

Implémentation numérique d'un modèle multi-échelle pour la modélisation de matériaux magnétoélectriques

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Journée thématique « multi-échelles »

Remerciements équipe « magnétoélectrique »

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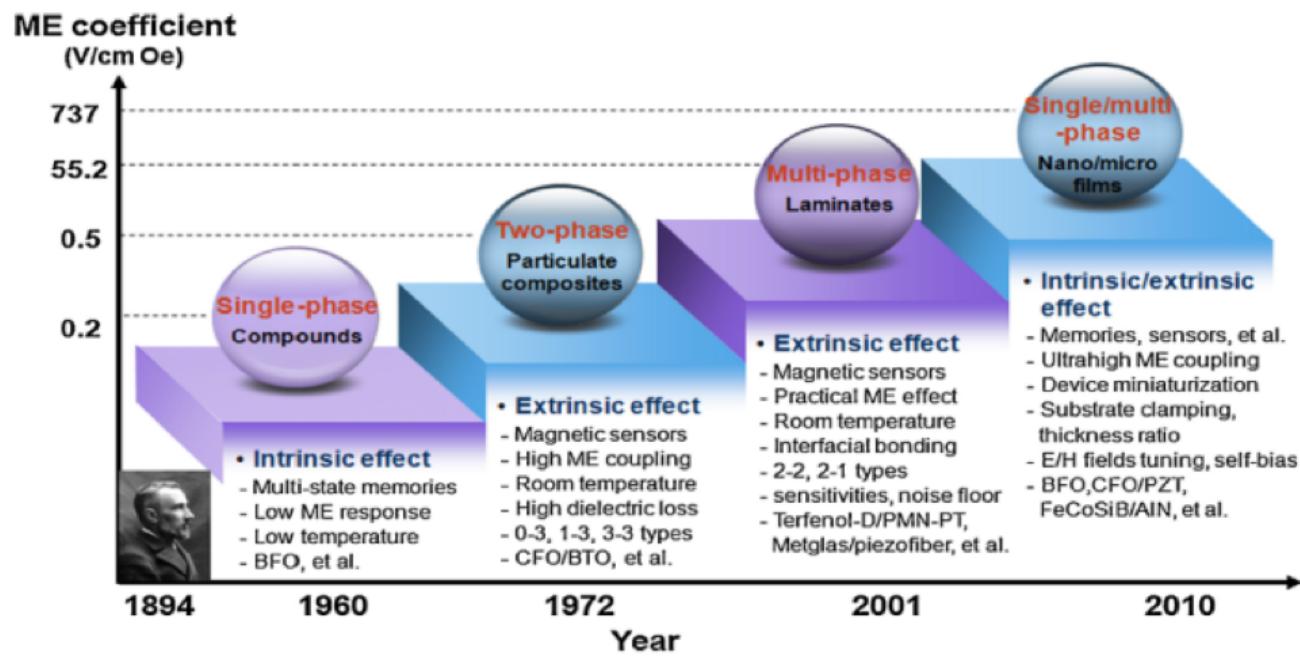
Doctorants en cours: Tianwen Huang et Sheno Karimi

Plan

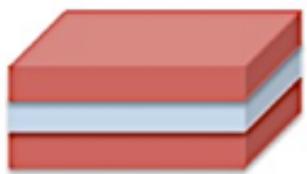
- Contexte : Matériaux magnétoélectriques
- Couplage multiphysique
- MME* simplifié
- Formulations analytiques
 - Cas 1 $\sigma=0$, cas 2 $\sigma\neq0$
- Limite de validité
- Validation des modèles
- Implémentation dans un code FEM 2D
- Résultats de simulation : Composites laminaires PZT/TD/PZT

* :MME = Modèle Multi-Échelles

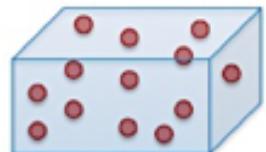
Contexte



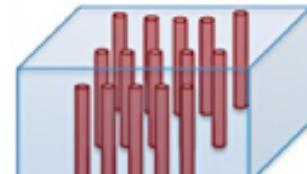
H. Palneedi, V. Annareddy, S. Priya and Jungho Ryu, "Status and Perspectives of Multiferroic Magnetoelectric Composite Materials and Applications", *Actuators* 2016, 5, 9; doi:10.3390/act5010009.



Type 2-2



Type 0-3

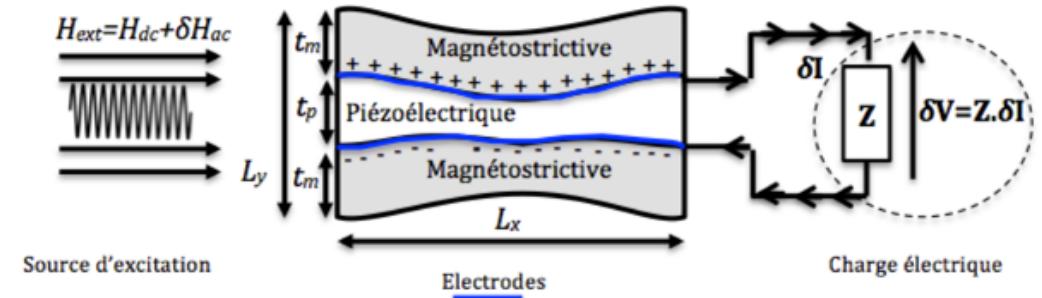
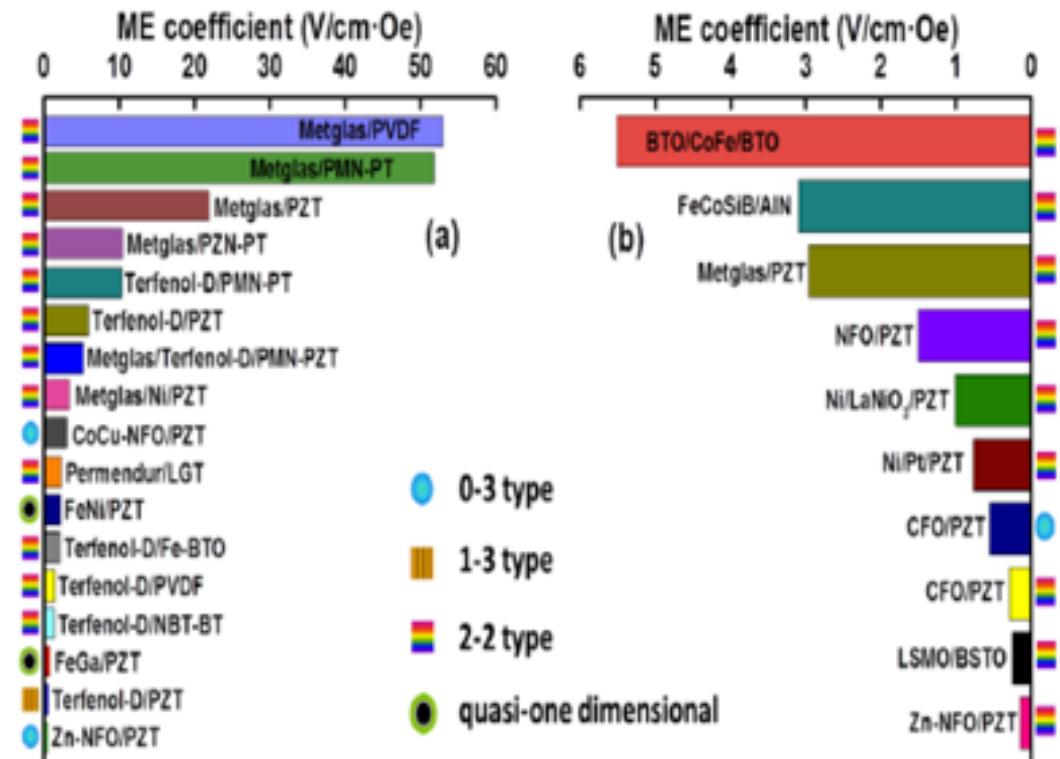


