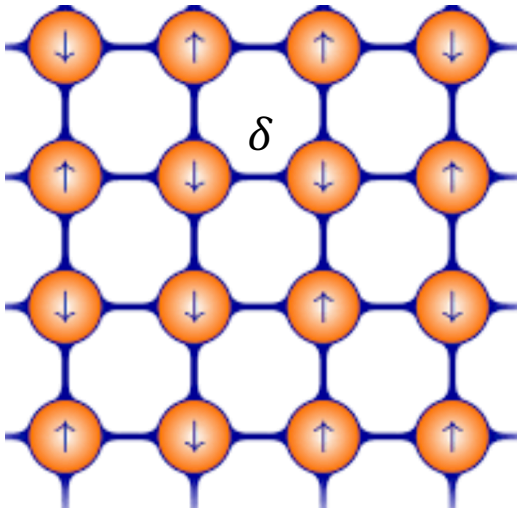


Figure 19. Geometry. The interface region is sketched in (*a*). The antiferromagnet is in the $y < \epsilon$ half space, and the ferromagnet is in the $y > \epsilon$ half space. The interface region contains magnetic moments from each material and the boundaries are defined to intercept only exchange couplings between like moments. In (*b*), the angles θ, ϕ, and ξ are defined, specifying the transformed magnetizations. The angles are functions of position, y.

Assumptions: (1)) $F(\vec{x})$ change slowly over lattice spacing length scales

(2) $F(\vec{x}) = F(y)$

(3) Nearest coordination neighbors



$$F(\vec{x}+\vec{\delta}) \approx F(\vec{x}) + \vec{\delta}\cdot\nabla F(\vec{x}) + \frac{1}{2}\left(\vec{\delta}\cdot\nabla\right)^2 F(\vec{x}) \ , \quad F = \vec{f}_i, \vec{l}_i, \vec{t}_i$$

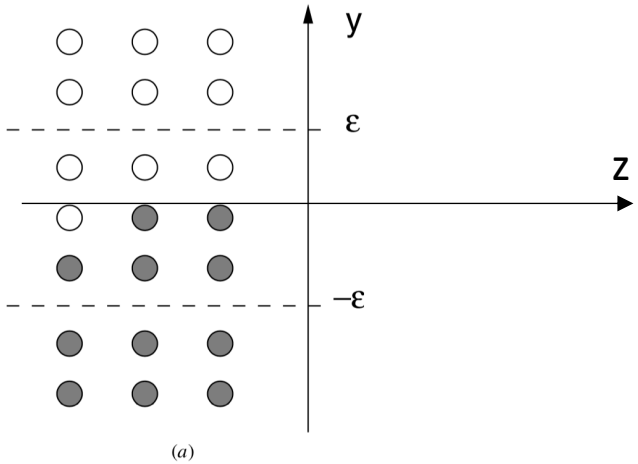
$$\mathcal{E}_{\text{inter}} = 2\epsilon\left[J_+ \boldsymbol{f}\cdot\boldsymbol{l} + J_- \boldsymbol{f}\cdot\boldsymbol{t}\right]$$

$$\mathcal{E}_{\text{f}} = \int_{\epsilon}^{\infty}\left[-\boldsymbol{H}\cdot\boldsymbol{f} - K_{\text{f}}\,(\boldsymbol{f}\cdot\boldsymbol{n}_{\text{f}})^2 - \boldsymbol{f}\cdot D_{\text{f}}\frac{\partial^2}{\partial y^2}\boldsymbol{f}\right]\mathrm{d}y$$

$$\mathcal{E}_{\text{af}} = \int_{-\infty}^{-\epsilon}\Bigg[-\boldsymbol{H}\cdot\boldsymbol{l} - K_{\text{af}}\left[(\boldsymbol{l}\cdot\boldsymbol{n}_{\text{af}})^2 + (\boldsymbol{t}\cdot\boldsymbol{n}_{\text{af}})^2\right] + D_{\text{af}}\left(\boldsymbol{t}\cdot\frac{\partial^2}{\partial y^2}\boldsymbol{t} - \boldsymbol{l}\cdot\frac{\partial^2}{\partial y^2}\boldsymbol{l}\right)\Bigg]\mathrm{d}y.$$

$$D_f = z_f\, J_f\, \delta^2/2,$$

$$D_{af} = z_{af}\, J_{af}\, \delta^2/2$$



$$\mathcal{E}_{inter} = 2\epsilon\left[J_+\vec{f}\cdot\vec{l} + J_-\vec{f}\cdot\vec{t}\right]$$

$$J_\pm = \frac{1}{4}(J_a \pm J_b)$$

$$\boldsymbol{l}_i = \boldsymbol{a}_i + \boldsymbol{b}_i$$
$$\boldsymbol{t}_i = \boldsymbol{a}_i - \boldsymbol{b}_i.$$

Minimizing $\mathcal{E} = \mathcal{E}_f + \mathcal{E}_{af} + \mathcal{E}_{inter}$ by considering variations of $\vec{f}$, $\vec{l}$ and $\vec{t}$ with constraints $|\vec{f}| = |\vec{a}| = |\vec{b}| = 1$, i.e., $|\vec{f}| = 1$, $l^2 + t^2 = 2$

$$|\boldsymbol{l}| = \sqrt{2}\cos\xi \qquad |\boldsymbol{t}| = \sqrt{2}\sin\xi$$

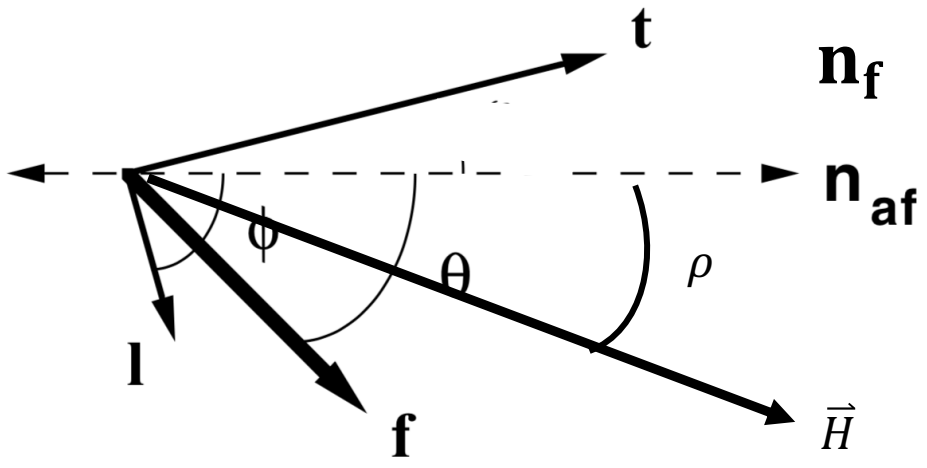
D_{af} is large and so AFM two sublattice magnetizations remain nearly antiparallel

