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Olivier Hubert, Xavier Milhet, Pascal Gadaud, Mathieu Tatat, Pierre-Olivier Renault, et al.. Modeling of Young's modulus variations with temperature of Ni and oxidized Ni using a magneto-mechanical approach. Materials Science and Engineering: A, 2015, 633, pp.76-91. <10.1016/j.msea.2015.03.014>. <hal-01530469>

HAL Id: hal-01530469

<https://hal.science/hal-01530469v1>

Submitted on 31 May 2017

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Modeling of Young's modulus variations with temperature of Ni and oxidized Ni using a magneto-mechanical approach.

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Abstract

Thin films and coatings are usually used to give functional properties to the surface of the underlying substrate but are never seen as load bearing due to a very low film to substrate thickness ratio. However, this ratio can increase in some specific domains (such as transportation), where the weight reduction is a high stake. This study deals with the influence of the thermally grown oxide (TGO) NiO on the evolution of the elastic modulus of nickel with temperature. For pure nickel, the Young's modulus evolves non-linearly with temperature, from room temperature up to 360°C, corresponding to the Curie temperature of nickel. The amplitude of these variations can be drastically reduced with the presence of the NiO TGO. The purpose of this study is to propose a modeling of these phenomenon using magneto-mechanical approach. A first analytical modeling takes the change of the saturation magnetization, of the initial anhysteretic susceptibility and of the maximal magnetostriction with a relaxation of magneto-crystalline anisotropy concomitant to increasing temperature, into account. The second modeling is a numerical modeling giving the average behavior of a representative volume element. It allows a continuous description of the change with temperature of the Young's modulus and a clear interpretation of the effect of a coating. This gives an insight for future promising applications.

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Keywords: Nickel, Thermally-Grown-Oxide, *Delta E* effect, Magneto-mechanical coupling, Magnetostriction, Multiscale modeling, Residual stresses

1. Introduction

Thin films and coatings are generally used to give functional properties to the surface of the underlying substrate. For example, they play an important role of diffusion barriers to prevent the degradation of the substrate by oxidation when used at high temperature [1]; they can be used to prevent wear and erosion, or to provide lubrication and thermal insulation [2]. Various chemical and/or physical deposition techniques (with various compositions) can be used or they can develop naturally, resulting for example from the oxidation of the surface in a controlled atmosphere (thermally grown oxide TGO) [3]. Generally, these films are very thin and are not seen as load bearing. In some particular applications, such as turbine blades for example, the coating to substrate thickness ratio increases, inducing some peculiar mechanical behaviors as observed for Young's modulus variation of oxidized nickel in a recent study [4, 5]. The elastic modulus has been measured from 20°C up to 600°C. Its evolution with temperature is non-linear and non monotonous from room temperature up to 360°C, corresponding to the Curie temperature of nickel. But the amplitude of these variations can be drastically reduced by the TGO.

The non-monotonous Young's modulus evolution with temperature was previously reported by many authors [6, 7, 8], known as temperature dependent ΔE effect. Its relation with the mechanical or magnetic state of material was discussed in the early work of Bozorth [6] who reported experiments from Siegel, Quimby and Köster [9].

The influence of TGO on this behavior was not reported since the work of Tatat [5] (except experiments of Huntz interpreted as internal stress rearrangement [10]) and no model was proposed to simulate the variation of pure nickel Young's modulus with temperature and model the influence of the oxide layer on this behavior. Actually, it was suspected to arise from a long-range modification of the internal stresses within the substrate. This interpretation seems accurate considering that stress is well known to change significantly the magnetic behavior [6, 7, 11] and the apparent Young's mod-

33 ulus of a wide range of magnetic materials [12].

34

35 The purpose of this paper is to propose a modeling of the variation of
36 Young's modulus of Ni and Ni-NiO layers with temperature using a magneto-
37 mechanical approach. As these approaches usually consider the influence of
38 multiaxial stress on the magneto-mechanical behavior, they allow an accu-
39 rate modeling of both Young's modulus (seen a stress *vs* strain ratio for a
40 low stress amplitude) and internal stress effect. Experimental results are first
41 reminded. Two modeling approaches are then proposed: an analytical mod-
42 eling first based on a room temperature ΔE effect modeling [12]; a numerical
43 implementation is secondly detailed based on the work of Daniel [13] allowing
44 a continuous description of the Young's modulus variations with temperature
45 and taking the TGO, or any other coating nature leading to residual stresses,
46 into account.

47 2. Experimental results and interpretation

48 2.1. Material and experimental features

49 A pure (>99%) 2 mm thick polycrystalline nickel has been used for the
50 experimental study [4, 5]; the initial grain size of the Ni samples is about
51 30 μm . After a soft mechanical polishing, samples have been oxidized in
52 synthetic air (80% nitrogen, 20% oxygen) during 1h30 at 1110°C to form
53 NiO coatings and then furnace cooled at approximately 300°C/h. The spec-
54 imen was exposed to an $Ar - H_2$ flow to limit the oxidation prior to the
55 target temperature and during cooling. The oxidation was simultaneously
56 performed on the two opposite free surfaces of the Ni samples. After oxida-
57 tion, the thickness of the NiO coatings has been estimated at 16 μm thick
58 (figure 1). Electron Back Scattered Diffraction (EBSD) measurements were
59 carried out on a polished sample after oxidation (for a 40mm² area - 10mm
60 \times 4mm). Figure 2 shows a typical example of inverse pole figure (with re-
61 spect to the normal direction ND) obtained after oxidizing. The grain size of
62 the Ni substrate has evolved substantially by growing up to about 280 μm .
63 Texture index concludes on the other hand to a quasi-isotropic distribution
64 of orientations: the material can be considered as isotropic.

65 The elastic properties of the specimens were investigated from room tem-
66 perature (RT) up to 600°C by means of the resonant frequency technique in
67 bending mode [14] in the 1-10 kHz range (the temperature range 20°C to
68 600°C was chosen in order to make sure to measure the material behavior

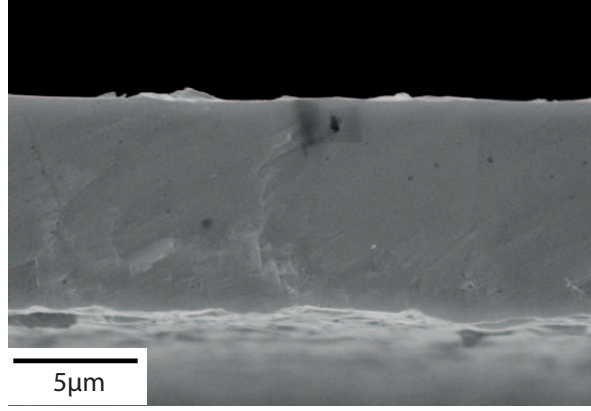


Figure 1: SEM observation of typical NiO oxide layer after oxidizing in synthetic air during 1h30 at 1110°C.

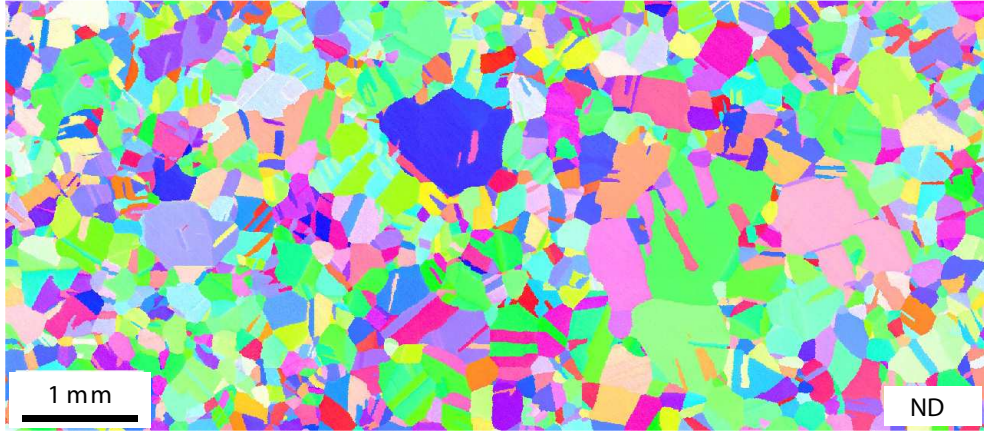


Figure 2: Inverse pole figure (normal direction ND) obtained by EBSD on the Ni sample after oxidizing treatment.

69 well above the Curie temperature). This method is detailed hereafter: In
 70 the case of a bulk material, the longitudinal Young's modulus (E) can be
 71 deduced using the following relation [15]:

$$E = 0.9464\rho f^2 \frac{L^4}{h^2} \zeta \quad (1)$$

72 where f is the flexural resonance frequency, ρ the density, h and L , the

73 beam thickness (0.5 to 2 mm) and span length (20 to 30 mm), and ζ , a
74 correcting factor close to 1. The sample is maintained horizontally between
75 steel wires located at the vibration nodes. Both excitation and detection
76 are performed using an electrostatic device (capacitance created between the
77 sample and a unique electrode). Using this set-up, the Young's modulus can
78 be measured from -150°C up to 1100°C without any harmful contact. The
79 heating rate can be as low as 1°C/min and high vacuum ($\approx 10^{-4}$ Pa) is used
80 to hinder or limit the specimen oxidation. The accuracy of this method is
81 better than 0.5% for conductive bulk materials whatever the rigidity range.
82 An important feature of this technique lies in the very low applied stress
83 level, less than 1 MPa.