Type 1-3

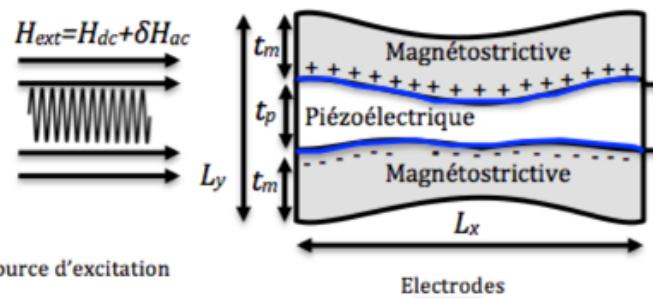
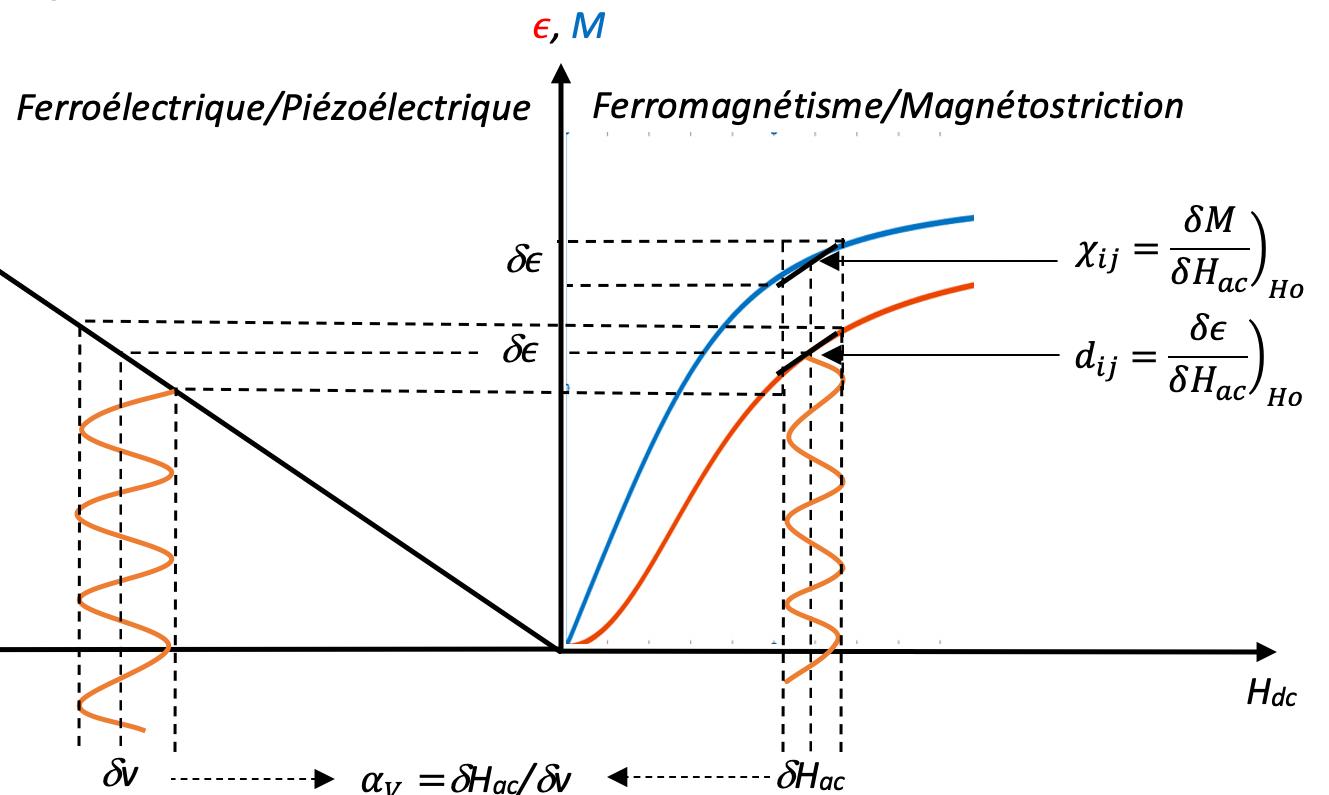
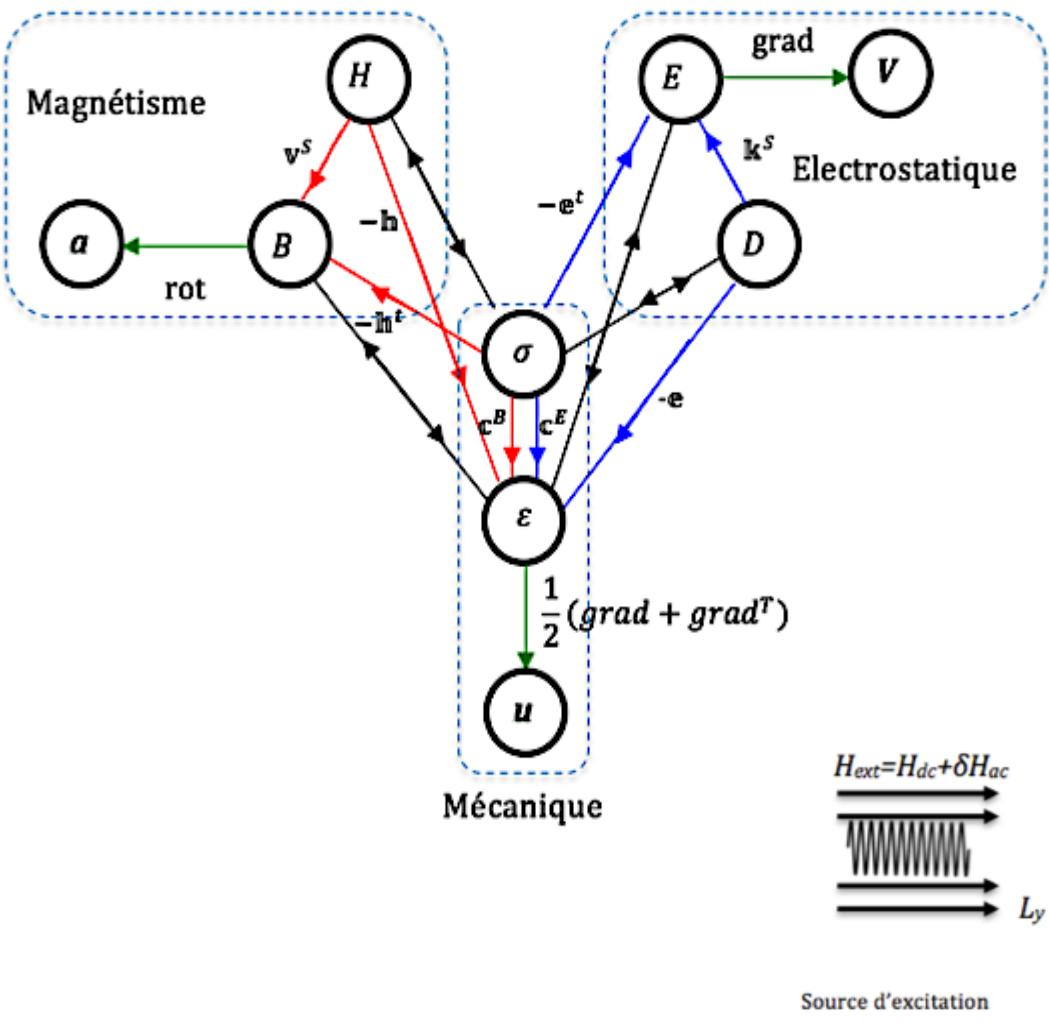
Laminate composite

Particulate composite

Fiber composite



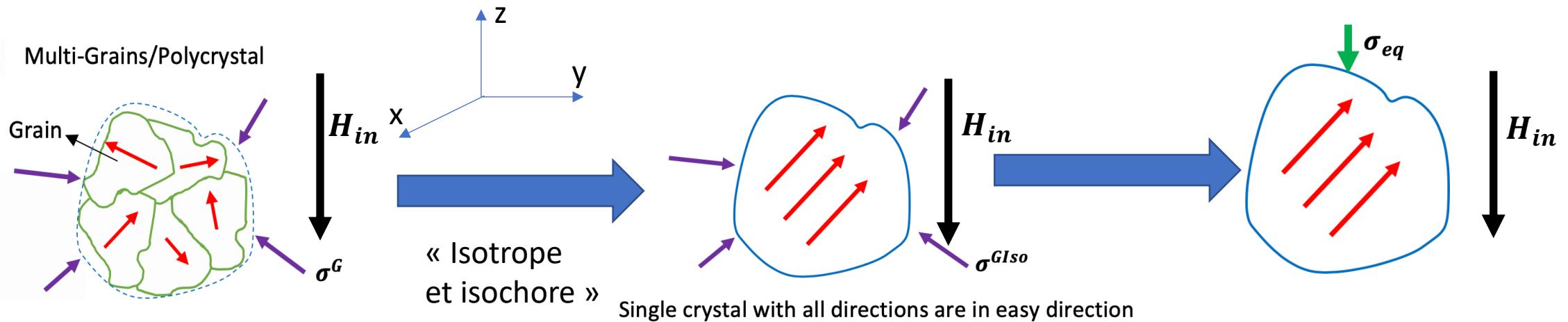
Couplage multi-physique



Code numérique :

- 1- Simulation non linéaire DC => Polarisation en fonction de l'effet structure
- 2- Simulation linéaire AC

MME simplifié



Déformation

$$\lambda_p(\theta) = \frac{3}{2} \lambda_s \left(\cos \theta^2 - \frac{1}{3} \right)$$

$$\theta = \langle \mathbf{M}, \mathbf{H} \rangle$$

Contraintes

$$\boldsymbol{\sigma}_G = \begin{pmatrix} \sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\ \sigma_{yx} & \sigma_{yy} & \sigma_{yz} \\ \sigma_{zx} & \sigma_{zy} & \sigma_{zz} \end{pmatrix}$$

Déformations de la magnétostriction

$$\boldsymbol{\varepsilon}_{SC}^m = \lambda_p(\theta) \begin{pmatrix} -\frac{1}{2} & 0 & 0 \\ 0 & -\frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Contraintes équivalentes

$$\boldsymbol{\sigma}_{eSC} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \sigma_Z \end{pmatrix}$$

$$\sigma_Z = \frac{3}{2} \mathbf{e}_z^t \mathbf{s} \mathbf{e}_z$$

$$\mathbf{s} = \boldsymbol{\sigma}_{SC} - \frac{1}{3} \text{tr}(\boldsymbol{\sigma}_{SC}) \mathbf{I}$$

Formulations analytiques 1/2

Energie de Gibbs

$$W_{SC}^F = W_{SC}^M + W_{SC}^E = -\mu_o H_{in} \cdot M_s \cos(\theta) - \frac{3}{2} \sigma_{\mathbb{Z}} \lambda_s \left(\cos \theta^2 - \frac{1}{3} \right)$$

$$\boldsymbol{M} = \langle \boldsymbol{M}_G \rangle = \int_G f_G \boldsymbol{M}_G \quad \boldsymbol{\varepsilon}^\mu = \langle \boldsymbol{\varepsilon}_G^\mu \rangle = \int_G f_G \boldsymbol{\varepsilon}_k^\mu \quad f_G = Z^{-1} e^{-A_s W_{SC}^F} \quad Z = \int_G e^{-A_s W_{SC}^M} dV \quad A_s = \frac{3\chi_o}{\mu_o M_s^2}$$