$\vec{l}$ is small and ξ approaches to $\frac{\pi}{2}$. Define $\beta = \frac{\pi}{2} - \xi$, $\beta \ll 1$

$$\mathcal{E} \approx \int_{\epsilon}^{+\infty}\left[-HM_f\cos(\theta-\rho) + D_f{\theta_y}^2 + K_f cos^2\theta\right]dy$$
$$+\int_{-\infty}^{\epsilon}\left[-HM_{af}\beta\cos(\phi-\rho) + 2D_{af}(1-2\beta^2)({\beta_y}^2 - {\phi_y}^2) - 2K_{af}(\beta^2 cos^2\phi + (1-\beta^2)sin^2\phi)\right]dy$$
$$+\sqrt{2}\epsilon[J_+\beta_0\cos(\theta_0-\phi_0) - J_-(1-\tfrac{1}{2}{\beta_0}^2)\sin(\theta_0-\phi_0)]$$

where $\theta_0, \phi_0, \beta_0$ denotes the values at $y = 0$

$$\frac{\delta\mathcal{E}}{\delta\theta} = \frac{\delta\mathcal{E}}{\delta\beta} = \frac{\delta\mathcal{E}}{\delta\phi} = 0$$



AFM ($\vec{l}(y)$)	Direction: $\frac{\delta\mathcal{E}}{\delta\phi} = 0$	Magnitude: $\frac{\delta\mathcal{E}}{\delta\beta} = 0$
Equations	$4D_{\mathrm{af}}\left(2\beta^2-1\right)\phi_{yy} + 16D_{\mathrm{af}}\beta\beta_y - \sqrt{2}\beta H M_{af}\sin(\phi-\rho)$ $-2K_{\mathrm{af}}\left(1-2\beta^2\right)\sin(2\phi) = 0.$	$4D_{\mathrm{af}}\left(2\beta^2-1\right)\beta_{yy} + 8D_{\mathrm{af}}\beta\beta_y^2 - \sqrt{2}HM_{af}\cos(\phi-\rho)$ $-4K_{\mathrm{af}}\beta\cos(2\phi) = 0$
Boundary Condition at $y = 0$	$4D_{\mathrm{af}}\left(2\beta_0^2-1\right)\phi_y(0) + \sqrt{2}\epsilon\left[J_+\beta_0\sin(\theta_0-\phi_0)\right.$ $\left.+J_-\left(1-\frac{1}{2}\beta^2\right)\cos(\theta_0-\phi_0)\right] = 0.$	$4D_{\mathrm{af}}\left(2\beta_0^2-1\right)\beta_y(0) - \sqrt{2}\epsilon$ $\times\left[J_+\cos(\theta_0-\phi_0) + J_-\beta_0\sin(\theta_0-\phi_0)\right] = 0.$

FM: neglecting any deformation of the ferromagnet order($\theta_y = 0$) and FM anisotropy($K_f = 0$)

$$x_{yy} = \frac{\partial^2 x}{\partial y^2}$$

$$\frac{\delta\mathcal{E}}{\delta\theta} = 0$$

$$\mathcal{E}_{\mathrm{f}} = -HMt_{\mathrm{f}}\cos(\theta-\rho).$$

$$HMt_{\mathrm{f}}\sin(\theta_0-\rho) - 2\sqrt{2}\epsilon \times\left[J_+\beta_0\sin(\theta_0-\phi_0) + J_-\cos(\theta_0-\phi_0)\right] = 0.$$

$$\mathcal{E} \approx \int_{\epsilon}^{+\infty}\left[-HM_f\cos(\theta-\rho) + D_f{\theta_y}^2 + K_f\cos^2\theta\right]dy + \int_{-\infty}^{\epsilon}\left[-HM_{af}\beta\cos(\phi-\rho) + 2D_{af}(1-2\beta^2)({\beta_y}^2-{\phi_y}^2) - 2K_{af}(\beta^2\cos^2\phi + (1-\beta^2)\sin^2\phi)\right]dy + \sqrt{2}\epsilon\left[J_+\beta_0\cos(\theta_0-\phi_0) - J_-(1-\frac{1}{2}{\beta_0}^2)\sin(\theta_0-\phi_0)\right]$$

Interface Exchange Energy

$$E_{\text{inter}} = -HMt_{\text{f}}\cdot f + J_1 f\cdot a + J_2 (f\cdot a)^2 + \sigma(1 - a\cdot n_{\text{af}})$$

Assumptions: (1) canting of the antiferromagnet at the interface is small $(\beta, \beta_y, \phi \ll 1)$
(2)there is no significant twist in the ferromagnet

$$\beta = C_{\pm}\exp(\pm\Delta y)$$

FM: neglecting any deformation of the ferromagnet order($\theta_y = 0$) and FM anisotropy($K_f = 0$)

$$\frac{\delta\mathcal{E}}{\delta\theta} = 0$$

$$\mathcal{E}_{\text{f}} = -HMt_{\text{f}}\cos(\theta - \rho).$$

$$\boxed{HMt_{\text{f}}\sin(\theta_0 - \rho) - 2\sqrt{2}\epsilon \times \left[J_+\beta_0\sin(\theta_0 - \phi_0) + J_-\cos(\theta_0 - \phi_0)\right] = 0.}$$

AFM ($\vec{l}(y)$)	Direction: $\frac{\delta\mathcal{E}}{\delta\phi} = 0$	Magnitude: $\frac{\delta\mathcal{E}}{\delta\beta} = 0$
Equations	$4D_{\text{af}}(2\beta^2 - 1)\phi_{yy} + 16D_{\text{af}}\beta\beta_y - \sqrt{2}\beta HM_{\text{f}}\sin(\phi - \rho) - 2K_{\text{af}}(1 - 2\beta^2)\sin(2\phi) = 0.$	$4D_{\text{af}}(2\beta^2 - 1)\beta_{yy} + 8D_{\text{af}}\beta\beta_y^2 - \sqrt{2}HM_{\text{f}}\cos(\phi - \rho) - 4K_{\text{af}}\beta\cos(2\phi) = 0$
Boundary Condition at $y = 0$	$4D_{\text{af}}(2\beta_0^2 - 1)\phi_y(0) + \sqrt{2}\epsilon\left[J_+\beta_0\sin(\theta_0 - \phi_0) + J_-(1 - \frac{1}{2}\beta^2)\cos(\theta_0 - \phi_0)\right] = 0.$	$4D_{\text{af}}(2\beta_0^2 - 1)\beta_y(0) - \sqrt{2}\epsilon \times \left[J_+\cos(\theta_0 - \phi_0) + J_-\beta_0\sin(\theta_0 - \phi_0)\right] = 0$