85 2.2. Variation of Young's modulus

86 Figure 3 shows the evolution of the Young's modulus of the specimens
87 with temperature [4]. The measurements reported here were performed us-
88 ing the same Ni substrate; the Young's modulus was first measured on the
89 laminated state before oxidation, secondly on the two-sides oxidized speci-
90 men (*i.e.* two NiO coatings) and, finally, after removing one and both NiO
91 coatings successively by fine polishing (noted as "peeled off samples" in the
92 following). The procedure to remove the oxide, based on conventional met-
93 allographic techniques, included an ultimate step of fine chemo-mechanical
94 polishing in order to reach a very low roughness without work hardening *i.e.*
95 no additional residual stresses in the sub-surface.

96 Two domains are clearly evidenced in figure 3, depending on the tempera-
97 ture. Above approximately $T = 360^\circ\text{C}$, the evolution of the elastic modulus is
98 quite similar regardless to the specimen state, characterized by the expected
99 linear decrease of the Young's modulus with the temperature. A slight dif-
100 ference between non-oxidized and oxidized substrates can be observed due
101 to composite effect: the Young's modulus of NiO is usually higher than the
102 Young's modulus of pure Ni; its value depends strongly on oxidizing temper-
103 ature and oxide porosity [4]. It must be emphasized that the increase of the
104 grain size from 30 to 280 μm does not act on the modulus of the substrate
105 (the experimental technique integrates all the sample volume).

106
107 Below this threshold temperature, the Young's modulus depends strik-
108 ingly on the structural configuration of the specimens:

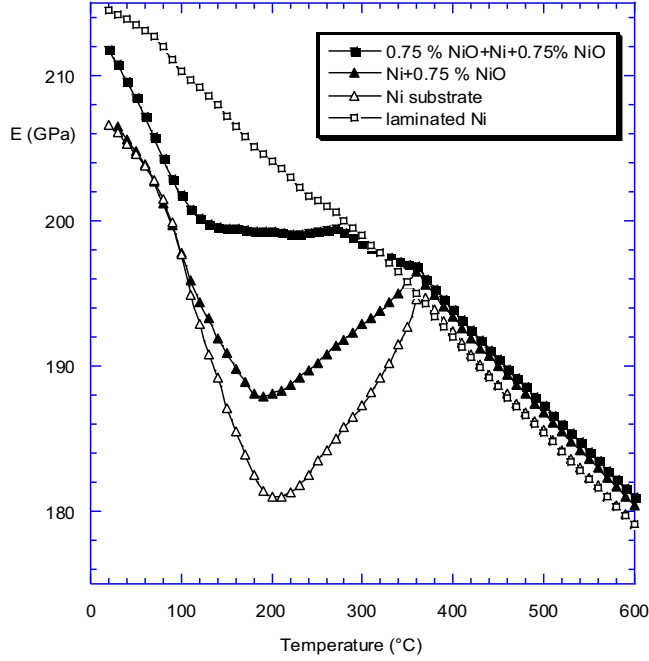


Figure 3: Variation of Young's modulus with temperature for different specimens.

- the presence of the NiO oxide layer representing only about 3% of the total thickness on the Ni substrate significantly influences the value of the elastic modulus (apparent Young's modulus E_a) at a temperature range between 90°C and 360°C.
- the variation of the Young's modulus at 260°C for oxidized samples can be associated to the Néel temperature transition of NiO.
- the maximum deviation of E_a is about 9% between nickel and nickel-oxide.

2.3. Estimation of residual stresses

The residual stresses have been determined at RT using the X-ray diffraction (XRD) so-called $\sin^2\psi$ method [16] where ψ is defined as the angle between the normal to the sample surface and the normal to the diffracting

121 planes. X-ray measurements were carried out using a four-circle diffractome-
 122 ter (Seifert XRD 3003) operating at 40 kV and 40 mA, with a Cu X-ray tube
 123 ($\lambda_{K\alpha} = 0.15418$ nm) equipped with a 1×1 mm² point focus and a Ni filter on
 124 the direct beam path to absorb the Cu $K\alpha$ radiation. The incident beam was
 125 collimated using a collimator 1 mm in diameter and targeted on the samples
 126 mounted on an Eulerian cradle for ψ tilting. The X-ray measurements have
 127 been performed for fourteen different ψ angles for two independent plane
 128 families, namely $\{331\}$ and $\{420\}$. The residual stress state was calculated
 129 from the lattice strains assuming a planar equibiaxial stress state and using
 130 the X-ray elastic constants [17]. For a polycrystalline quasi-isotropic mate-
 131 rial of Young's modulus E and Poisson's ratio ν , the biaxial residual stress
 132 state of magnitude σ^r is given by the slope of $\sin(\theta)^{-1} = f(\sin^2\psi)$ function
 133 following:

$$\frac{\sin(\theta_0)}{\sin(\theta)} = \sigma^r \left(\frac{(1 + \nu)\sin^2\psi - 2\nu}{E} \right) + 1 \quad (2)$$

134 where θ and θ_0 indicate the Bragg's angle of the diffracting plane with
 135 or without stress respectively. The technique was used to evaluate the resid-
 136 ual stress level inside both the as-received material and the material after
 137 oxidation [5]. In the as-received state the material exhibits a high level of
 138 residual stress in sub-surface that corresponds to a biaxial compression of
 139 amplitude -130 ± 30 MPa. This surface stress state should be equilibrated by
 140 an internal bi-tension stress that can unfortunately not be estimated because
 141 the transition area between these two fields cannot clearly be defined. It can
 142 be considered that thermal treatment completely reduces this stress field to
 143 zero since a global recrystallization mechanism occurs.

144
 145 After oxidation, the internal stresses have only been determined in the
 146 NiO coatings. Actually the X-Ray diffraction analysis is not possible in the
 147 Ni layer due to the large grain size. Internal stresses in NiO correspond
 148 to an equibicompensation of amplitude -550 ± 50 MPa [5]. Similar compressive
 149 stresses values are reported in literature [10, 19]. They mainly result from the
 150 thermal mismatch coefficients between the coating and the substrate. Indeed
 151 dilatation coefficients for NiO and Ni are respectively: $\alpha_{NiO} = 14.5 \times 10^{-6} \text{K}^{-1}$
 152 and $\alpha_{Ni} = 17.5 \times 10^{-6} \text{K}^{-1}$ [18, 19]. The thermal stresses distribution in the
 153 Ni layer has been determined from a simple beam analysis integrating the
 154 experimental values obtained for the oxide coatings thickness and residual
 155 stress, and considering a global equilibrium (force and momentum equilib-

rium). For NiO-Ni-NiO system, the in-plane stress in the Ni substrate is a bi-tension and remains constant over the entire thickness ($+9\pm 1$ MPa), while for Ni-NiO the stress decreases linearly from a bi-tension ($+18\pm 2$ MPa) to a bi-compression state (-9 ± 1 MPa) giving an average value of $+3\pm 1$ MPa. After removal of the double oxide coating, it may be assumed that the Ni layer is completely internal stress free.

As seen in figure 3 and table 1, internal stresses of few MPa are sufficient to significantly modify the apparent Young's modulus of nickel. Results reported in table 1 correspond to the estimated average biaxial stress inside the Ni Layer.

Table 1: Change of ΔE effect with biaxial residual stress level of amplitude σ^r .

Configuration	Cold rolled	2-sides oxidized	1-side oxidized	Peeled-off
$\Delta E/E(\%)$	0	-3	-8	-11
$\sigma^r(\text{MPa})$	unknown	+9	+3 (average)	0

2.4. Results interpretation

The non monotonous change of Young's modulus with temperature and effect of TGO cannot be explained by a classical mechanical rule of mixture but by magneto-elastic considerations. Ni is a ferromagnetic material exhibiting magnetic domains below its Curie temperature, T_C , equal to 360°C [6].

The observed evolution of pure Ni Young's modulus for increasing temperature was already experimentally reported in literature [6, 7, 8]. This deviation from the Hooke's law is known as the ΔE effect ("Δ" for variation) and can only be highlighted in the very first stage of stress-strain curves [13]. A relation with the magnetic character of the material can be made considering:

1. The phenomenon is strongly dependent on the magnetization M of the layer: at the magnetic saturation ($M = M_s$; M_s : saturation magnetization of the material) the non-linear variation of Young's modulus progressively vanishes.

183 2. Young's modulus recovers its linear variation with temperature above
 184 the Curie temperature of the layer (360°C).