Fct probabilité Boltzmann Fct de partition Paramètre matériau

Cas 1: $\sigma_{\mathbb{Z}}=0$

$$Z = \int_G e^{-A_s W_{SC}^M} dV = \frac{1}{2} \int_0^\pi \sin \theta e^{A_s \mu_o H_{in} \cdot M_s \cos(\theta)} d\theta$$

$$\boldsymbol{M} = \frac{1}{2} \int_0^\pi \sin \theta \frac{e^{A_s \mu_o H_{in} \cdot M_s \cos(\theta)}}{Z} d\theta = M_s \mathcal{L}(\alpha)$$

$$\boldsymbol{\varepsilon}_{zz}^m = \frac{1}{2} \int_0^\pi \sin \theta \frac{e^{A_s \mu_o H_{in} \cdot M_s \cos(\theta)}}{Z} \lambda_p(\theta) d\theta = \lambda_s \left(1 - 3 \frac{\mathcal{L}(\alpha)}{\alpha} \right)$$

$$\mathcal{L}(\alpha) = \coth(\alpha) - \alpha^{-1} = \frac{\boldsymbol{M}}{M_s}$$

$$\alpha = \kappa H_{in} \quad \kappa = A_s \mu_o M_s$$

$$\boldsymbol{\varepsilon}_{zz}^m = \lambda_s \left(1 - \frac{3}{\alpha} \frac{\boldsymbol{M}}{M_s} \right)$$

$$\frac{3\boldsymbol{M}}{\alpha M_s} = \gamma^{-1} \frac{\boldsymbol{M}}{M_s^2} = \frac{\chi}{\chi_o}$$

$$\boldsymbol{\varepsilon}_{zz}^m = \lambda_s (1 - \kappa) \quad \kappa = \chi / \chi_o$$

Formulations analytiques 2/2

Cas 1: $\sigma_{\mathbb{Z}}=0$

$$Z = \int_G e^{-A_s W_{SC}^M} dV = e^{-\frac{A_s}{2} \lambda_s \sigma_z} \frac{1}{2} \int_0^\pi \sin \theta e^{A_s (\mu_o H_{in} \cdot M_s \cos(\theta) + \frac{3}{2} \lambda_s \sigma_{\mathbb{Z}} \cos \theta^2)} d\theta$$

$$M_{\sigma_e} = -\frac{1}{A_s \mu_o} \frac{1}{Z} \frac{\partial Z}{\partial H_{in}}$$

$$\varepsilon_{zz,\sigma_e}^m = -\frac{1}{A_s} \frac{1}{Z} \frac{\partial Z}{\partial \sigma_{\mathbb{Z}}}$$

$$M_{\sigma_e} = \frac{M_s}{3\Delta} \left(-\alpha - \sqrt{A_s} \frac{P_1}{P_2} \right)$$

$$P_1 = \sqrt{\frac{3}{2}} (-1 + e^{2\alpha}) \sqrt{\Delta} / \sqrt{A_s}$$

$$P_2 = (D(a_-) - e^{2\alpha} D(a_+))$$

$$\Delta = A_s \lambda_s \sigma_{\mathbb{Z}}$$

$$\alpha = \kappa H_{in} \quad \kappa = A_s \mu_o M_s$$

$$a_{\pm} = (\alpha \pm 3\Delta) / \sqrt{6\Delta}$$

$$D(x) = e^{-x^2} \int_0^t e^{t^2} dt$$

$$\varepsilon^m = \frac{1}{6\Delta \sigma_e} \left(\frac{\alpha^2 - 3\Delta}{A_s} - \sqrt{6\Delta} e^{\alpha} \frac{P_3}{P_2} \right)$$

$$P_2 = (D(a_-) - e^{2\alpha} D(a_+))$$

$$P_3 = [\alpha \sinh(\alpha) - 3\Delta \cosh(\alpha)] / A_s$$

Les coefficients incrémentaux

La perméabilité

$$\mu_{ij} = \mu_o \partial_H (\mathbf{H}_{in} + \mathbf{M}) = \mu_o (1 + \partial_H \mathbf{M}) = \mu_o (1 + \chi_{ij})$$

$$\mu_{33r} = \begin{cases} 1 + M_s \left[\left(\frac{1}{\kappa H^2} \right) - \kappa R \right], & \sigma = 0 \\ 1 + M_s^2 [-3(-1 + e^{2\alpha})^2 \sqrt{\Delta/A_s} - 2P_2 U_o], & \sigma \neq 0 \end{cases}$$

$$R = [\csc h(\kappa H)]^2$$

$$\mu_{ij} = \mu_o \begin{pmatrix} \mu_{11r} & 0 & 0 \\ 0 & \mu_{22r} & 0 \\ 0 & 0 & \mu_{33r} \end{pmatrix}$$

Coefficients piézomagnétiques

$$d_{ij}^H = \partial_H \boldsymbol{\varepsilon}$$

$$d_{33}^H = \begin{cases} 3\lambda_s [-2 + \kappa H [\coth(\kappa H) + \kappa H R]] / ((\kappa H)^2 H), & \sigma = 0 \\ 6M_s e^{2\alpha} [\sqrt{\Delta} \sinh(\alpha) P_3 + V_o] / V_1, & \sigma \neq 0 \end{cases}$$

$$d_{31}^H = d_{32}^H = -d_{33}^H / 2$$

$$d_{14}^H = d_{25}^H = 3 \boldsymbol{\varepsilon}^m / H$$

S. Huang, S. Wang, W. Li and Q. Wang, "Chapter 3 Analytical Method of EMAT Based on Magnetostrictive Mechanism", Electromagnetic Ultrasonic Guided, Springer Series in Measurement Science and Technology, ISBN-10 : 9789811005626

$$d_{ij}^H = \begin{bmatrix} 0 & 0 & d_{31}^H \\ 0 & 0 & d_{32}^H \\ 0 & 0 & d_{33}^H \\ d_{14}^H & 0 & 0 \\ 0 & d_{25}^H & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

Limite de validité. : Singularité $P_2=0$

$$\Delta = A_s \lambda_s \sigma_{\mathbb{Z}}$$

$$\alpha = \kappa H_{in}$$

$$\kappa = A_s \mu_o M_s$$

$$a_{\pm} = (\alpha \pm 3\Delta)/\sqrt{6\Delta}$$

$$P_2 = (D(a_-) - e^{2\alpha} D(a_+))$$

$$D(a_-) = e^{-a_-^2} \int_0^t e^{t^2} dt$$

$$e^{2\alpha} D(a_+) = e^{-(a_+^2 - 2\alpha)} \int_0^t e^{t^2} dt$$

$$P_2 = 0$$

$$a_+^2 - 2\alpha = a_-^2$$

$$a_+ - a_- = \sqrt{6\Delta}$$

$$a_+^2 - a_-^2 = (a_+ - a_-)(a_+ + a_-) = 2\alpha$$

$$a_+ = -n\sqrt{6\Delta} \quad a_- = -(n+1)\sqrt{6\Delta}$$

$$(a_+ + a_-) = \frac{2\alpha}{\sqrt{6\Delta}}$$

$$-(2n+1)\sqrt{6\Delta} = \frac{2\alpha}{\sqrt{6\Delta}} = \frac{\kappa H_{in}}{3\Delta}$$

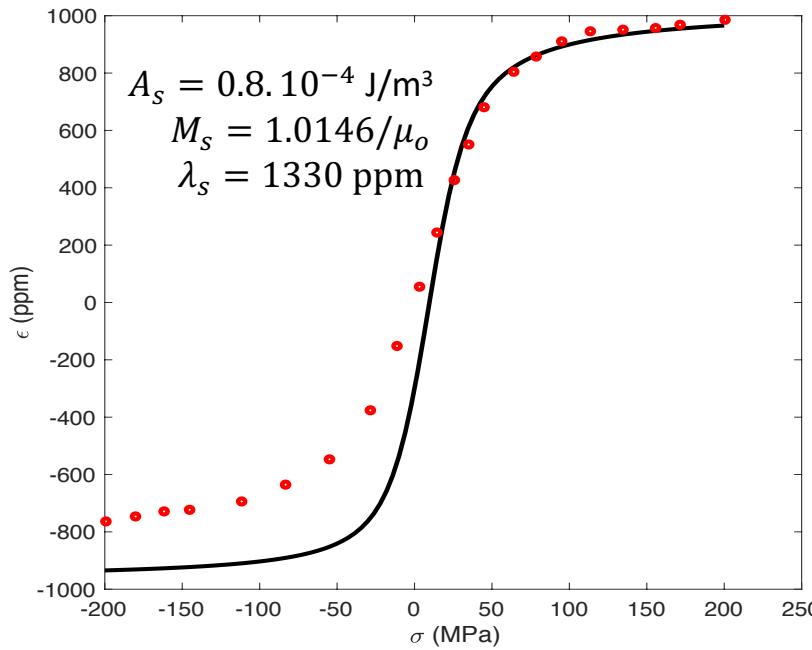
$$H_{in_lim} = -\frac{3\Delta(2n+1)}{\kappa} = -3(2n+1) \frac{\lambda_s \sigma_{\mathbb{Z}-}}{\mu_o M_s}$$