$$\boldsymbol{\beta = Ce^{\Delta y}}$$

$$\Delta = \sqrt{\frac{K_{\text{af}}}{D_{\text{af}}}\cos(2\phi_0)} \approx \sqrt{\frac{K_{\text{af}}}{D_{\text{af}}}}$$

$$C = -\frac{J_+\cos(\theta_0 - \phi_0)}{\sigma_\beta + J_-\sin(\theta_0 - \phi_0)} = -\frac{J_+\cos(\theta_0 - \phi_0)}{\sigma_\beta}\left[\frac{1}{1 + \frac{J_-\sin(\theta_0 - \phi_0)}{\sigma_\beta}}\right]$$

$$= \boxed{-\frac{J_+\cos(\theta_0 - \phi_0)}{\sigma_\beta}}\left[1 - \frac{J_-\sin(\theta_0 - \phi_0)}{\sigma_\beta} + \left(\frac{J_-\sin(\theta_0 - \phi_0)}{\sigma_\beta}\right)^2 - \left(\frac{J_-\sin(\theta_0 - \phi_0)}{\sigma_\beta}\right)^3 + \cdots\right]$$

$$C = -\frac{J_+\cos(\theta_0 - \phi_0)}{\sigma_\beta + J_-\sin(\theta_0 - \phi_0)}$$

$$\sigma_\beta = 4\sqrt{K_{\text{af}}D_{\text{af}}}/\sqrt{2}.$$

$\frac{J_-}{\sigma_\beta} \ll 1$ **(interlayer exchange relatively weak)**

Boundary Condition at $y = 0$

$$HMt_{\text{f}}\sin(\theta_0 - \rho) - \theta_-\sin(\theta_0 + \alpha_0) - \frac{\theta_+^2}{\sigma_{\text{a}}}\sin(\theta_0 + \alpha_0)\cos(\theta_0 + \alpha_0) = 0.$$

Where $\alpha = -\phi$; $\sigma_a = 2\sqrt{2}\sigma_b$;
$\theta_\pm = 2\sqrt{2}\epsilon J_\pm$

$$E_{\text{inter}} = -\boldsymbol{H} M t_{\text{f}} \cdot \boldsymbol{f} + J_1 \boldsymbol{f} \cdot \boldsymbol{a} + J_2 (\boldsymbol{f} \cdot \boldsymbol{a})^2 + \sigma (1 - \boldsymbol{a} \cdot \boldsymbol{n}_{\text{af}})$$

AFM ($\vec{l}(y)$)	Direction: $\frac{\delta\varepsilon}{\delta\phi} = 0$	Magnitude: $\frac{\delta\varepsilon}{\delta\beta} = 0$
Equations	$4D_{\text{af}}\left(2\beta^2 - 1\right)\phi_{yy} + 16D_{\text{af}}\beta\beta_y - \sqrt{2}\beta H M_{\text{f}}\sin(\phi - \rho)$ $-2K_{\text{af}}\left(1 - 2\beta^2\right)\sin(2\phi) = 0.$	$4D_{\text{af}}\left(2\beta^2 - 1\right)\beta_{yy} + 8D_{\text{af}}\beta\beta_y^2 - \sqrt{2}H M_{\text{f}}\cos(\phi - \rho)$ $-4K_{\text{af}}\beta\cos(2\phi) = 0$
Boundary Condition at $y = 0$	$4D_{\text{af}}\left(2\beta_0^2 - 1\right)\phi_y(0) + \sqrt{2}\epsilon\left[J_+\beta_0\sin(\theta_0 - \phi_0)\right.$ $\left.+J_-\left(1 - \frac{1}{2}\beta^2\right)\cos(\theta_0 - \phi_0)\right] = 0.$	$4D_{\text{af}}\left(2\beta_0^2 - 1\right)\beta_y(0) - \sqrt{2}\epsilon$ $\times\left[J_+\cos(\theta_0 - \phi_0) + J_-\beta_0\sin(\theta_0 - \phi_0)\right] = 0.$

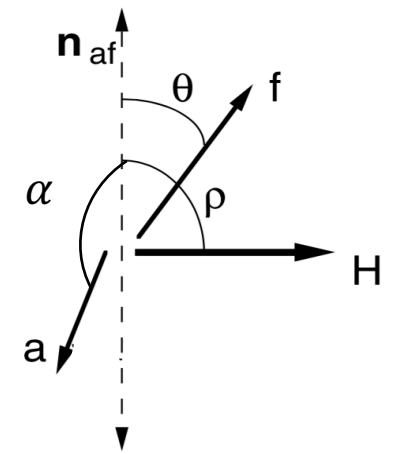


Figure 5. Angles for the applied field, ferromagnet, and antiferromagnet defined in reference to the antiferromagnet uniaxial anisotropy axis $\boldsymbol{n}_{\text{af}}$.

$$\sigma_{\text{a}}\sin\phi_0 - \theta_-\sin(\theta_0 + \alpha_0) - \frac{\theta_+^2}{\sigma_{\text{a}}}\sin(\theta_0 + \alpha_0)\cos(\theta_0 + \alpha_0 = 0$$

$$H M t_{\text{f}}\sin(\theta_0 - \rho) - \theta_-\sin(\theta_0 + \alpha_0 - \frac{\theta_+^2}{\sigma_{\text{a}}}\sin(\theta_0 + \alpha_0)\cos(\theta_0 + \alpha_0) = 0.$$

You can also derive these two equations from phenomenological model !

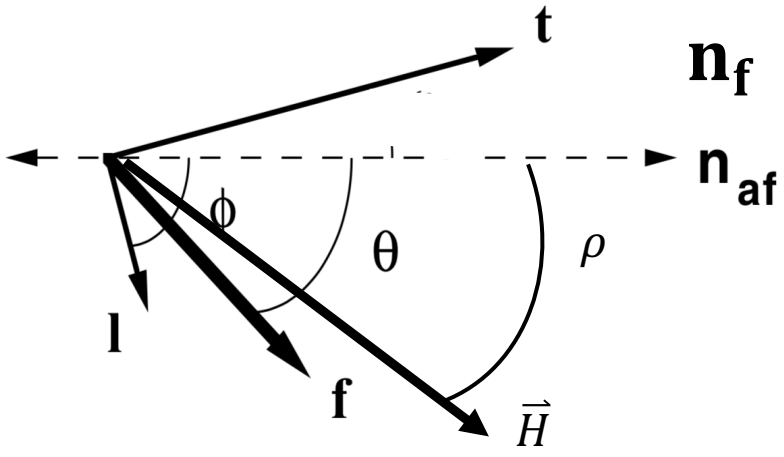
$$J_1 = 2\sqrt{2} \in (J_{\text{a}} - J_{\text{b}})$$

$$J_2 = \frac{\left[2\sqrt{2} \in (J_{\text{a}} + J_{\text{b}})\right]^2}{2\sigma_{\text{a}}}.$$

$$J_1/\sqrt{J_2} = \frac{J_{\text{a}} - J_{\text{b}}}{J_{\text{a}} + J_{\text{b}}}$$

(1) Uncompensated case: $J_a = 0, or\ J_b = 0,$
$J_1 \neq 0, J_2 \neq 0$

(2) compensated case: $J_a = J_b,$
$J_1 = 0, J_2 \neq 0$



FM Partial Wall Models

FM partial wall could exist!