185 These points are illustrated in figure 4a.

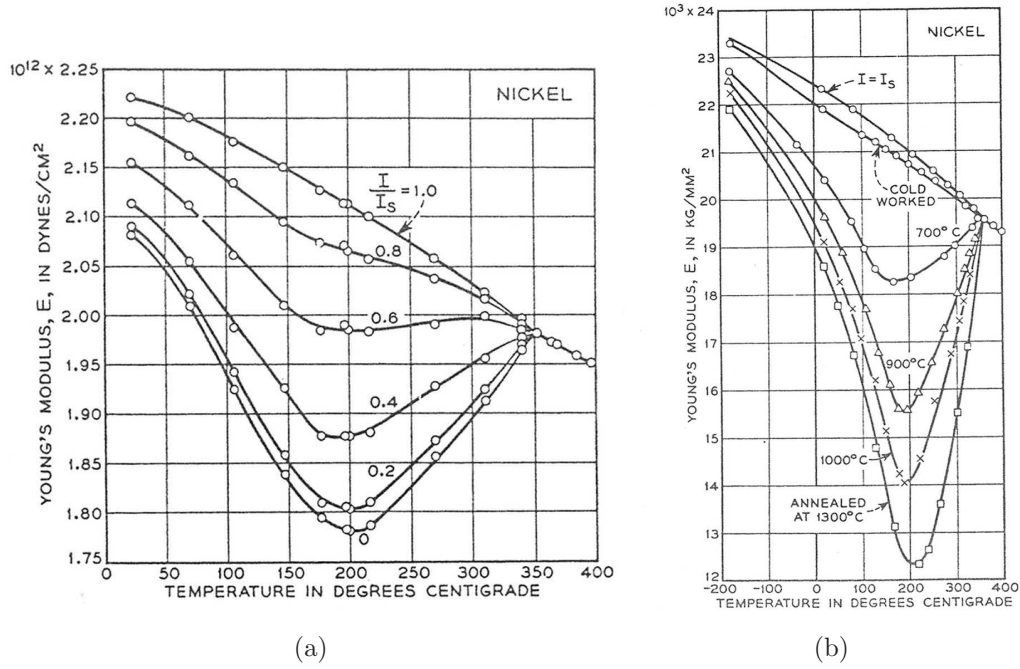


Figure 4: Apparent Young's modulus of nickel vs. Temperature: (a) effect of magnetization to saturation magnetization ratio (I/I_s); (b) effect of mechanical condition ("internal stress") and thermal annealing [6] - NB: $10^{12}[\text{Dynes/cm}^2]=10^2[\text{GPa}]$; $10^3[\text{Kg/mm}^2]=9.81[\text{GPa}]\approx 10[\text{GPa}]$.

186 As magnetic properties of ferromagnetic materials depend on the tem-
 187 perature, the amplitude of ΔE effect can change. In particular, the magne-
 188 tocrystalline anisotropy (determining for a single crystal the most favorable
 189 magnetization direction) decreases significantly while the temperature in-
 190 creases, especially from RT up to 100°C for Ni [6]. Hence, with increasing
 191 temperature, the magnetic moments direction becomes progressively more
 192 sensitive to the mechanical stress, enhancing the ΔE effect. From approxi-
 193 mately $T=200^\circ\text{C}$ to the Curie temperature, the spontaneous magnetization
 194 (and consequently the magnetostriction) of Ni quickly decreases down to 0:
 195 the ferromagnetic properties disappear (magnetostrictive and exchange con-
 196 stants progressively decrease to zero). This latter point explains that the ΔE

197 effect is gradually weakened and vanishes at T_C when the material becomes
198 paramagnetic.

199
200 The role of stress is another point to consider. For cold worked nickel (as
201 received material), the decrease of Young's modulus is regular following a
202 classical linear variation with temperature (figure 3). Thermal annealing at
203 increasing temperature progressively enhances the non-linear phenomenon as
204 experimentally observed and reported in figure 4b [6]. The internal stress as-
205 sociated to plasticity acts as a magnetic saturation; the stress relieving at in-
206 creasing annealing temperature acts as a demagnetization. The effect of oxide
207 layers is another typical example of coupling to stress. X-rays measurements
208 indicates that the substrate is submitted to residual stresses. Single-layer or
209 two-layers situations do not lead to the same stress level. The amplitude of
210 non-linearity of Young's modulus is changed. The highest amplitude of ΔE
211 effect is reached for peeled off sample where residual stress reduces to zero.

212
213 Considering finally that the measurement method is based on a stress
214 loading, a quantitative modeling of these phenomena requires to use a fully
215 coupled magneto-mechanical approach and to consider the effect of temper-
216 ature on the parameters involved in this coupling.

217 3. Modeling

218 3.1. ΔE effect definition

219 The so-called ΔE effect is one of the manifestations of magneto-elastic
220 couplings in ferromagnetic materials [7]. It can be defined as the depen-
221 dence of Young's modulus E of a material on its state of magnetization. The
222 Young's modulus of an originally demagnetized specimen appears to be lower
223 (by an amount ΔE) than the Young's modulus of the same specimen magne-
224 tized at saturation (figure 5). Indeed a ferromagnetic material is subdivided
225 in magnetic domains. A magnetic domain corresponds to microscopic or-
226 ganization of magnetic moments aligned together to minimize the so-called
227 exchange energy. Each magnetic domain is magnetized at saturation and
228 characterized by a free isochoric strain called magnetostriction. Due to mag-
229 neto crystalline energy, orientation of magnetic domains is usually associated
230 to crystallographic axes (8 easy directions for nickel - 8 domain families). At
231 zero applied stress or magnetic field and without boundary effect, domains
232 are equally distributed so that the initial deformation and magnetization are

233 null. An increasing magnetic field leads to a progressive increase of the well
 234 oriented domain families volume so that macroscopic magnetization and de-
 235 formation occur (macroscopic magnetostriction ϵ^μ). An increasing uniaxial
 236 stress σ leads to a progressive increase of the well oriented domain fami-
 237 lies of opposite sign so that a macroscopic magnetostriction ϵ^μ occurs while
 238 macroscopic magnetization remains null.

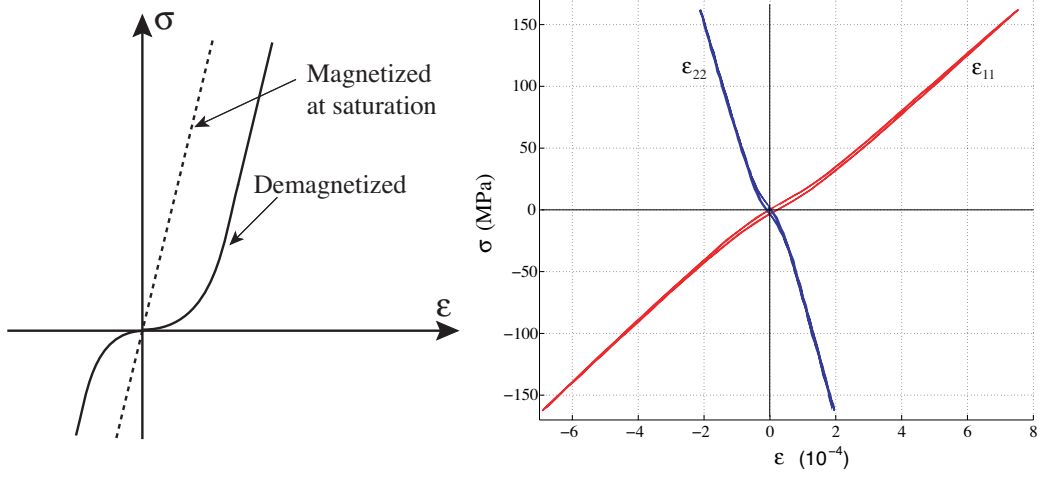


Figure 5: Illustration of the ΔE effect for a tensile-compressive test (ϵ is the total strain); (a) principle (b) illustration for iron-cobalt alloy [20].

This magnetostriction strain ϵ^μ is superimposed to the elastic strain ϵ^{el} , so that the total measured strain ϵ is higher than foreseen without magnetostriction phenomenon. It is defined by equation (3), all the strains being measured in the direction parallel to the applied stress.

$$\epsilon = \epsilon^\mu + \epsilon^{el} \quad (3)$$

Because ϵ^μ is usually non-linear with stress and saturates, the apparent Young's modulus appears non-linear and saturates too. The stress level investigated using the resonant technique for measurement of Young's modulus is very small ($< 1\text{MPa}$). The apparent Young's modulus E_a is given by:

$$E_a = \left(\left. \frac{d\epsilon^\mu}{d\sigma} \right|_{\sigma=0} + \left. \frac{d\epsilon^{el}}{d\sigma} \right|_{\sigma=0} \right)^{-1} \quad (4)$$

In case of a saturated material, the magnetic domain structure has reached a saturated configuration and the magnetostriction strain cannot evolve anymore. The apparent Young's modulus is then defined as:

$$E_a = \left. \frac{d\sigma}{d\epsilon^{el}} \right|_{\sigma=0} \quad (5)$$

leading to a higher value because $\frac{d\epsilon^\mu}{d\sigma}$ is always positive [12]. This phenomenon is described by Bozorth [6] and reported in figure 4. In case of a highly deformed material, the internal stresses saturate the magnetostriction leading to the same effect.