Terfenol-D

$$n \approx \sqrt{\frac{20}{\sigma_o}}$$

$$\sigma_o = |\sigma_{\mathbb{Z}-}|/1 \text{ [Mpa]}$$

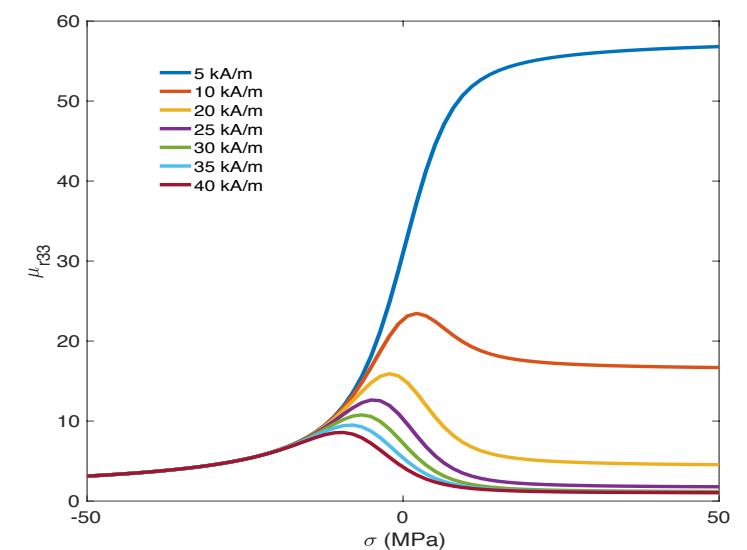
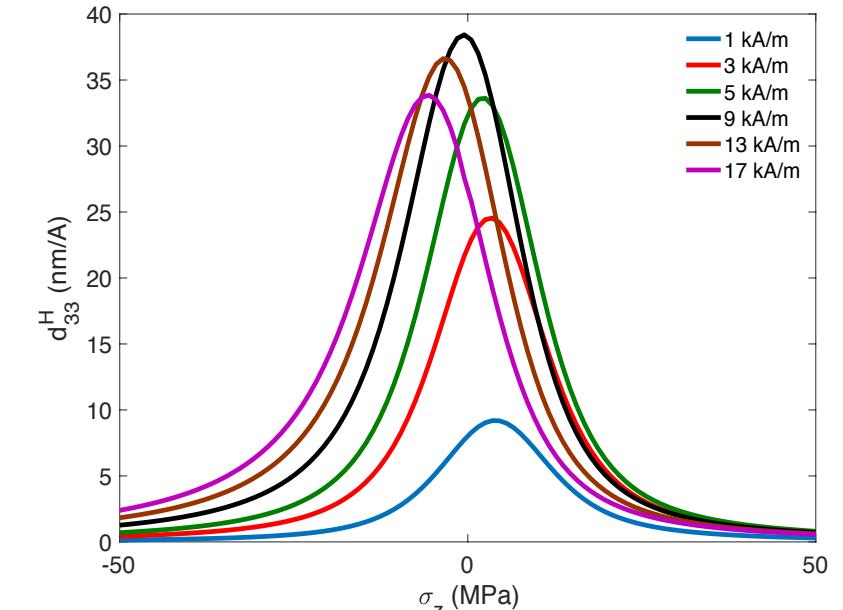
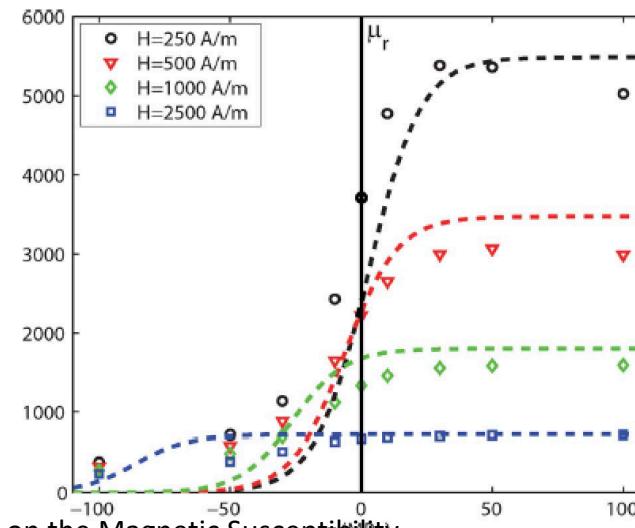
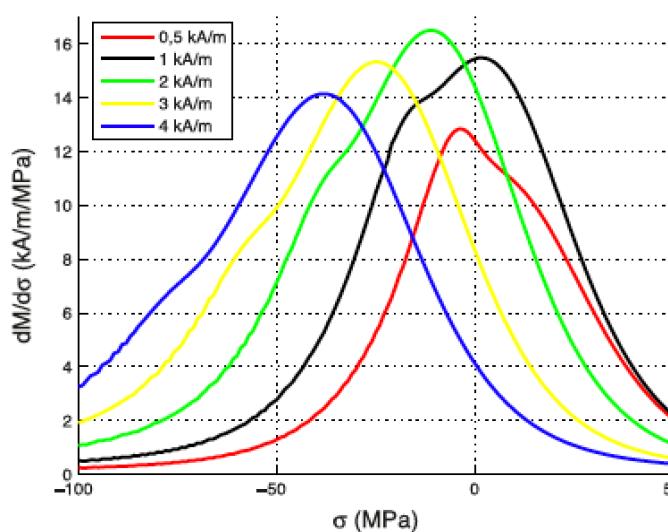
Validation pour contraintes compressives ou extensives

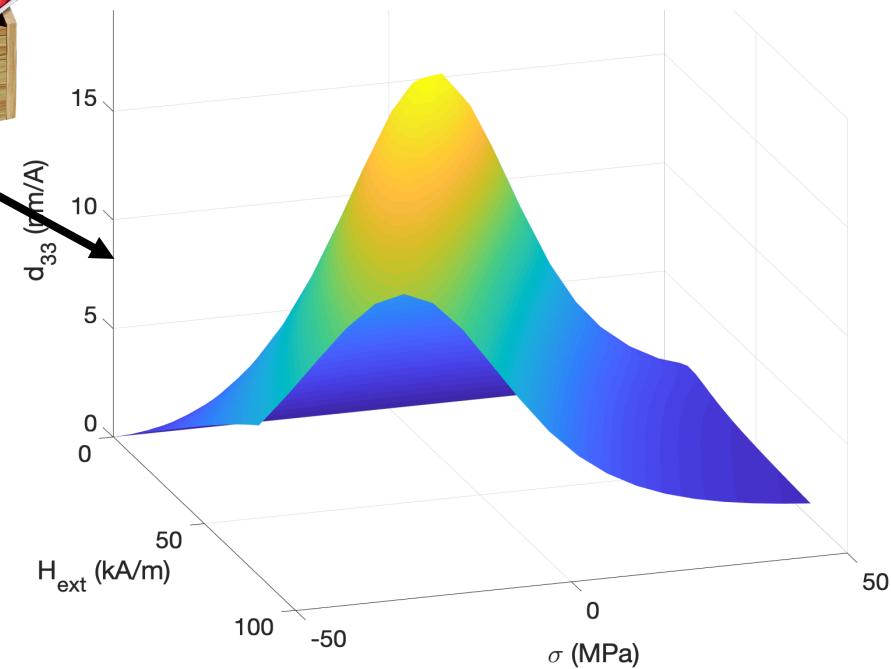
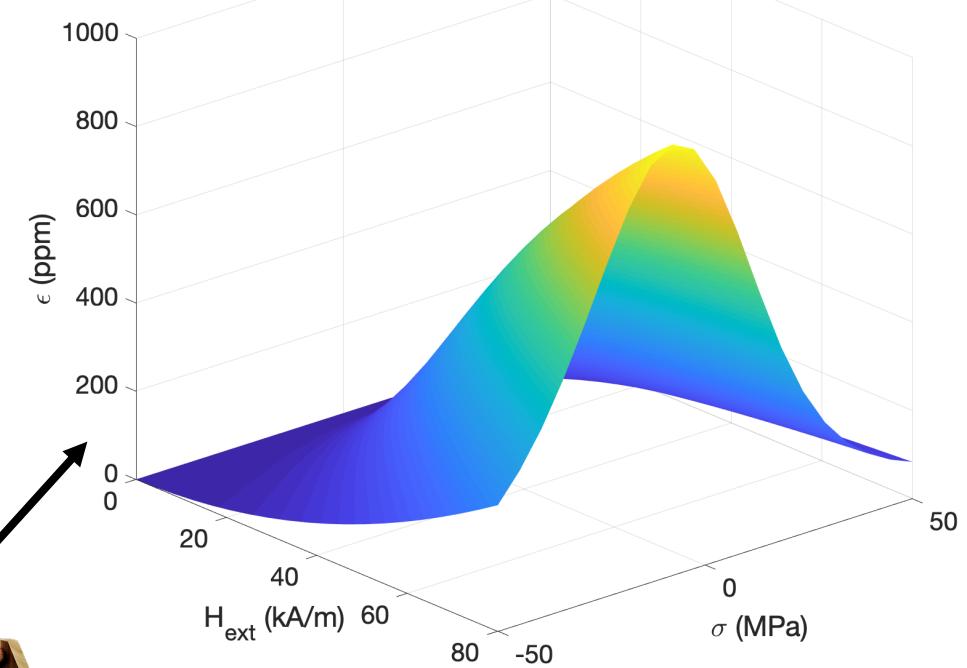
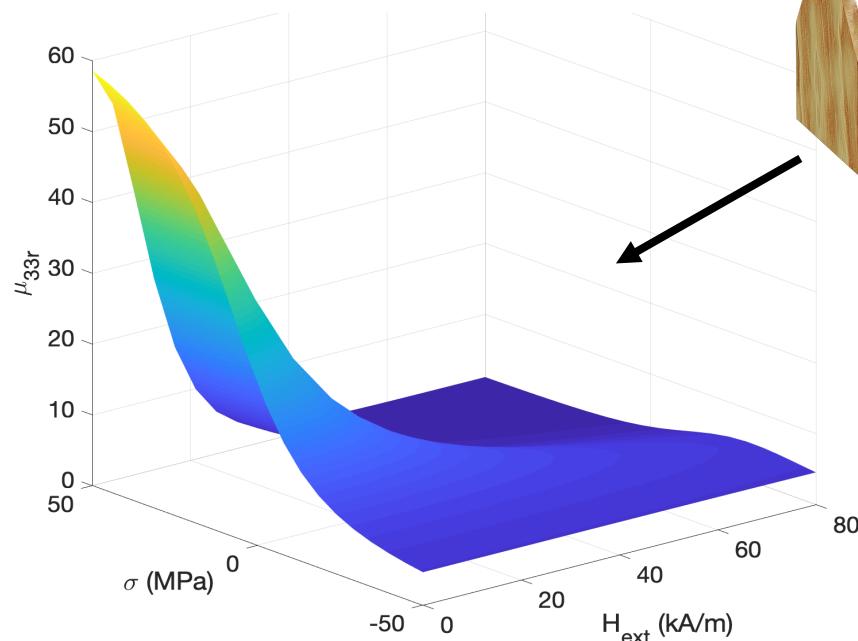
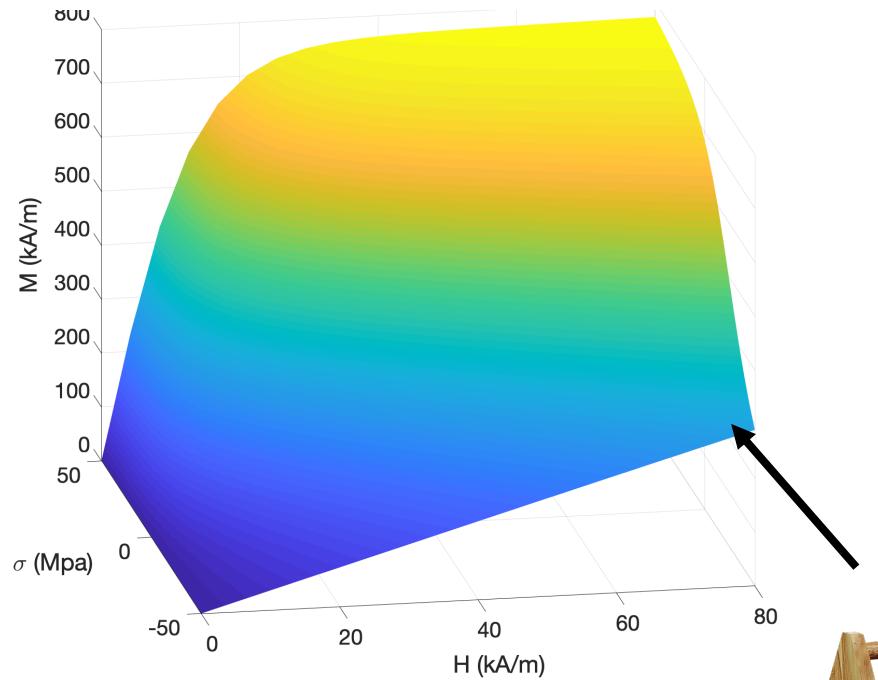