FM: neglecting any deformation of the ferromagnet order($\theta_y = 0$) and FM anisotropy($K_f = 0$)

$$\frac{\delta \mathcal{E}}{\delta \theta} = 0$$

$$\mathcal{E}_f = -HMt_f \cos(\theta - \rho).$$

$$HMt_f \sin(\theta_0 - \rho) - 2\sqrt{2}\epsilon \times \left[J_+\beta_0 \sin(\theta_0 - \phi_0) + J_- \cos(\theta_0 - \phi_0)\right] = 0.$$

$$\mathcal{E} \approx \int_{\epsilon}^{+\infty} \left[-HM_f \cos(\theta - \rho) + D_f {\theta_y}^2 + K_f cos^2\theta\right] dy$$
$$+ \int_{-\infty}^{\epsilon} \left[-HM_{af}\beta \cos(\phi - \rho) + 2D_{af}(1 - 2\beta^2)({\beta_y}^2 - {\phi_y}^2) - 2K_{af}(\beta^2 cos^2\phi + (1 - \beta^2) sin^2\phi)\right] dy$$
$$+\sqrt{2}\epsilon[J_+\beta_0 \cos(\theta_0 - \phi_0) - J_-(1 - \tfrac{1}{2}{\beta_0}^2) \sin(\theta_0 - \phi_0)]$$

$$\frac{\delta \mathcal{E}}{\delta \theta} = 0$$

$$2D_f\theta_{yy} - HM \sin(\theta - \rho) - K_f \sin(2\theta) = 0$$

$$2D_f\theta_y(0) + 2\sqrt{2}\epsilon \left[J_+\beta_0 \sin(\theta_0 - \phi_0) + J_- \cos(\theta_0 - \phi_0)\right] = 0.$$

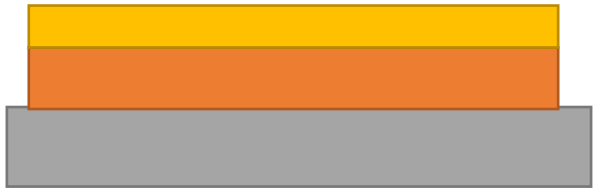
Neglecting FM anisotropy($K_f = 0$),

$$\mathcal{E}_f = 2HMt_f + \tfrac{1}{2}\sqrt{HMD_f} \sin\left(\theta_0 - \rho - t_f\sqrt{2HM/D_f}\right)$$

$$E_{\text{inter}} = -\boldsymbol{H}Mt_f \cdot \boldsymbol{f} + J_1 \boldsymbol{f} \cdot \boldsymbol{a} + J_2(\boldsymbol{f} \cdot \boldsymbol{a})^2 + \boxed{\sigma(1 - \boldsymbol{a} \cdot \boldsymbol{n}_{\text{af}})}$$

FM Partial Wall Models in FeF_2/Fe

Prototype system

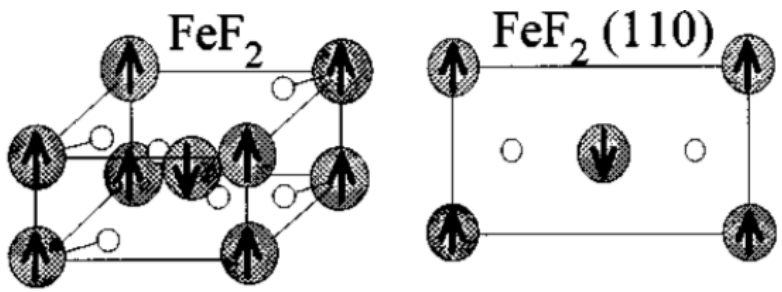


Fe polycrystalline (110) (100) 6.7nm, **13nm**, 130nm

FeF_2 (110) 90nm

MgO (100)

sequential *e*-beam evaporations



Compensated AFM interface

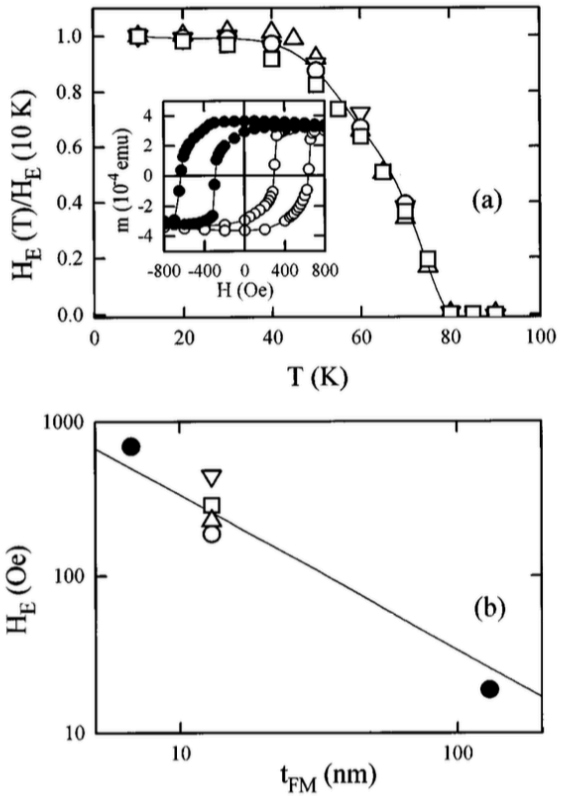


FIG. 3. Exchange bias H_E for samples I (∇), II (□), III (△), and IV (○) in Fig. 1. (a) H_E as a function of temperature normalized to H_E(10 K). Inset: Hysteresis loops at $T = 10$ K for FeF_2 (90 nm)–Fe (13 nm)–Ag (9 nm) grown at $T_S = 200$ °C (sample I in Fig. 1) field cooled in 2000 Oe (●) and −2000 Oe (○). (b) Log-log plot of H_E(10 K) as a function of Fe thickness t_{FM}. (●) are samples grown at $T_S = 200$ °C with thicknesses of 6.7 and 130 nm.