3.2. Analytical modeling of apparent Young's modulus

An analytical modeling of the ΔE effect at RT has been recently proposed [12]. This approach is inspired from a multiscale model for the prediction of magneto-elastic reversible behavior of ferromagnetic materials presented in [13] and in Appendix A. The full multiscale model is used for a numerical resolution in section 4. The simplified approach is limited to the situation where no magnetic field is applied, so that the magneto-static energy does not appear in the definition of the magnetic equilibrium. On the other hand it has been supposed that the magneto-crystalline anisotropy energy does not participate to the evolution of the magnetostriction strain. In such conditions, the elastic energy is the only energy term explicitly considered in the description of the magnetic equilibrium of a domain.

On the other hand, an isotropic polycrystal can be seen as an aggregate of single crystals with random orientation. Polycrystal can be considered as a single crystal for which all directions would be easy directions. In one domain of such a single crystal, the magnetostriction strain tensor can be written (in its own framework):

$$\epsilon_m^\mu = \frac{1}{2} \lambda_{max} \begin{pmatrix} 2 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \quad (6)$$

λ_{max} denotes the maximum magnetostriction strain of the considered polycrystal.

A multi-axial eigen-stress tensor is considered in the macroscopic frame $(\vec{e}_1, \vec{e}_2, \vec{e}_3)$ following:

$$\boldsymbol{\sigma} = \begin{pmatrix} \sigma_{11} & 0 & 0 \\ 0 & \sigma_{22} & 0 \\ 0 & 0 & \sigma_{33} \end{pmatrix} \quad (7)$$

265 The transformation matrix from macroscale to domain scale is given by:

$$\mathbf{P} = \begin{pmatrix} \cos\theta \sin\varphi & \sin\theta & \cos\theta \cos\varphi \\ \sin\theta \sin\varphi & -\cos\theta & \sin\theta \sin\varphi \\ \cos\varphi & 0 & -\sin\varphi \end{pmatrix} \quad (8)$$

266 leading to:

$$\boldsymbol{\epsilon}_p^\mu = {}^t \mathbf{P} \boldsymbol{\epsilon}_m^\mu \mathbf{P} \quad (9)$$

267 The magneto-elastic energy is given for a constant by:

$$W_\sigma^\alpha = -\boldsymbol{\sigma} : \boldsymbol{\epsilon}_p^\mu \quad (10)$$

that can be expressed as function of strain and stress components following:

$$W_\sigma^\alpha = -\frac{\lambda_{max}}{2} (\sigma_{11}(3 \cos^2\theta \sin^2\varphi - 1) + \sigma_{22}(3 \sin^2\theta \sin^2\varphi - 1) + \sigma_{33}(3 \cos^2\varphi - 1)) \quad (11)$$

268 Angles θ ($0-2\pi$) and φ ($0-\pi$) define the orientation of domain in the macro-
269 scopic frame.

270

271 Considering homogeneous stiffness, localization operation is avoided. The
272 average magnetostriction is given by:

$$\boldsymbol{\epsilon}^\mu = \int_\alpha f_\alpha \boldsymbol{\epsilon}_p^\mu \quad (12)$$

273 f_α indicates the volume fraction of domain α (see equation A.8 in Ap-
274 pendix A) calculated using:

$$f_\alpha = \frac{\exp(-A_s \cdot W_\sigma^\alpha)}{\int_0^{2\pi} \int_0^\pi \exp(-A_s \cdot W_\sigma^\alpha) \sin\varphi \, d\varphi \, d\theta} \quad (13)$$

with (see equation A.11 in Appendix A):

$$A_s = \frac{3\chi_0(T)}{\mu_0 M_s(T)^2} \frac{T^{RT}}{T} \quad (14)$$

χ_0 and M_s are the initial anhysteretic susceptibility (variation of anhysteretic magnetization with magnetic field) and saturation magnetization. μ_0 is the vacuum permeability ($=4\pi \times 10^{-7}$ Henry/m). T indicates the actual temperature and T^{RT} the room temperature.

A tensile test of magnitude σ along the macroscopic unit vector \vec{e}_3 is now considered. The magneto-elastic energy expression is simplified into:

$$W_\sigma^\alpha = -\frac{1}{2}\lambda_{max}\sigma(3\cos^2\varphi - 1) \quad (15)$$

The magnetostriction strain tensor is diagonal:

$$\epsilon^\mu = \frac{\pi\lambda_{max}S_2}{2S_1} \exp\left(-\frac{1}{2}A_s\lambda_{max}\sigma\right) \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 2 \end{pmatrix} \quad (16)$$

with

$$S_1 = 2\pi \exp\left(-\frac{1}{2}A_s\lambda_{max}\sigma\right) \int_0^\pi \exp\left(\frac{3}{2}A_s\lambda_{max}\sigma\cos^2\varphi\right) \sin\varphi d\varphi \quad (17)$$

and,

$$S_2 = \int_0^\pi (3\cos^2\varphi - 1) \exp\left(\frac{3}{2}A_s\lambda_{max}\sigma\cos^2\varphi\right) \sin\varphi d\varphi \quad (18)$$

The apparent Young's modulus is measured by the resonance method corresponding to a low magnitude tensile loading. Considering the additivity of deformation (homogeneous stress) at a physical point, the apparent Young's modulus verifies:

$$\frac{1}{E_a} = \frac{1}{E} + \frac{1}{E_m} \quad (19)$$

with E the ideal Young's modulus and E_m the magnetostriction modulus. The latter satisfies:

$$\frac{1}{E_m} = \left. \frac{d\epsilon_{33}^\mu}{d\sigma} \right|_{\sigma=0} \quad (20)$$

289 Since an analytical expression of magnetostriction *vs* stress is available,
 290 the calculation is developed:

$$\epsilon_{33}^\mu = \frac{\pi \lambda_{max} S_2(\sigma)}{S_1(\sigma)} \exp\left(-\frac{1}{2} A_s \lambda_{max} \sigma\right) \quad (21)$$

A derivation of ϵ_{33}^μ function with respect to stress at $\sigma = 0$, leads to, after few calculations:

$$\frac{1}{E_m} = \left. \frac{d\epsilon_{33}^\mu}{d\sigma} \right|_{\sigma=0} = \frac{\lambda_{max}^2 A_s}{5} = \frac{3\chi_0(T) \lambda_{max}^2}{5\mu_0 M_s(T)^2} \frac{T^{RT}}{T} \quad (22)$$

291 Most of the terms are temperature dependent, including λ_{max} , that may
 292 lead to a complex variation of the magnetostriction modulus with temper-
 293 ature. It is possible to extend the proposed approach to other hypotheses
 294 than homogeneous stiffness by reporting the localization operation in the
 295 definition of λ_{max} . This point is addressed in the next section.

296 3.3. Numerical applications for pure isotropic polycrystalline nickel and in- 297 fluence of temperature

298 The parameter λ_{max} can be derived from magnetostrictive constants of
 299 single crystal λ_{100} and λ_{111} following different assumptions, depending of ei-
 300 ther or not the magnetization rotation is considered, and depending on the
 301 elastic behavior of the domain (single crystal stiffness constants) and the
 302 average medium. An analytical calculation of the average magnetostrictive
 303 tensor can be strictly made only at magnetic saturation, when the magne-
 304 tization is uniformly aligned along the external field direction. Grains g are
 305 composed of single domains α so that the magnetostriction strain in each
 306 grain is the magnetostriction strain of the domain in the crystallographic
 307 frame (CF) :

$$\epsilon_\mu^g = \epsilon_\mu^\alpha = \frac{3}{2} \begin{pmatrix} \lambda_{100}(\gamma_1^2 - \frac{1}{3}) & \lambda_{111}\gamma_1\gamma_2 & \lambda_{111}\gamma_1\gamma_3 \\ \lambda_{111}\gamma_1\gamma_2 & \lambda_{100}(\gamma_2^2 - \frac{1}{3}) & \lambda_{111}\gamma_2\gamma_3 \\ \lambda_{111}\gamma_1\gamma_3 & \lambda_{111}\gamma_2\gamma_3 & \lambda_{100}(\gamma_3^2 - \frac{1}{3}) \end{pmatrix}_{CF} \quad (23)$$

The average magnetostriction strain is the solution of a thermo-elasticity problem [21]:

$$\epsilon_\mu^{sat} = \langle {}^t\mathbb{B}^g : \epsilon_\mu^g \rangle \quad (24)$$

308 where ${}^t\mathbb{B}^g$ indicates the transpose of the stress concentration tensor and
 309 $\langle \dots \rangle$ denotes the averaging operation over the volume. The macroscopic
 310 behavior being isotropic, previously defined equation (6) gives the average
 311 saturation magnetostriction strain tensor with $\lambda_{max} = \lambda_{sat}$ the saturation
 312 magnetostriction. In case of high magneto crystalline anisotropy, domain
 313 wall displacement and magnetization rotation can be considered as succes-
 314 sive (they are usually considered as concomitant) so that it is possible to
 315 estimate another average magnetostriction tensor denoted average *maximal*
 316 magnetostriction strain tensor. A calculation of analytical values is possible
 317 using $\lambda_{100} = 0$ for $\langle 111 \rangle$ easy directions materials or $\lambda_{111} = 0$ for $\langle 100 \rangle$
 318 easy directions materials:

- in case of low magneto crystalline energy (free rotation) or at the mag-
netic saturation:

$$\lambda_{max} = \lambda_{sat} = \frac{2}{5}\lambda_{100}k^a + \frac{3}{5}\lambda_{111}k^b$$

319 This value corresponds to the theoretical magnetostriction at the mag-
 320 netic saturation.

- in case of high magneto crystalline energy (no rotation):

$$\begin{aligned}
 \lambda_{max} &= \frac{2}{5}\lambda_{100}k^a && \text{for materials with} \\
 &&& \langle 100 \rangle \text{ easy directions} \\
 \lambda_{max} &= \frac{3}{5}\lambda_{111}k^b && \text{for materials with} \\
 &&& \langle 111 \rangle \text{ easy directions}
 \end{aligned}$$

321 k^a and k^b are homogenization parameters depending on the elastic prop-
 322 erties. They are given by:

$$\begin{cases} k^a = \frac{\mu_a}{\mu_{eff}} \frac{\mu_{eff} + \mu^*}{\mu_a + \mu^*} \\ k^b = \frac{\mu_b}{\mu_{eff}} \frac{\mu_{eff} + \mu^*}{\mu_b + \mu^*} \end{cases} \quad (25)$$

323 μ_a and μ_b are the the single crystal shear moduli (equation 26 - with
 324 C_{ij} the stiffness constants of the cubic symmetry single crystal). μ_{eff} is the
 325 shear modulus of the effective medium given by equation (27). μ^* (eq. 28)
 326 is the Hill's shear modulus, whose definition depends on μ_o and κ_o the shear

327 and compression moduli of the reference medium supposed isotropic (NB:
328 $\kappa_o = \kappa$).

$$\begin{cases} \mu_a &= \frac{1}{2}(C_{11} - C_{12}) \\ \mu_b &= \frac{1}{2}(C_{44}) \\ \kappa &= \frac{1}{3}(C_{11} + 2C_{12}) \end{cases} \quad (26)$$

$$\mu_{eff} = \frac{5(\mu_a + \mu^*)(\mu_b + \mu^*)}{(3\mu_a + 2\mu_b + 5\mu^*)} - \mu^* \quad (27)$$

$$\mu^* = \frac{1}{6}\mu_o \frac{9\kappa_o + 8\mu_o}{\kappa_o + 2\mu_o} \quad (28)$$

329 The value of these parameters (and finally of k^a and k^b) depends on the
330 homogenization approximations made:

- 331 • Homogeneous stress (Reuss hypothesis - ie: $\mu_o=0$): $k^a = k^b = 1$
- 332 • Homogeneous deformation (Voigt hypothesis - ie: $\mu_o = \infty$): $k^a =$
333 $5\mu_a/(2\mu_a + 3\mu_b)$ and $k^b = 5\mu_b/(2\mu_a + 3\mu_b)$
- 334 • Hashin and Shtrikman upper estimation (ie: $\mu_o = \mu_b$ - considering that
335 $\mu_b > \mu_a$)
- 336 • Hashin and Shtrikman lower estimation (ie: $\mu_o = \mu_a$ - considering that
337 $\mu_b > \mu_a$)
- Self-consistent estimation (ie: $\mu_o = \mu_{eff}$ so that μ_{eff} is the result of
the self-consistent equation:

$$8\mu_{eff}^3 + (9\kappa + 4\mu_a)\mu_{eff}^2 - (12\mu_a\mu_b + 3\kappa\mu_b)\mu_{eff} - 6\kappa\mu_a\mu_b = 0 \quad (29)$$

338 Analytical expressions of k_a and k_b are not reported for the three last
339 estimations due to their complicated expressions.

3.3.1. Apparent Young's modulus at the room temperature

The physical constants for nickel used for the calculations are reported in table 2. They are given at RT. The value of the second magneto crystalline constant K_2 strongly varies from one author to another (from one value to its opposite) [6, 7]. The effect of this term is usually negligible when its amplitude is close or inferior to the amplitude of the first magneto crystalline constant K_1 . Equation (30) gives the magneto crystalline energy expression function of constants K_1 and K_2 and direction cosines γ_i of magnetization in the crystal frame.

$$W_K^\alpha = K_1(\gamma_1^2\gamma_2^2 + \gamma_2^2\gamma_3^2 + \gamma_3^2\gamma_1^2) + K_2(\gamma_1^2\gamma_2^2\gamma_3^2) \quad (30)$$

The magneto elastic energy can be calculated for a uniaxial stress σ_u along the direction [100] of the single crystal and a magnetostriction strain at the domain scale (23). It gives:

$$W_\sigma^\alpha = -\frac{1}{2}\lambda_{100}\sigma_u (3\gamma_1^2 - 1) \quad (31)$$

To estimate if rotation has to be or not taken into account at RT, a material with positive K_1 ($< 100 >$ easy magnetization direction) and a magnetization rotation of angle θ in the (\vec{e}_1, \vec{e}_2) plane are considered. The magnetoelastic and magnetocrystalline energy of a domain α_1 oriented along \vec{e}_1 can be written following:

$$\begin{cases} W_K^{\alpha_1} &= K_1(\cos^2\theta \sin^2\theta) \\ W_\sigma^{\alpha_1} &= -\frac{1}{2}\lambda_{100}\sigma_u(3\cos^2\theta - 1) \end{cases} \quad (32)$$

If no other magnetization mechanism or energy is considered, the variation of total energy is null at equilibrium so that:

$$\frac{dW_K^{\alpha_1}}{d\theta} = -\frac{dW_\sigma^{\alpha_1}}{d\theta} \quad (33)$$

An equalization of the two expressions for $\theta = 0$ allows to estimate an uniaxial stress amplitude σ_u able to initiate a magnetization rotation. Its expression is reported in equation (34).

$$\sigma_u \approx \left| \frac{2K_1}{3\lambda_{100}} \right| \quad (34)$$

Using the numerical values reported in table 2, a stress σ_u higher than 100 MPa is obtained. This value is much larger than the value expected during

the Young's modulus measurements (less than 1 MPa). The no rotation assumption can be made at RT so that λ_{max} is defined by:

$$\lambda_{max} = \frac{3}{5} \lambda_{111} k_b \quad (35)$$

Table 2: Physical constants of pure nickel at RT [6, 7]; see figure 10 for χ_0 value.

K_1	K_2	M_s	λ_{100}	λ_{111}	χ_0	C_{11}	C_{12}	C_{44}
-5×10^3	$\pm 2 \times 10^3$	4.84×10^5	-50	-25	800	246	147	248
J.m ⁻³	J.m ⁻³	A/m	ppm	ppm	-	GPa	GPa	GPa

Assuming finally an effective Young's modulus E of 223 GPa (in accordance with C_{ij} values), different estimations of the apparent Young's modulus can be made depending on the different estimations of k_b . They are reported in the following table:

Table 3: Different estimations of k_b , λ_{max} , E_m , E_a and $\Delta E/E(\%) = (E_a - E)/E \times 100$ at RT - magnetostriction is given in ppm ($\times 10^{-6}$) and moduli in GPa - V: Voigt estimation, R: Reuss estimation, HS+: Hashin-Shtrikman upper estimation, HS-: Hashin-Shtrikman lower estimation, SC: self-consistent estimation.

	V	HS+	SC	HS-	R
k_b	1.316	1.209	1.187	1.151	1
λ_{max}	-19.7	-18.1	-17.8	-17.3	-15.0
E_m	1573	1866	1934	2057	2726
E_a	195	199	200	201	206
$\Delta E/E(\%)$	-12.4	-10.7	-10.3	-9.8	-7.6

The sequence of estimations reported in the table is classical. Values are roughly consistent with the experimental results reported in figure 3 and [5, 6]. The homogeneous stress hypothesis giving an apparent Young's modulus of 206 GPa leads nevertheless to the best result. Since the EBSD measurement did not reveal any crystallographic texture, this result could be linked to an anisotropic distribution of domains.

3.3.2. Effect of increasing temperature on apparent Young's modulus

Temperature has a significant effect on the physical constants of nickel used in the analytical modeling.

- Figure 6 shows the experimental results obtained by Kirkham [22] and Döring reported in [6] for the magnetostriction of a polycrystalline nickel (confirmed by the more recent measurements of Tatsumoto [23]). Magnetostriction is decreasing with increasing temperature. It reaches zero at T_C . No data are available for single crystal parameters λ_{100} and λ_{111} . One admissible assumption is to suppose that they behave similarly than the saturation magnetostriction of the isotropic medium. λ_{max} would evolve similarly.