N. Buiron, L. Hirsinger et al
J. Phys. IV France 09 (1999) Pr9-187-Pr9-196

C. Bormio-Nunes, O. Hubert, Piezomagnetic behavior of Fe-Al-B alloys, Journal of Magnetism and Magnetic Materials, 2015,

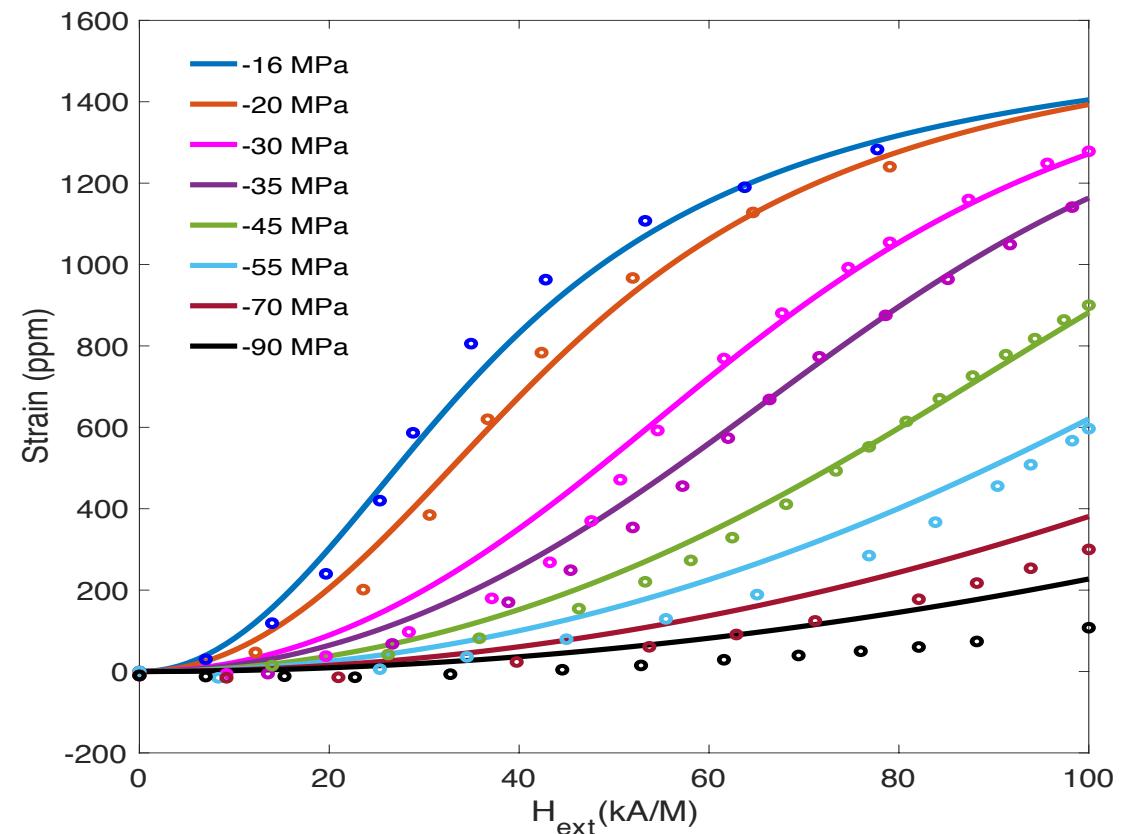
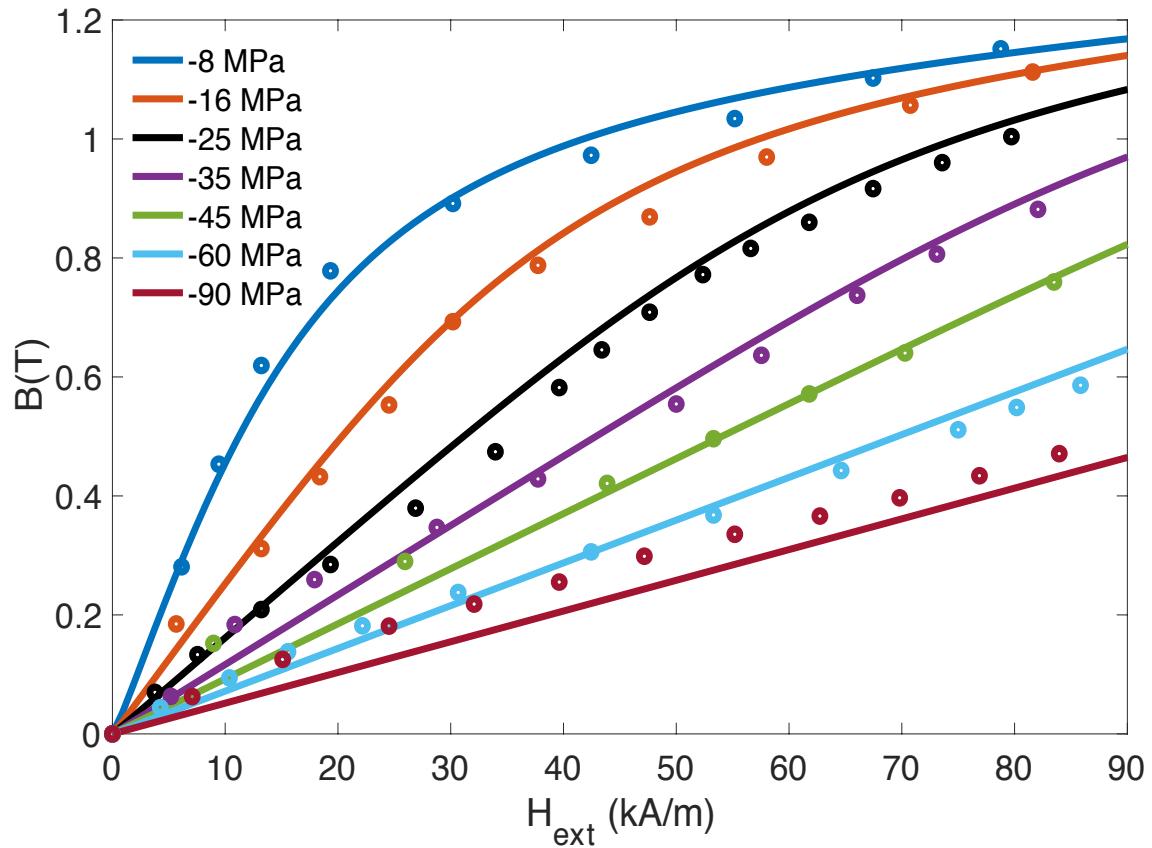
L. Daniel, "An Analytical Model for the Effect of Multiaxial Stress on the Magnetic Susceptibility of Ferromagnetic Materials," IEEE Transactions on Magnetics, May 2013,