$T_S =$ 200 °C (I), 200 °C (II), 250 °C (III), 300 °C (IV)

J. Nogués, D. Lederman, T. J. Moran, Ivan K. Schuller, and K. V. Rao, Appl. Phys. Lett. **68**, 3186 (1996)

M. Kiwi, J. Mejia-Lopez, R. D. Portugal and R. Ramirez, Europhys. Lett., 48 (5), pp. 573-579 (1999)

FM Partial Wall Models in FeF_2/Fe

Pre-theoretical Simulations

$$E = -\sum_{\langle i \neq j \rangle}^{N} J_{ij}\ \vec{S}_i \cdot \vec{S}_j - \sum_{i=1}^{N} [K_i\ (\vec{S}_i \cdot \hat{e}_i)^2 + \mu_B g_i\ \vec{S}_i \cdot \vec{H}]\,.$$

Range: A unit interface magnetic cell extends up to 65 F, and many AF monolayers;

Methods: ***Stimulated annealing and Camley's method***;

$$d_W \sim \sqrt{A/K}$$

Results and Conclusions:

(0) $d_W^{FM} \sim 100nm$, $d_W^{AFM} \sim$a few monolayers

(1) When measurement field points opposite to the cooling field, a long-range FM partial wall develops;

(2) Interface layer AF spins deviate significantly relative to the AF bulk, only a tiny deviation develops in the second AF layer and no appreciable canting in the third;

(3) The presence of canted spins at the AF interface layer is no guarantee for $H_E \neq 0$ in the absence of a ***symmetry-breaking mechanism***

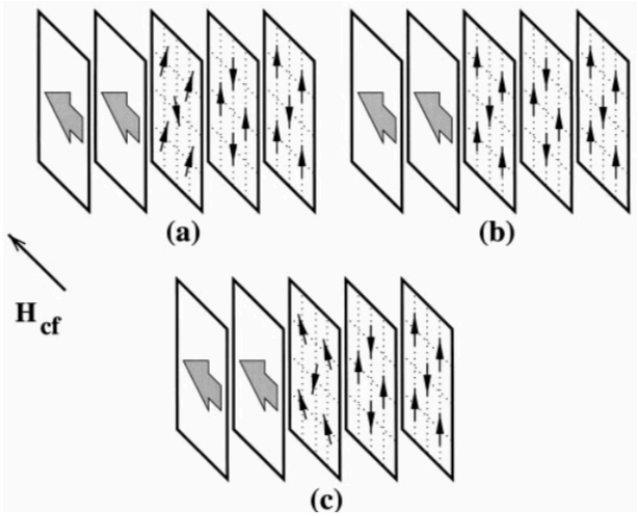


Fig. 1. Spin configuration of the AFM interface monolayer and both the two FM and the two AFM monolayers closest to the interface, after it is field-cooled through T_N. The canting angle θ_c is measured relative to the cooling field $\vec{H}_{cf}$, applied parallel to the $(\bar{1}10)$ AFM crystal direction: (a) corresponds to weak; (b) to the critical; and (c) to strong $|\vec{H}_{cf}|$ values.

Kirkpatrick S., Gelatt C. D. and Vechi M. P., Science, 220 (1983) 671

Camley R. E., Phys. Rev. B, 35 (1987) 3608;

Camley R. E. and Tilley D. R., Phys. Rev. B, 37 (1988) 3413.

FM Partial Wall Models in FeF_2/Fe

Assumptions:

(1) Perfect, flat, compensated two-sublattice AFM interface;

(2) Strong AFM anisotropy

(3)**Symmetry-breaking Mechanism: During field cooling, the first AF interface layer freezes into the canted spin configuration when $T \to T_N$, and remains frozen in a metastable state during the cycling of H, where $|H| < H_{cf}$**

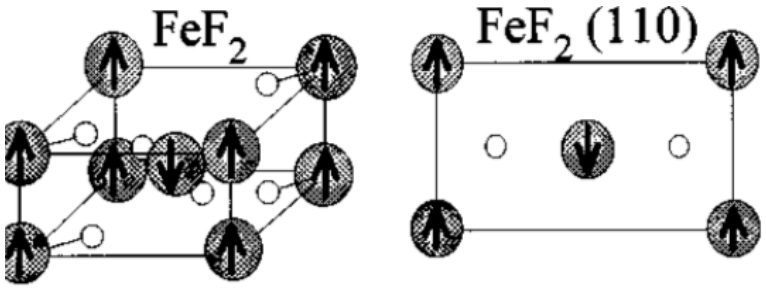
For a single magnetic cell $\mathcal{H} = \mathcal{H}_{\rm AF} + \mathcal{H}_{\rm F/AF} + \mathcal{H}_{\rm F}$

$$\mathcal{H}_{\rm AF} = -\, J_{\rm AF}\, [\, S\, \hat{e}_{\rm AF} \cdot (\vec{S}^{(\alpha)} - \vec{S}^{(\beta)}) + 2\vec{S}^{(\alpha)} \cdot \vec{S}^{(\beta)}\,] -$$

$$-\quad K_{\rm AF}\, [\, (\vec{S}^{(\alpha)} \cdot \hat{e}_{\rm AF})^2 \;+\; (\vec{S}^{(\beta)} \cdot \hat{e}_{\rm AF})^2\,] - \quad \mu_{\rm B} g\, (\vec{S}^{(\alpha)} + \vec{S}^{(\beta)}) \cdot \vec{H}\ ,$$

$$\mathcal{H}_{\rm F/AF} = -\, J_{\rm F/AF}\, (\vec{S}^{(\alpha)} + \vec{S}^{(\beta)}) \cdot \vec{S}_1\ ,$$

$$\mathcal{H}_{\rm F} = -\, 2J_{\rm F} \sum_{k=1}^{N-1} \vec{S}_k \cdot \vec{S}_{k+1} - \sum_{k=1}^{N} \left[\, \frac{K_{\rm F}}{H^2}\, (\vec{S}_k \cdot \vec{H})^2 + \mu_{\rm B} g\, \vec{S}_k \cdot \vec{H}\, \right]\ .$$



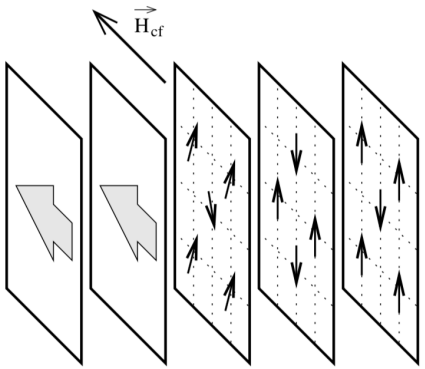


Fig. 1. – Zero applied field spin configuration of the AF interface monolayer and the two F and AF monolayers closest to the interface. The canting angle θ_c is measured relative to the cooling field $\vec{H}_{cf}$, applied parallel to the $(\bar{1}10)$ AF crystal direction.