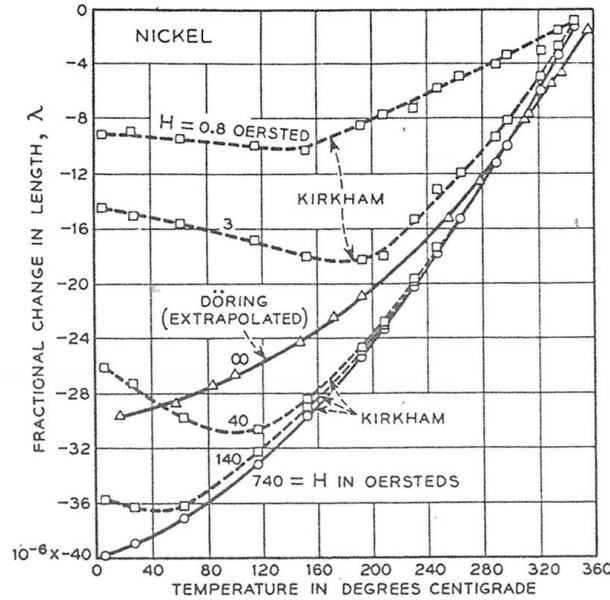


Figure 6: Effect of temperature on the magnetostriction of polycrystalline nickel [6, 22].

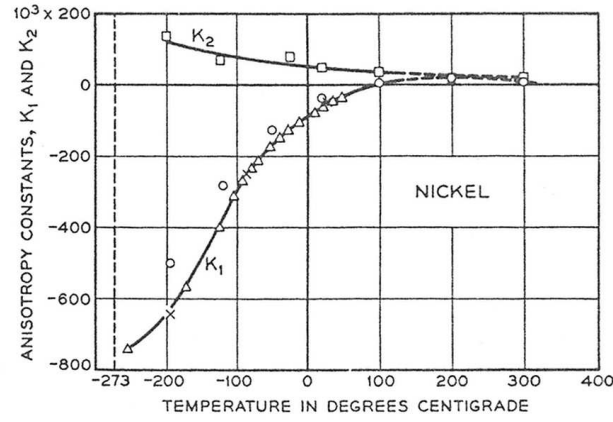
- Figure 7 shows the experimental results obtained by Honda [6] and Tatsumoto [24] for the magnetostriction constants of nickel. The amplitude of constants decreases drastically with increasing temperature. K_1 , initially negative, reaches zero at approximately 100°C for Honda

391 or 200°C for Tatsumoto, then becomes slightly positive before coming
 392 back to zero close to T_C . K_2 is positive and of lower amplitude than
 393 K_1 . It decreases regularly to zero when temperature is approaching
 394 T_C .

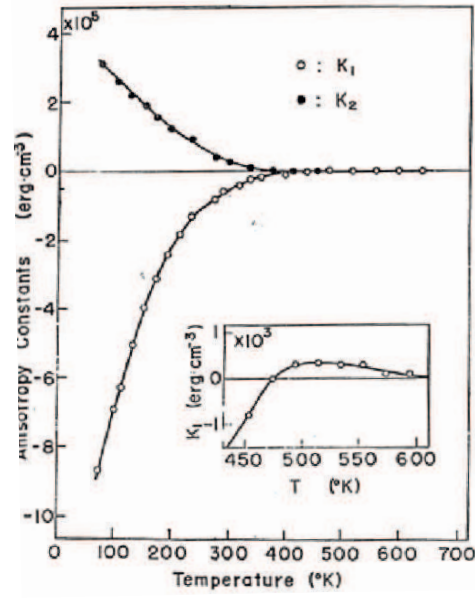
395 • Figure 8 shows the experimental results obtained by Kneller and re-
 396 ported by Ascher [25] for the saturation magnetization of nickel. The
 397 decrease of M_s with temperature is much less regular than magne-
 398 tostrictive and magneto crystalline constants. M_s remains high up to
 399 a high temperature level. It drastically decreases to zero when the
 400 temperature approaches T_C .

401 • Finally, figure 9 shows the experimental results obtained by Kirkham
 402 [22] for the initial susceptibility of nickel. A global strong increase
 403 of susceptibility before a sharp decrease at T_C is observed. The ini-
 404 tial increasing is strongly modified by a non monotonous evolution at
 405 a temperature (local maximum at $T \approx 200^\circ\text{C}$) that is interpreted by
 406 Kirkham as a direct effect of the change of K_1 sign (modifying the easy
 407 magnetization axis from the $\langle 111 \rangle$ to the $\langle 100 \rangle$ direction). The
 408 evolution of this term can be seen as a result of a new magnetic equilib-
 409 rium associated to new physical constants, as for Young's modulus. It
 410 must be noticed that the susceptibility used in the analytical modeling
 411 is the *anhysteretic* initial susceptibility, but the data reported are the
 412 initial susceptibility of the first magnetization curve. Figure 10 reports
 413 the typical cyclic and anhysteretic behaviors of pure polycrystalline
 414 nickel measured at RT. The initial susceptibility of the first magne-
 415 tization curve is drastically different from initial susceptibility of the
 416 anhysteretic curve. At RT, initial susceptibility of the first magnetiza-
 417 tion curve is close to 60 (in accordance with Kirkham measurements)
 418 while initial susceptibility of the anhysteretic curve is at minimum ten
 419 times higher (about 800). The variations with temperature of initial
 420 susceptibility of the first magnetization curve give only a survey of the
 421 anhysteretic susceptibility variations.

422 Let reconsider now the analytical expression of E_m equation 22, tempera-
 423 ture dependent parameters are: λ_{max} , χ_0 and M_s . K_1 quickly decreases while
 424 the temperature increases, meaning that the rotation becomes progressively
 425 dominant (for a temperature around 100°C up to 200°C). The maximum



(a)



(b)

Figure 7: Effect of temperature on the magnetocrystalline constants of nickel - (a) results of Honda [6]; (b) results of Tatsumoto [24] - NB: K_1 and K_2 are given in $\text{erg/cm}^3 - 10 [\text{erg/cm}^3] = 1 [\text{J/m}^3]$.

426 magnetostriction definition has to be reconsidered because it tends progres-

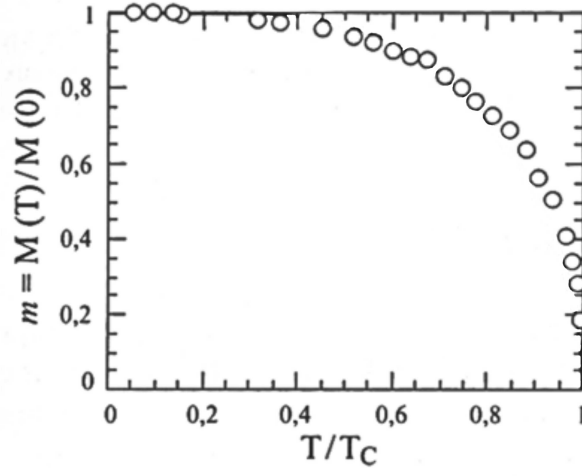


Figure 8: Effect of temperature on the saturation magnetization of nickel [25].

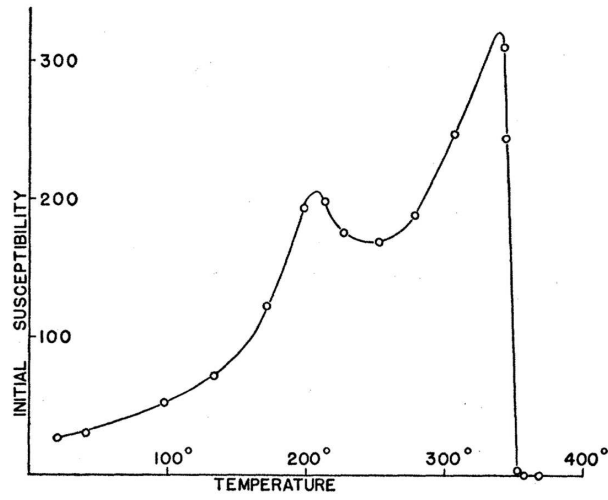


Figure 9: Effect of temperature on the initial susceptibility of nickel [22].

427 sively to the saturation magnetostriction:

$$\lambda_{max} = \frac{2}{5}\lambda_{100}k_a + \frac{3}{5}\lambda_{111}k_b \quad (36)$$

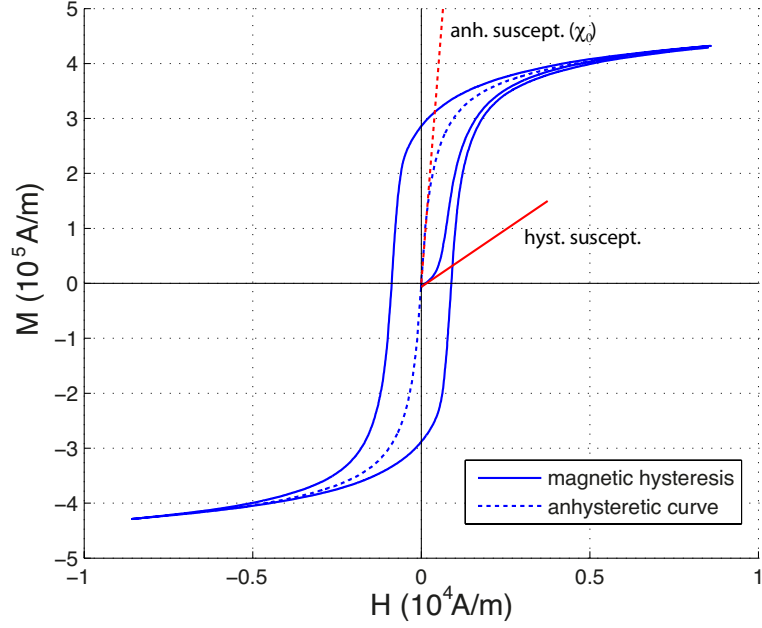


Figure 10: Typical cyclic and anhysteretic behaviors of pure polycrystalline nickel at RT.