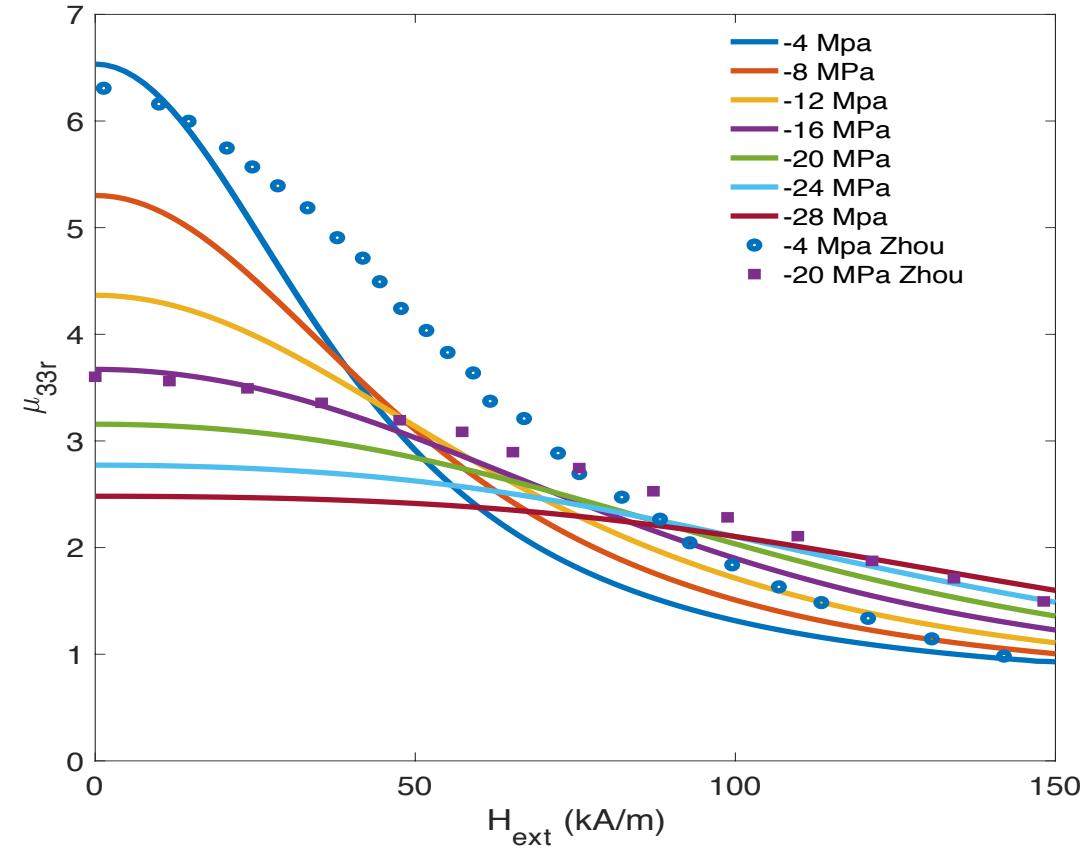
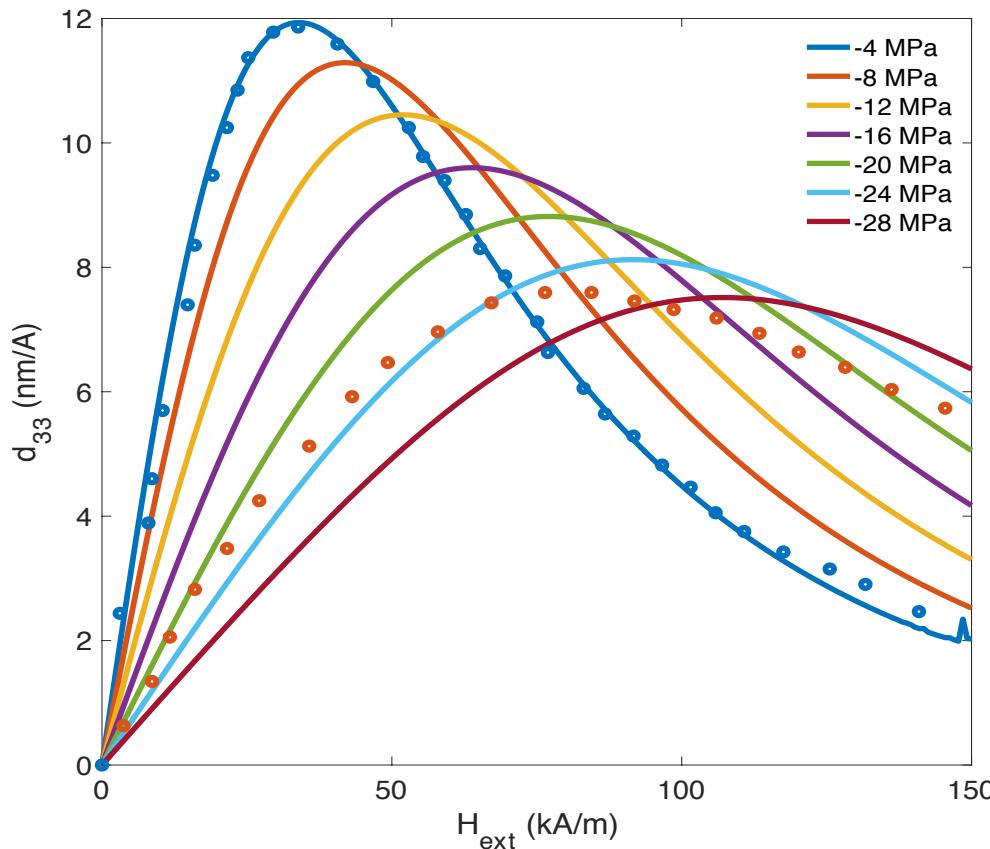
Validation des modèles 1/2

Mesures « o », Modèles « - »

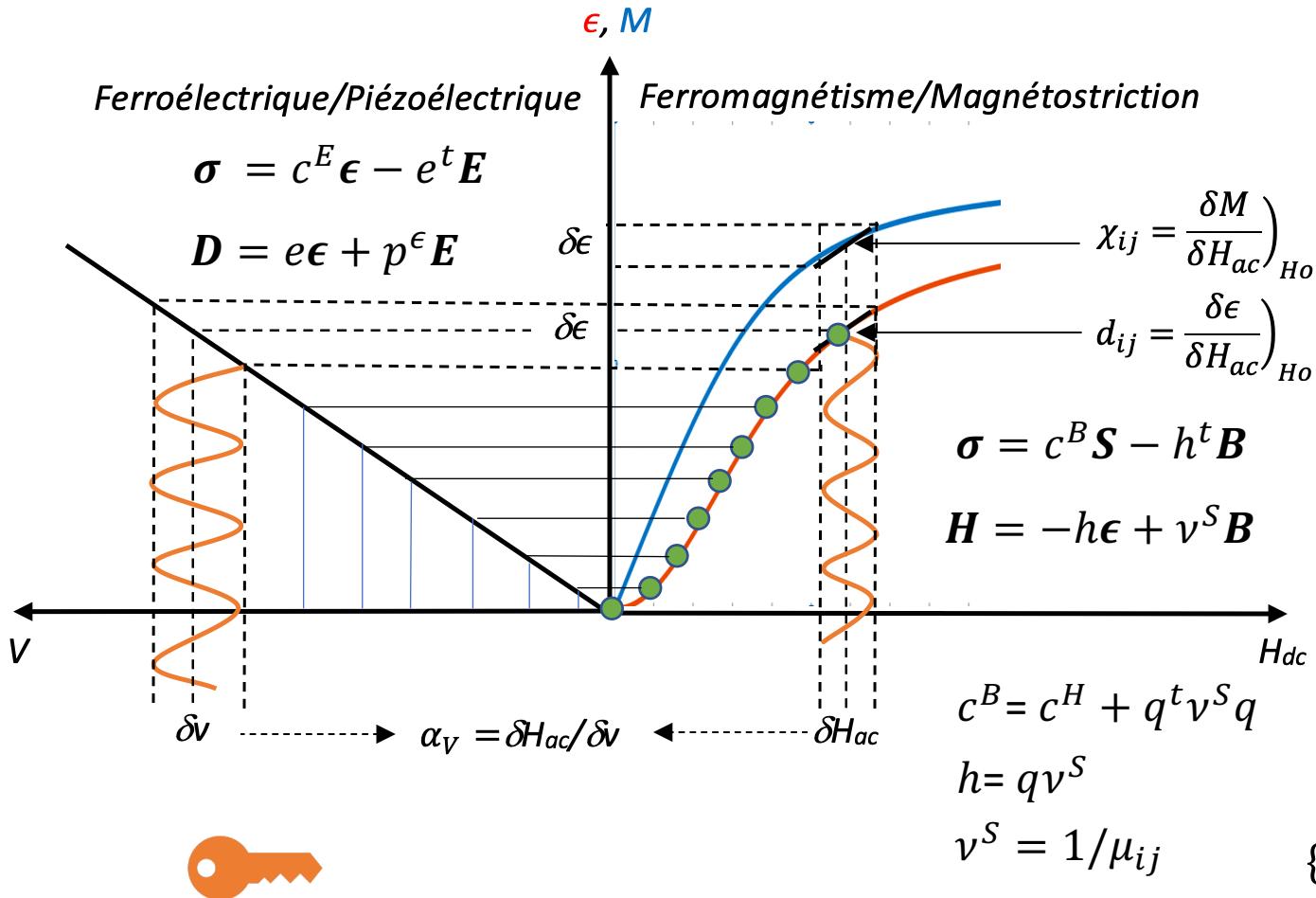


Validation des modèles 2/2

Mesures « o », Modèles « - »



Code FEM : Cas statique-Régime non linéaire



$$\begin{bmatrix} H \\ \sigma \end{bmatrix} = \begin{bmatrix} v_{ij} & -h_{ij}' \\ -h & C_{ijkl}^B \end{bmatrix} \begin{bmatrix} B \\ \epsilon \end{bmatrix} \quad jac = \begin{bmatrix} v_{ij} & -h_{ij}' \\ -h & C_{ijkl}^B \end{bmatrix}$$