Where $S = |\vec{S}|$; μ_B: Bohr magneton; g: Fe gyromagnetic ratio

$\vec{H}$:external magnetic field; J_μ: Heisenberg exchange parameter;

K_υ: uniaxial anisotropy; $\hat{e}_{AF}$: unit vector along AF uniaxial anisotropy direction;

$\vec{S}^{(\alpha)}, \vec{S}^{(\beta)}$: canted spin vectors in the AF interface, belonging to α- and β- sublattices;

$\vec{S}_k$: spin vectors of the k-th FM layer, with $1 \le k \le N$, k=1 labeling FM interface;

FM Partial Wall Models in FeF_2/Fe

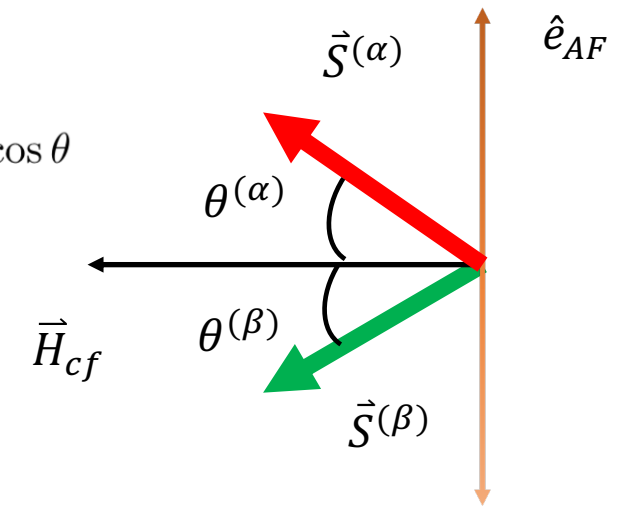
Part I : field cool process

$$\mathcal{H}_{\mathrm{AF}} = -\, J_{\mathrm{AF}}\, [\, S\, \hat{e}_{\mathrm{AF}} \cdot (\vec{S}^{(\alpha)} - \vec{S}^{(\beta)}) + 2\vec{S}^{(\alpha)} \cdot \vec{S}^{(\beta)}\,] - K_{\mathrm{AF}}\, [\, (\vec{S}^{(\alpha)} \cdot \hat{e}_{\mathrm{AF}})^2 + (\vec{S}^{(\beta)} \cdot \hat{e}_{\mathrm{AF}})^2\,] - \mu_{\mathrm{B}} g\, (\vec{S}^{(\alpha)} + \vec{S}^{(\beta)}) \cdot \vec{H}$$

$$\mathcal{H}_{\mathrm{F/AF}} = -\, J_{\mathrm{F/AF}}\, (\vec{S}^{(\alpha)} + \vec{S}^{(\beta)}) \cdot \vec{S}_1$$

$$\mathrm{E} = \frac{\mathcal{H}_{\mathrm{AF}} + \mathcal{H}_{\mathrm{F/AF}}}{\mathrm{S}^2} = 2|J_{\mathrm{AF}}|\, \left[\cos(2\theta) + \cos\left(\theta + \frac{\pi}{2}\right)\right] - K_{\mathrm{AF}} \cos^2(\theta - \frac{\pi}{2}) + (\, 2\, |J_{\mathrm{F/AF}}| - \mu_{\mathrm{B}} g H_{\mathrm{cf}})\cos\theta$$

describes the behavior of the system during the cooling process and the removal of the cooling field



$$\frac{\delta E}{\delta \theta} = 0, \quad \frac{\delta^2 E}{\delta \theta^2} > 0 \quad \Rightarrow \quad \theta = \theta_c$$

$$\theta = \theta^{(\alpha)} = -\, \theta^{(\beta)}$$

This provides the symmetry breaking required for EB to develop !

(1) $|\vec{H}_{cf}| < 2J_{F/AF} / \mu_B g, \theta = \theta_c > \frac{\pi}{2}$, Negative EB

(2) $|\vec{H}_{cf}| > 2J_{F/AF} / \mu_B g, \theta = \theta_c < \frac{\pi}{2}$, Positive EB

(3) $|\vec{H}_{cf}| = 2J_{F/AF} / \mu_B g, \theta = \theta_c = \frac{\pi}{2}$, No EB

$J_{F/AF} = J_{AF} = -1.2$ meV $\quad K_{AF} = 2.5$ meV/spin

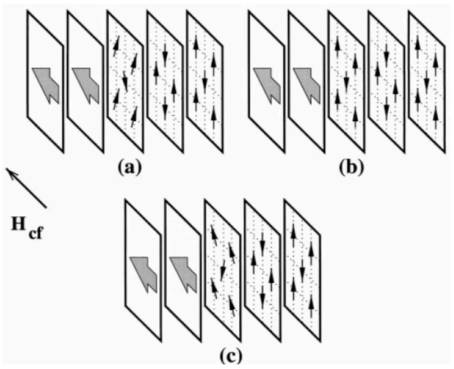
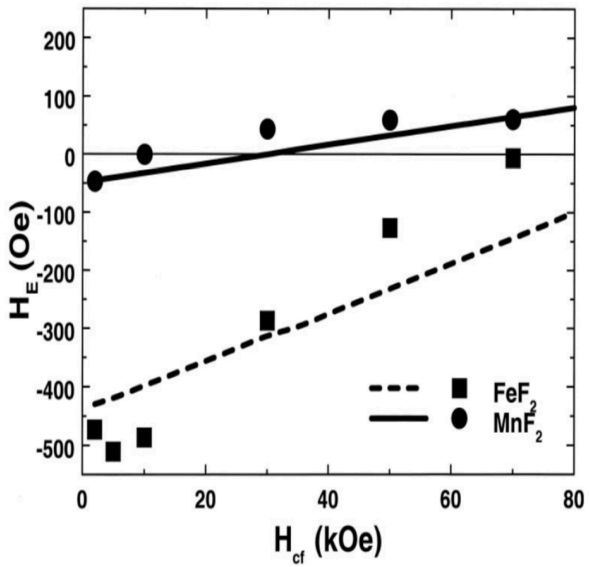