Variations of λ_{100} and λ_{111} with temperature must be taken into account too. They are considered to follow the same variation with temperature than λ_s plotted in figure 6.

Variation of the anhysteretic initial susceptibility χ_0 with temperature is unknown since figure 9 refers to the hysteretic initial susceptibility. To simplify, a linear increasement of χ_0 with temperature is considered:

$$\chi_0(T) = \chi_0^{RT} \frac{T}{T_{RT}} \quad (37)$$

Such relation is in global accordance with the experimental variation of hysteretic initial susceptibility and allows a simplification of the magnetostriction modulus expression:

$$\frac{1}{E_m} = \frac{3\chi_0^{RT}}{5\mu_0} \left(\frac{\lambda_{max}(T)}{M_s(T)} \right)^2 \quad (38)$$

Therefore new assessments of the magnetostriction modulus can be obtained considering the different previous estimations at a temperature of

439 200°C. Parameters values at this temperature come from experimental re-
440 sults. They are reported in table 4.

Table 4: Physical constants of pure nickel at 200°C used for the estimation of the apparent Young's modulus (a linear variation of the ideal Young's modulus with temperature has been used to estimate the C_{ij} values using equation (40) - Poisson's ratio variations are not considered); χ_0 is supposed unchanged with temperature.

M_s	λ_{100}	λ_{111}	χ_0	C_{11}	C_{12}	C_{44}
3.9×10^5	-33.3	-16.7	800	227	136	229
A/m	ppm	ppm	-	GPa	GPa	GPa

441 The effective Young's modulus E is 206 GPa at 200°C (in accordance with
442 C_{ij} values and experimental results). Different estimations of the apparent
443 Young's modulus can be made depending on the different estimations of k_a
444 and k_b . They are reported in table 5.

Table 5: Different estimations of k_a , k_b , λ_{max} , E_m , E_a and $\Delta E/E(\%) = (E_a - E)/E \times 100$ at 200°C - magnetostriction is given in ppm ($\times 10^{-6}$) and moduli in GPa - V: Voigt estimation, R: Reuss estimation, HS+: Hashin-Shtrikman upper estimation, HS-: Hashin-Shtrikman lower estimation, SC: self-consistent estimation.

	V	HS+	SC	HS-	R
k_a	0.525	0.687	0.719	0.773	1
k_b	1.316	1.209	1.187	1.151	1
λ_{max}	-20.2	-21.3	-21.5	-21.8	-23.3
E_m	977	881	863	835	731
E_a	170	167	166	165	161
$\Delta E/E(\%)$	-17.4	-19.0	-19.3	-19.8	-22.0

445 Whatever the estimation, a decrease of the apparent Young's mod-
446 ulus with temperature is clearly observed. This decrease fluctuates be-
447 tween 36 MPa and 45 MPa depending on the estimation. These values are
448 in good agreement with values observed in figure 3 and those reported in [6]
449 (figure 4a and 4a after annealing). It can be noticed that the homogeneous
450 stress estimation leads now to the lowest apparent Young's modulus (it was
451 corresponding to the highest value for the calculations at RT). Homogeneous

stress estimation allows to get the highest variation of ΔE effect with temperature. On the other hand it is interesting to compare these values with those reported in table 6, where the no rotation condition has been maintained. A clear increase of the apparent Young's modulus is observed, that does not fit to the experimental results. It confirms that the variation of the apparent Young's modulus with temperature is due to a combined effect of variation of intrinsic physical constants and a relaxation of the magnetization rotation enhancing the magnetostriction strain variation with stress.

The Young's modulus remains to its effective value (196 MPa) when temperature reaches the Curie temperature (disappearance of ferromagnetic coupling), leading to the sharp increase of apparent Young's modulus.

Table 6: Different estimations of k_b , λ_{max} , E_m , E_a and $\Delta E/E(\%) = (E_a - E)/E \times 100$ at 200°C **using the no-rotation condition:** $\lambda_{max} = \frac{3}{5}\lambda_{111}k_b$ - magnetostriction is given in ppm ($\times 10^{-6}$) and moduli in GPa - V: Voigt estimation, R: Reuss estimation, HS+: Hashin-Shtrikman upper estimation, HS-: Hashin-Shtrikman lower estimation, SC: self-consistent estimation.

	V	HS+	SC	HS-	R
k_b	1.316	1.209	1.187	1.151	1
λ_{max}	-13.2	-12.1	-11.9	-11.5	-10.0
E_m	2289	2715	2813	2993	3966
E_a	189	191	192	193	196
$\Delta E/E(\%)$	-8.3	-7.1	-6.8	-6.4	-4.9

4. Numerical implementation of $E(T)$ and comparisons between experiments and modeling

4.1. Multiscale model and simulation of apparent Young's modulus at the room temperature

The variations of nickel physical constants with temperature are now considered to propose a modeling of $E_a(T)$ curve and compare it to the measurements. The previous calculations used the assumption of no effect of magnetization rotation on the magnetostrictive response. This assumption is acceptable for a high K_1 . When K_1 reaches 0, this assumption is not valid

anymore. The analytical modeling can be made on the other hand when λ_{max} is known. The definition of λ_{max} is nevertheless not unique (known only for free rotation or no rotation situations). These different arguments motivate the choice of a numerical approach.

A multiscale (MS) model originally dedicated to build magneto-mechanical constitutive laws for anisotropic polycrystalline media is used [13]. The main characteristics of this model are recalled in Appendix A. MS model involves three scales: domain scale, grain scale and polycrystalline scale (representative volume element - *RVE*). Initially proposed by [26] at the grain scale, it was extended to polycrystals by [13] and [27]. In the present study, an isotropic grain distribution has been used (546 grains [13]). This model allows, among others, to simulate the ΔE effect of nickel ($\epsilon_{33}^{\mu}(\sigma)$) as reported in figure 11 where the effect of homogeneous stress or self consistent conditions are compared.

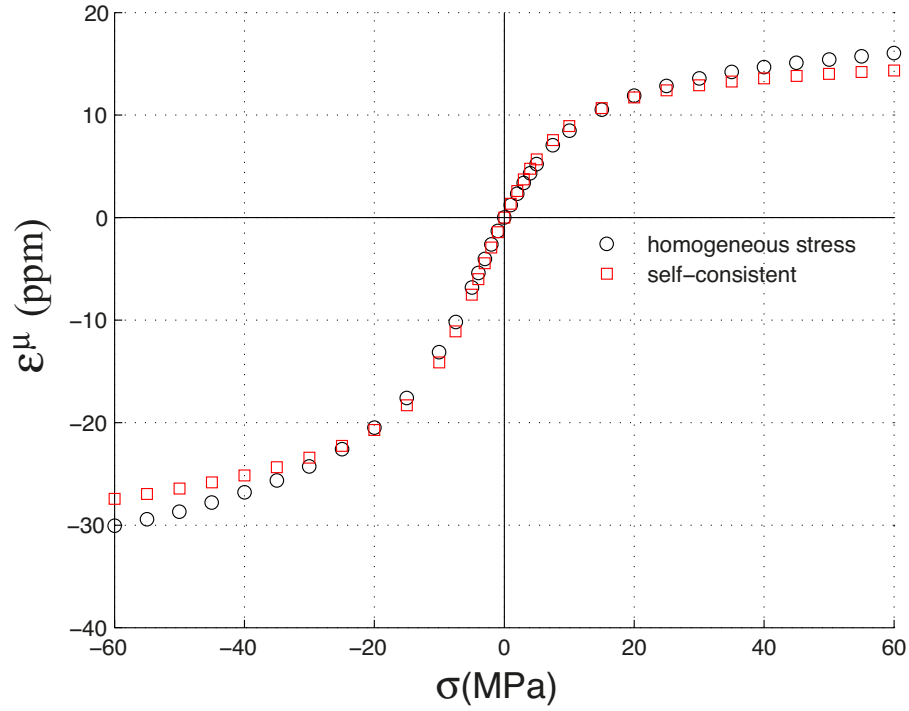


Figure 11: ΔE effect for isotropic polycrystalline nickel as estimated by MS model at RT for homogeneous stress and self-consistent conditions.