Équations d'équilibre (EQ) Relations potentiels (RP)

$$\operatorname{div} \mathbf{D} = 0$$

$$\mathbf{E} = -\operatorname{grad}(V)$$

$$\operatorname{rot} \mathbf{H} - J_{dc} = 0$$

$$\mathbf{B} = \operatorname{rot}(\mathbf{a})$$

$$\operatorname{div} \boldsymbol{\sigma} + \mathbf{f} = 0$$

$$\epsilon = \frac{1}{2} (\operatorname{grad} \mathbf{u} + \operatorname{grad}^t \mathbf{u})$$

Méthode des résidus pondérés

$$W(z) = \int_V \langle \varphi \rangle \{R(z)dV\} = 0 \quad R(z)$$

Équations d'équilibre

RP+ LC +conditions Dirichlet & Neumann

$$[K]\{X\} = [F]$$

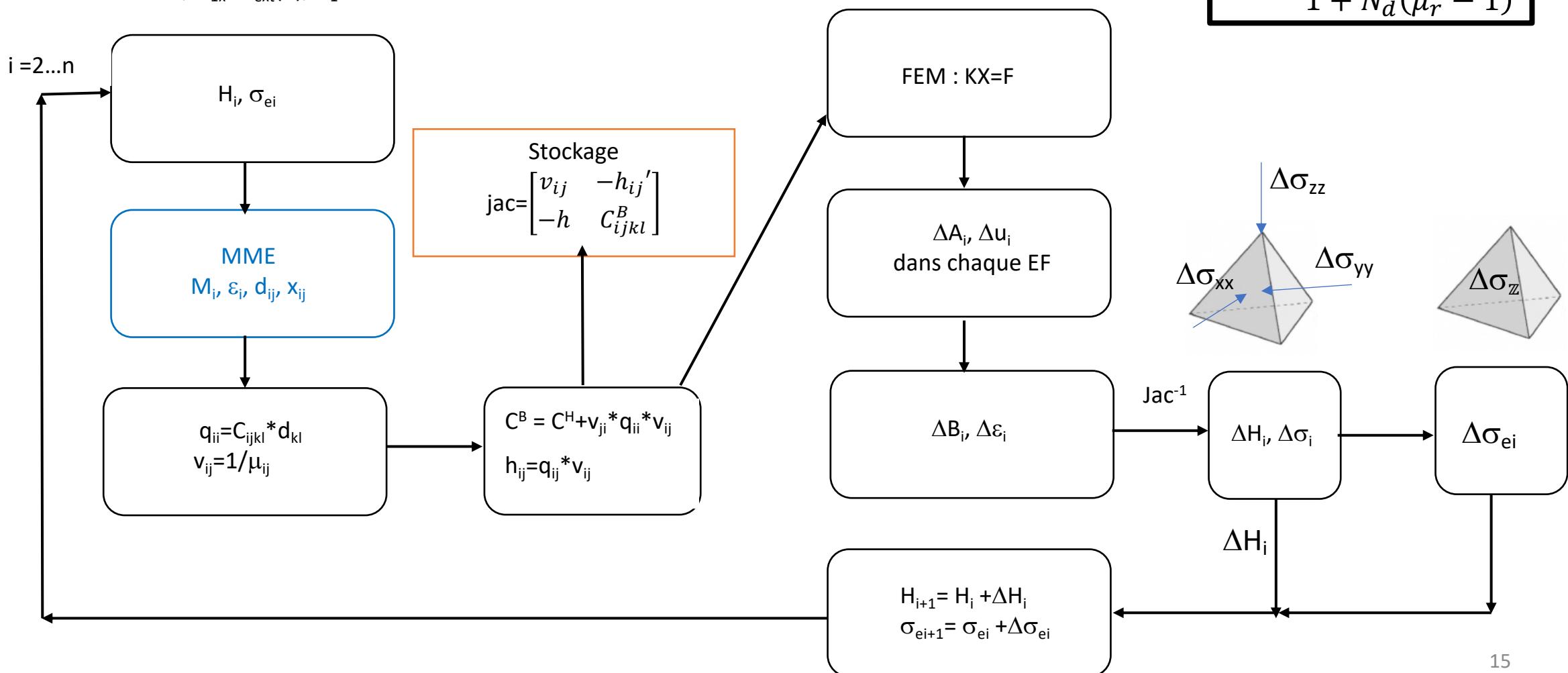
$$\{X\} = \{u \quad \mathbf{a} \quad V\}^t$$

$$[F] = [F \quad F_{dc} \quad 0]^t$$

$$[K] = \begin{bmatrix} K_{uu} & -K_{au}^t & K_{uv} \\ -K_{au} & K_{aa} & 0 \\ K_{uv}^t & 0 & -K_{vv} \end{bmatrix}$$

Algorithme d'implémentation

$H_{ext} = H_{min} \dots H_{max}$
 (n valeurs) $i = 1, H_{1x} = H_{ext}(1), \sigma_1 = 0$



Code FEM: Cas dynamique-Régime linéaire

Equations d'équilibre (EQ)

$$\operatorname{div} \boldsymbol{D} = 0$$

$$\operatorname{rot} \boldsymbol{H} - \boldsymbol{J}_{ac} = 0$$

$$\operatorname{div} \boldsymbol{\sigma} + \boldsymbol{f} = \rho_m \frac{\partial^2 \boldsymbol{u}}{\partial t^2}$$

Relations potentiels (RP)

$$\boldsymbol{E} = -\operatorname{grad}(V)$$

$$\boldsymbol{B} = \operatorname{rot}(\boldsymbol{a})$$

$$\boldsymbol{\epsilon} = \frac{1}{2} (\operatorname{grad} \boldsymbol{u} + \operatorname{grad}^t \boldsymbol{u})$$

Méthode des résidus pondérés

$$W(z) = \int_V \langle \varphi \rangle \{R(z)dV\} = 0 \quad R(z)$$

Equations d'équilibre

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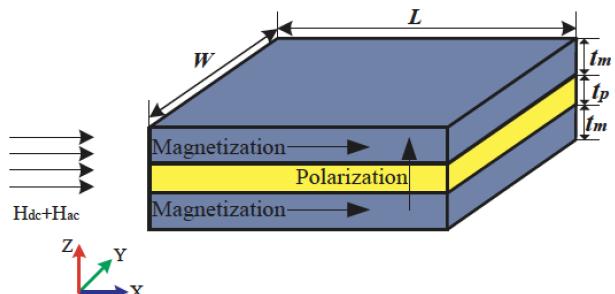
$$[\boldsymbol{K}_{ac}]\{X\} = [F]$$

$$C_{uu} = \beta K_{uu} + \alpha M$$

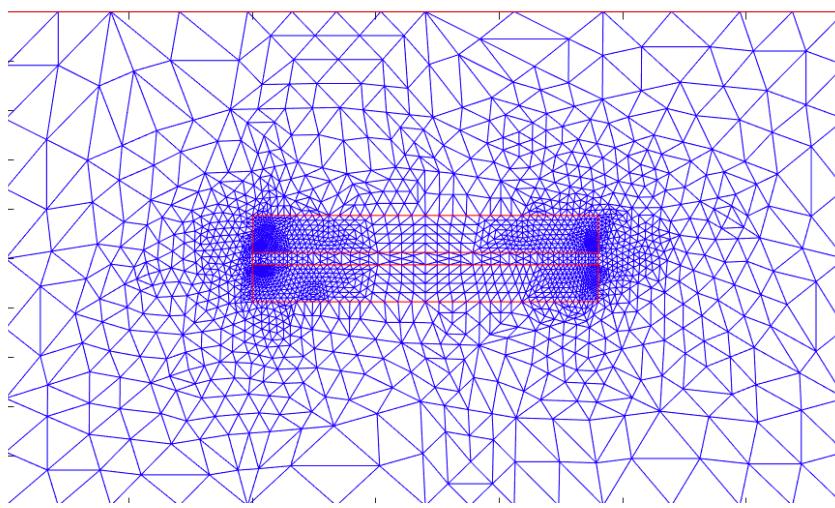
$$[\boldsymbol{K}_{ac}] = \begin{bmatrix} K_{uu} - \omega^2 \mathbf{M} + j\omega C_{uu} & -K_{au}^t & K_{uv} \\ -K_{au} & K_{aa} & 0 \\ K_{uv}^t & 0 & -K_{vv} \end{bmatrix}$$

Non-damped ($\alpha=0$ and $\beta=0$);
 Viscous damping ($\alpha=0$ and $\beta>0$);
 Damping proportional to the mass ($\alpha>0$ and $\beta=0$)
 Rayleigh damping ($\alpha>0$ and $\beta>0$).