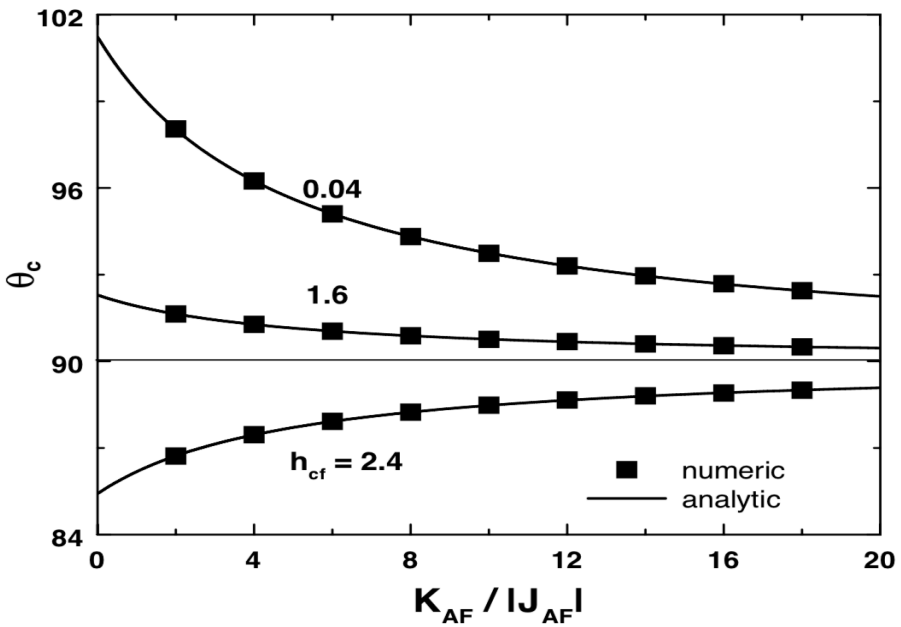
Fig. 1. Spin configuration of the AFM interface monolayer and bo
the two FM and the two AFM monolayers closest to the interfa
after it is field-cooled through T_N. The canting angle θ_c is measur
relative to the cooling field $\vec{H}_{cf}$, applied parallel to the $(\bar{1}10)$ AF
crystal direction: (a) corresponds to weak; (b) to the critical; and
to strong $|\vec{H}_{cf}|$ values.



Analytical Results:

Define $\theta = \frac{\pi}{2} + \gamma$, and expand $E(\theta)$ relative to γ, then minimizing $E(\theta)$, to the second order of γ, we get

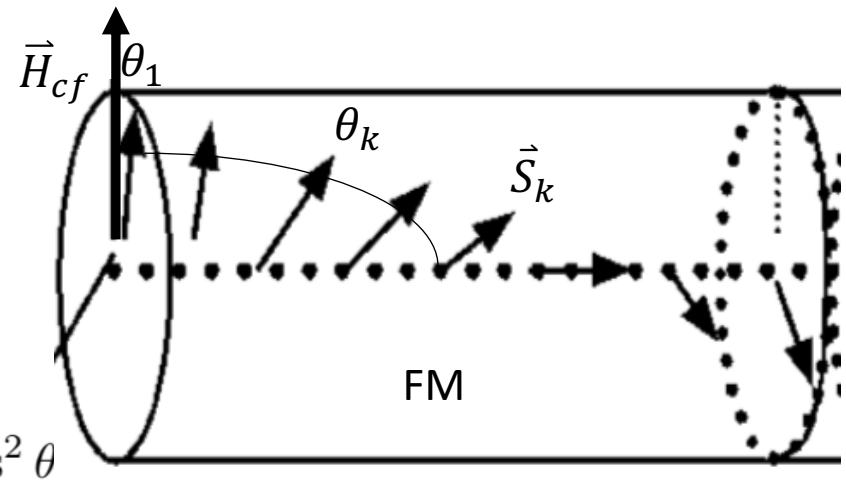
$$\theta_c = \frac{\pi}{2} + \frac{2\ |J_{F/AF}| - g_{AF}\mu_B H_{cf}}{10\ |J_{AF}| + 2K_{AF}}$$



$$h_{cf} = g_{AF}\mu_B H_{cf}/|J_{AF}|$$

FM Partial wall Models in FeF_2/Fe

Part II : measurement process



$$\mathcal{H}_{\mathrm{F/AF}} = -\, J_{\mathrm{F/AF}}\, (\vec{S}^{(\alpha)} + \vec{S}^{(\beta)}) \cdot \vec{S}_1$$

$$\mathcal{H}_{\mathrm{F}} = -\, 2J_{\mathrm{F}} \sum_{k=1}^{N-1} \vec{S}_k \cdot \vec{S}_{k+1} - \sum_{k=1}^{N} \left[\frac{K_{\mathrm{F}}}{H^2} (\vec{S}_k \cdot \vec{H})^2 + \mu_{\mathrm{B}} g\, \vec{S}_k \cdot \vec{H} \right]$$

$$\epsilon = \frac{\mathcal{H}_{\mathrm{AF}} + \mathcal{H}_{\mathrm{F/AF}}}{J_F S^2} = -h \sum_{k=1}^{N} \cos\theta_k - \sum_{k=1}^{N-1} \cos\,(\theta_{k+1} - \theta_k) - \kappa \cos\theta_1 - D \sum_{k=1}^{N} \cos^2\theta$$

$$J_{\mathrm{F/AF}} = J_{\mathrm{AF}} = -1.2\ \mathrm{meV}$$

$$K_{\mathrm{F}} = 5 \times 10^{-4}\ \mathrm{meV/spin}$$

$$J_{\mathrm{F}} = 16\ \mathrm{meV}$$

$$h = \mu_{\mathrm{B}} g H / 2J_{\mathrm{F}} < 10^{-3} \qquad \kappa = -(|J_{\mathrm{F/AF}}|/J_{\mathrm{F}}) \cos\theta_{\mathrm{c}} \qquad D = K_{\mathrm{F}}/2J_{\mathrm{F}} < 10^{-5}$$

$$\frac{\partial\epsilon}{\partial\theta_j} = h \sin\theta_j - (1-\delta_{j,N}) \sin(\theta_{j+1} - \theta_j) + (1-\delta_{j,1}) \sin(\theta_j - \theta_{j-1}) + \delta_{j,1}\, \kappa \sin\theta_1 + D \sin 2\theta_j = 0$$

$\delta_{i,j}$ is the Kronecker symbol. $\quad (1 \le j \le N)$

$$h \sum_{k=1}^{N} \sin\theta_k + \kappa \sin\theta_1 + 2D \sum_{k=1}^{N} \sin\theta_k \cos\theta_k = 0$$

If $\kappa = 0, \theta = 0, \pi$

$$\kappa > 0, \quad h < 0 \qquad \kappa \gg |h| \qquad 0 < \theta_k < \pi$$

$$0 < |\theta_{\mathrm{N}} - \theta_1| < 20^\circ \qquad |\theta_j - \theta_{j\pm1}| \ll 1$$

$$\frac{\partial \epsilon}{\partial \theta_j} = h \sin\theta_j - (1-\delta_{j,N}) \sin(\theta_{j+1}-\theta_j) + (1-\delta_{j,1}) \sin(\theta_j - \theta_{j-1}) + \delta_{j,1}\, \kappa \sin\theta_1 + D \sin 2\theta_j = 0$$

$$h \sum_{k=1}^{N} \sin\theta_k + \kappa \sin\theta_1 + 2D \sum_{k=1}^{N} \sin\theta_k \cos\theta_k = 0$$

TABLE I. Magnetization vector angle θ_k, relative to the direction of the cooling field $\mathbf{H}_{cf}$, for the five layers $k=-3, -2, -1, 1$, and 2 of Fig. 1 (H_{cf}=2000 Oe).