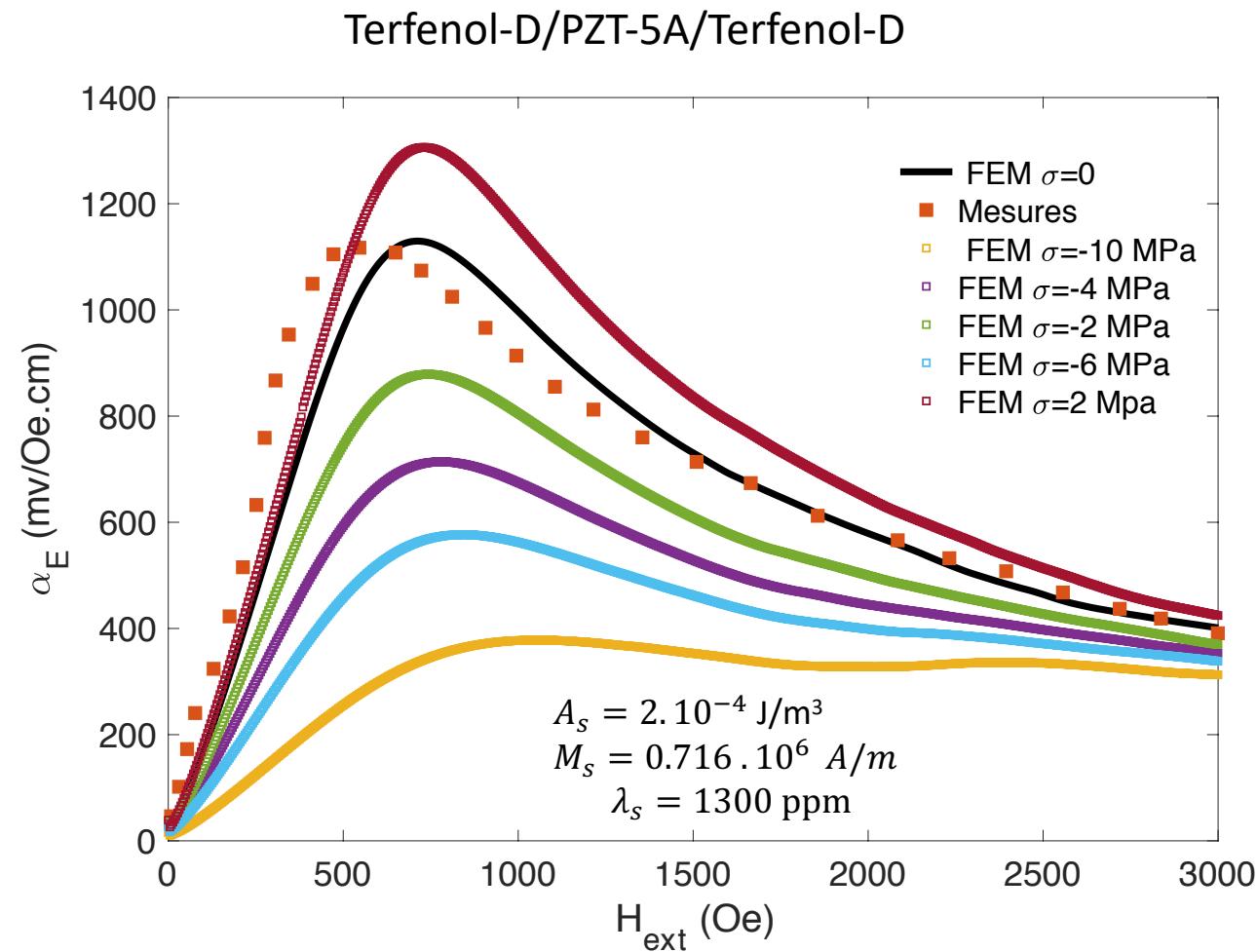
Mesure vs FEM 2D



Jian Han, Juanjuan Zhang, Yuanwen Gao, A nonlinear magneto-mechanical-thermal-electric coupling model of Terfenol-D/PZT/Terfenol-D and Ni/PZT/Ni laminates, Journal of Magnetism and Magnetic Materials, Vol 466, 2018,



$$N_d \approx (w t / l^2) [\ln(4l/(w+t)) - 1]$$



Conclusion

- Modèles analytiques ($\sigma=0$ et $\neq 0$) MME simplifié=> Energie de Gibbs
- Domaine de validité $\sigma \neq 0$, facteur « n » à définir
- Validation comportementale des modèles pour $\sigma>0$ et < 0
- Validation via des mesures Terfenol-D
- Implémentation réussie code FEM 2D
- Ajout de la température en cours....

Effet de la température (1/2)

$$\Delta T = T - T_r$$

$$M_s^T = M_{\text{so}} \left(1 - \left(\frac{T}{T_c} \right)^{3/2} \right)$$

$$\lambda_s(T) = \lambda_{\text{so}} \left(1 - \left(\frac{T}{T_c} \right)^{3/2} \right)$$

Expressions de \mathbf{M} et μ_{33r} $M_s \Rightarrow M_s^T$

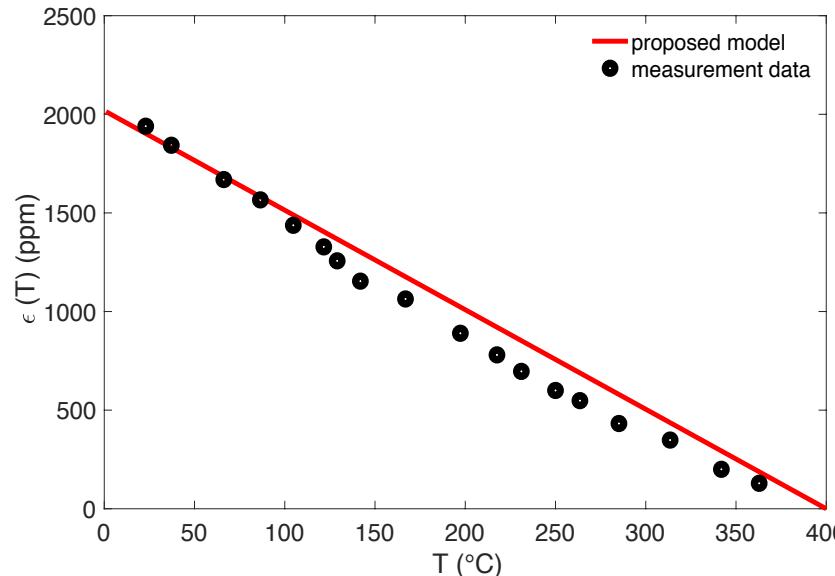
$$\beta = \frac{\partial \lambda_s(T_r)}{\partial T} = \left. \frac{\partial \lambda_s(T)}{\partial T} \right|_{T=T_r} = -\frac{3\lambda_{\text{so}}}{2T_c}$$

$$\lambda_s^T = \lambda_s(T) \approx \lambda_s(T_r) + \frac{\partial \lambda_s(T_r)}{\partial T} \Delta T$$

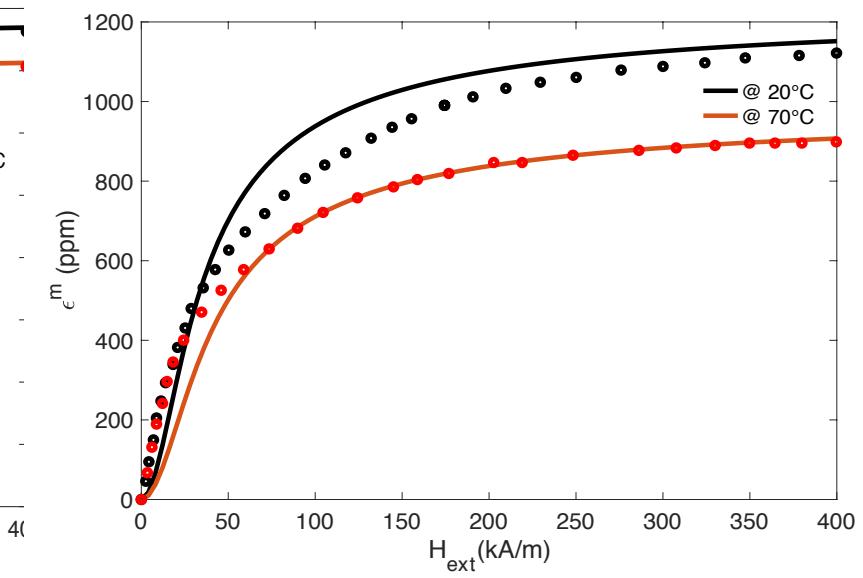
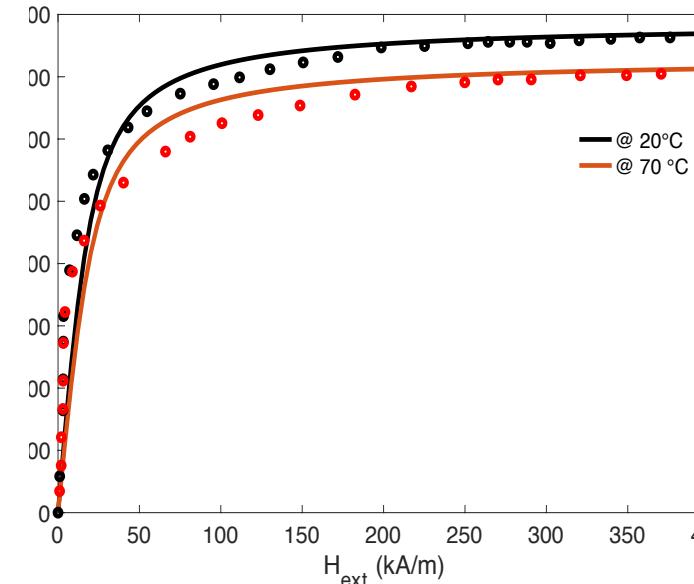
$$\lambda_s(T) \approx \lambda_{\text{so}} - \beta T$$

$$\boldsymbol{\varepsilon}_{zz}^{m,T} = (\lambda_{\text{so}} - \beta T)(1 - \kappa) = \boldsymbol{\varepsilon}_{zz}^m - \frac{\beta T}{\lambda_{\text{so}}} \boldsymbol{\varepsilon}_{zz}^m$$

A. Clark and D. Crowder, "High temperature magnetostriction of TbFe2 and Tb_{0.27}Dy_{0.73}Fe2," in IEEE Transactions on Magnetics, vol. 21, no. 5, pp. 1945-1947, September 1985, .



Xiao Jing Zheng and Le Sun, A nonlinear constitutive model of magneto-thermo-mechanical coupling for giant magnetostrictive materials, Journal of Applied Physics 100, 063906 (2006); doi: 10.1063/1.2338834



Effet de la température (2/2)