Layer	θ_k (Fe/FeF$_2$)	θ_k (Fe/MnF$_2$)
$F(k=2)$	0.17°	0.04°
$F(k=1)$	0.85°	0.26°
AF($k=-1$)	98.16°	93.04°
AF($k=-2$)	88.91°	89.41°
AF($k=-3$)	90.07°	90.03°

Analytical Results:

Define $\theta_k = \theta_1 + (k-1)\delta$, to the second order of δ

$$\varepsilon = (N_F - 1)\delta^2 - hN_F M(\theta_1, \delta) - \kappa \cos(\theta_1),$$

$$M(\theta_1, \delta) = \cos\theta_1 - (N_F - 1) \times \left[\tfrac{1}{2}\,\delta\, \sin\theta_1 - \tfrac{1}{12}\,(2N_F - 1)\delta^2\, \cos\theta_1\right]$$

$$\frac{1}{2\,(N_F - 1)} \frac{\partial \varepsilon}{\partial \delta} = \delta + \frac{1}{4}\, h\, N_F \left[\sin\theta_1 - \frac{1}{3}(2\, N_F - 1)\, \delta \cos\theta_1\right] = 0,$$

$$\frac{\partial \varepsilon}{\partial \theta_1} = -h\, N_F\, \frac{\partial M(\theta_1, \delta)}{\partial \theta_1} + \kappa \sin\theta_1 = 0$$

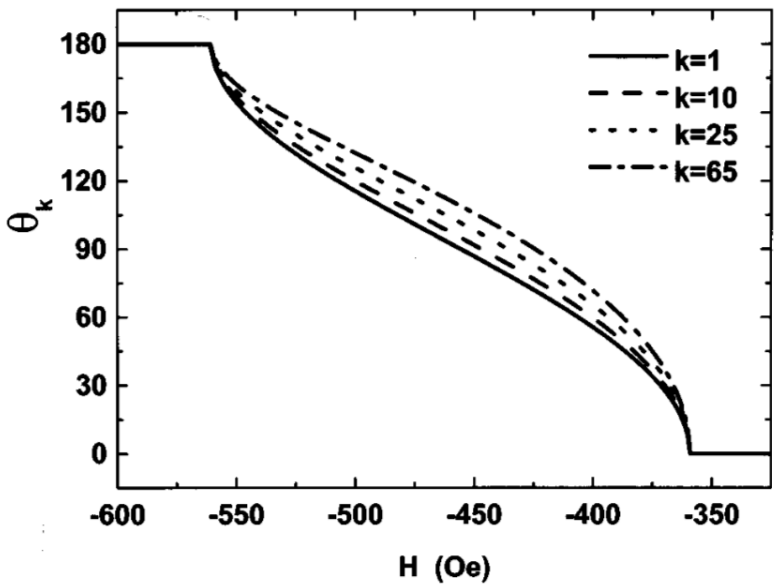


FIG. 4. Magnetization angle θ_k of the kth Fe layer with the cooling field $\mathbf{H}_{cf}$ vs applied field H.

$$M(\theta_1, \delta) = 0 \quad \Rightarrow \quad \cos\theta_1 - (N_F - 1) \times \left[\tfrac{1}{2}\delta \sin\theta_1 - \tfrac{1}{12}(2N_F - 1)\delta^2 \cos\theta_1\right] = 0 \quad \Rightarrow \quad h_{EB} = -\frac{x[\kappa x(2N_F - 1)(1 - x^2) + 24]}{N_F\ [x^2(N_F + 1) + 3(N_F - 1)]}$$

$$\delta = \frac{3hN \sin\theta_1}{2hN^2 \cos\theta_1 - hN \cos\theta_1 - 12} \qquad \kappa = \frac{|J_{F/AF}|}{J_F} \sin\left[\frac{2|J_{F/AF}| - g_{AF}\ \mu_B\ H_{cf}}{10|J_{AF}| + 2K_{AF}}\right]$$

$$\begin{aligned}
&\kappa^2\left(20N_F^2 - 4N_F + 5 + \frac{4}{N_F - 1}\right)x^7 \\
&- 2\kappa^2\ \left[(2N_F + 1)^2 + \left(\frac{2}{N_F - 1}\right)\right]x^5 \\
&+ 72\kappa\ (5N_F - 1)x^4 - 12\kappa^2 N_F \\
&\times (N_F - 1)\ x^3 - 144\kappa\ (N_F + 1)\ x^2 \\
&+ 1728\ x - 216\kappa(N_F - 1) = 0\ .
\end{aligned}$$

In the weak interface coupling limit $|\kappa| < \kappa_0$, where $\kappa_0 = \sqrt{24/(N_F^2 - 1)}$, the expression for h_{EB} reduces to

$$h_{EB} = -\frac{\kappa}{N_F}\ ,$$

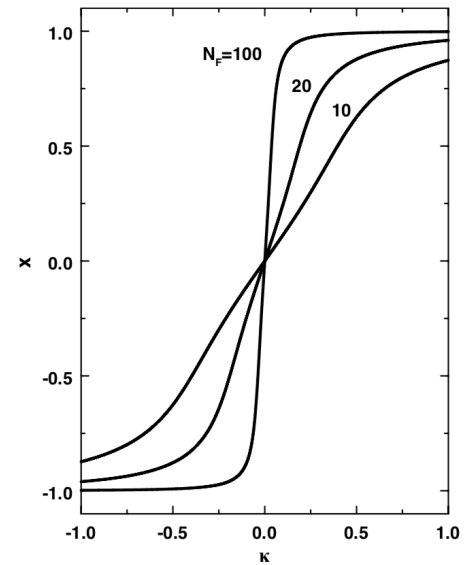


Fig. 2. Solutions of Eq. (16) for three FM film thickness (N_F) values.

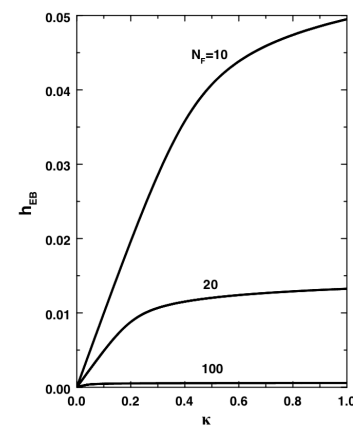


Fig. 3. EB field h_{EB} versus κ, for three values of the FM film thickness, N_F.