487 The difference of slope a zero applied stress between the two simulations
 488 is low: a slope of $1.212 \times 10^{-12} \text{Pa}^{-1}$ is obtained for the homogeneous stress
 489 condition and of $1.345 \times 10^{-12} \text{Pa}^{-1}$ for the self-consistent condition. These
 490 values correspond to E_m^{-1} . The corresponding apparent Young's modulus is
 491 evaluated to 176 GPa and 172 GPa respectively (for a ideal Young's modu-
 492 lus of 223 GPa). These values are lower than the experimental values at RT
 493 reported in figure 3 and different from the value obtained after the analyti-
 494 cal approach (206 GPa for homogeneous stress estimation and 200 GPa for
 495 the self-consistent one) which considered that rotation was not occurring at
 496 RT. Another estimation by the analytical approach of the apparent Young's
 497 modulus at RT has been made, now considering a free rotation mechanism
 498 (*i.e.* $\lambda_{max} = \frac{2}{5}\lambda_{100}k_a + \frac{3}{5}\lambda_{111}k_b$). The different estimations of E_a (numerical
 499 and analytic approaches for homogeneous stress and self-consistent estima-
 500 tions) are reported in table 7. The analytical estimation considering a free
 501 magnetization rotation leads to results closer to the numerical solution than
 502 the no-rotation assumption, especially for the self-consistent estimation. The
 503 variation of magnetostriction with stress must be considered as the result of
 504 both wall displacement and magnetization rotation at RT.

Table 7: Various estimations of apparent Young's moduli E_a (GPa) T=20°C. R: homoge-
neous stress: SC: self-consistent

R num.	SC num.	R no rot.	SC no rot.	R rot.	SC rot.
176	172	206	200	154	162

505 4.2. Simulation of $E_a(T)$ for isotropic polycrystalline nickel

506 The simulation of the apparent Young's modulus with temperature re-
 507 quires to use relations between physical constants (ideal Young's modu-
 508 lus, magnetostriction, magnetocrystalline constant, saturation magnetiza-
 509 tion) and temperature. Some of these relations have a theoretical back-
 510 ground, others have been built in former papers by different authors so that
 511 they fit properly the experimental data. The following functions are pro-
 512 posed:

- Ideal Young's modulus - All experiments (recent and former) show a linear decrease of ideal Young's modulus E with temperature T .

The following linear relation is implemented in the model:

$$E = E_0 - k_0 T \quad (39)$$

513 with $E_0=237.6$ GPa: Young's modulus at 0K; $k_0=0.06603$ GPa/K.
 514 Figure 12 allows the comparison between the linear approximation and
 515 the experimental results. The same relation is used to consider the
 516 variation of C_{ij} stiffness constants with temperature (in the range of
 517 temperature considered in this paper):

$$C_{ij}(T) = C_{ij}(T^{RT}) \frac{E(T)}{E(T^{RT})} \quad (40)$$

- Saturation magnetization - the theoretical variation of the saturation magnetization M_s with temperature is given by the self-consistent equation [32]:

$$\frac{M_s}{M_{s0}} = \tanh\left(\frac{M_s/M_{s0}}{T/T_C}\right) \quad (41)$$

518 with M_{s0} the magnetization at 0K ($M_{s0}=4.956 \times 10^5$ A/m). The tem-
 519 perature T is expressed in Kelvin.

520 Figure 13 allows the comparison between the experimental and modeled
 521 evolution of the saturation magnetization with the temperature. The
 522 model gives high quality results.

- 523 • Magnetocrystalline constants - The variation of magnetocrystalline con-
 524 stant K with temperature has been studied theoretically by Zener [28].
 525 It is expressed as function of magnetization ratio, K^0 the magnetocrys-
 526 talline constant at 0K, and a constant n :

$$K(T) = K^0 (M_s/M_s^0)^n \quad (42)$$

527 $n=10$ for a cubic symmetry. This value is justified considering that the
 528 amplitude of magneto crystalline K_1 is higher than the amplitude of
 529 K_2 , and considering the cubic symmetry (4^{th} order of direction cosines).
 530 This model is denoted model 1.

531 It has been shown that this relation did not fit very well the experi-
 532 mental results obtained for nickel. The relation has been modified by

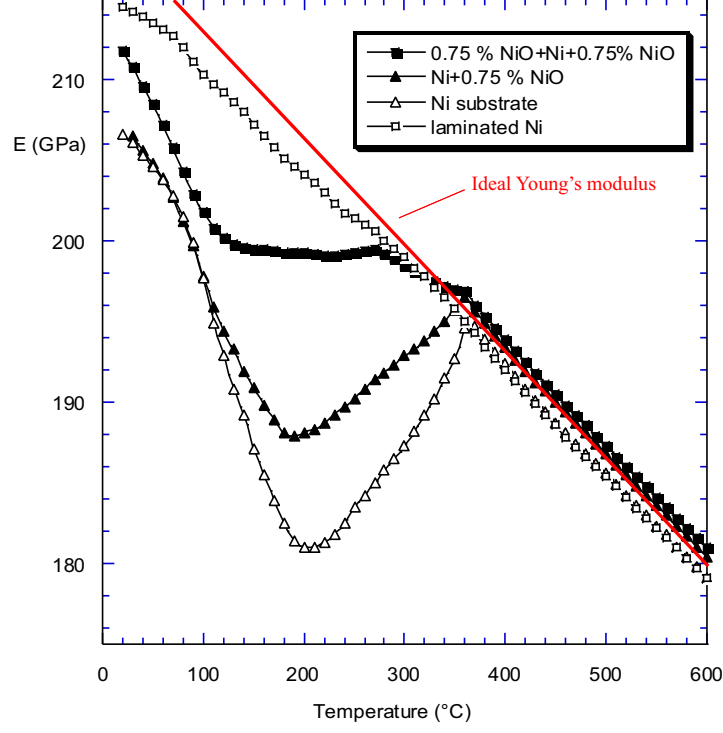


Figure 12: Variation of Young's modulus with temperature for different specimens complemented by a linear approximation of ideal Young's modulus.

533 Carr [30] to take account of the change of sign of K_1 and an earlier
 534 decrease of magneto crystalline amplitude. This model is denoted
 535 model 2.

$$K(T) = K^0 \left(\frac{M_s}{M_s^0} \right)^n \left(1 - \alpha \frac{T}{T_C} \right) \quad (43)$$

536 with $n=10$ and $\alpha > 1$

Williams and Bozorth [6] proposed on the other hand to use the following empirical relation to define the evolution of magneto crystalline constants with temperature:

$$K(T) = K^0 \exp(-kT^2) \quad (44)$$

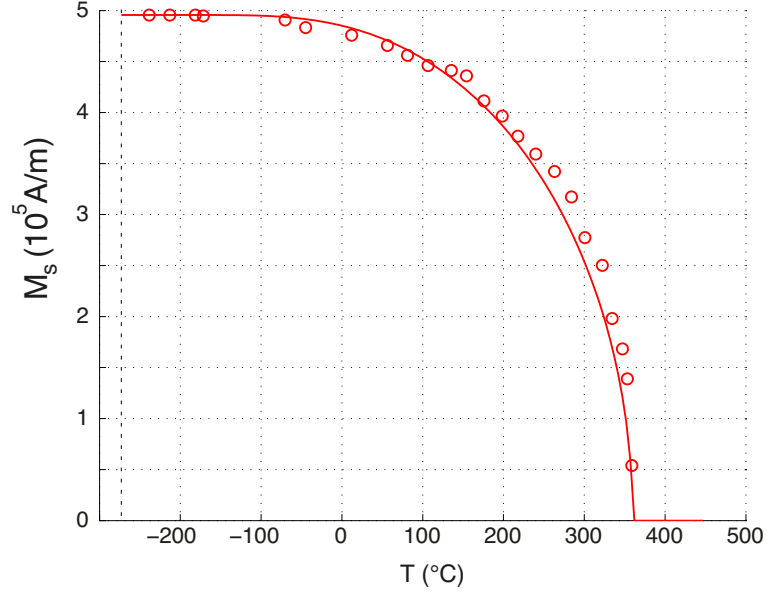


Figure 13: Comparison between experiment (circles) and modeling (full line - see eq. 41) of the evolution of saturation magnetization with temperature.

537 It has been decided to use this formulation multiplied by a linear func-
538 tion of temperature in order to represent the change of sign of K_1 . This
539 model denoted model 3 is given by:

$$K_1(T) = K_1^0 \exp(-k_1 T^2) \left(1 - \alpha \frac{T}{T_C}\right) \quad (45)$$

540 with: $K_1^0 = -82 \times 10^3 \text{ J/m}^3$, $k_1 = 1.562 \times 10^{-5} \text{ K}^{-2}$, $\alpha = 1.338$.
541 Figure 14 gathers experimental points from various authors [6, 24, 29]
542 and the results of the three models. The figure 15 is a zoom of figure
543 14. Model 3 gives clearly the best results.

544

Following Williams and Bozorth [6], equation (46) has been used to
model the variations of K_2 with temperature:

$$K_2(T) = K_2^0 \exp(-k_2 T^2) \quad (46)$$

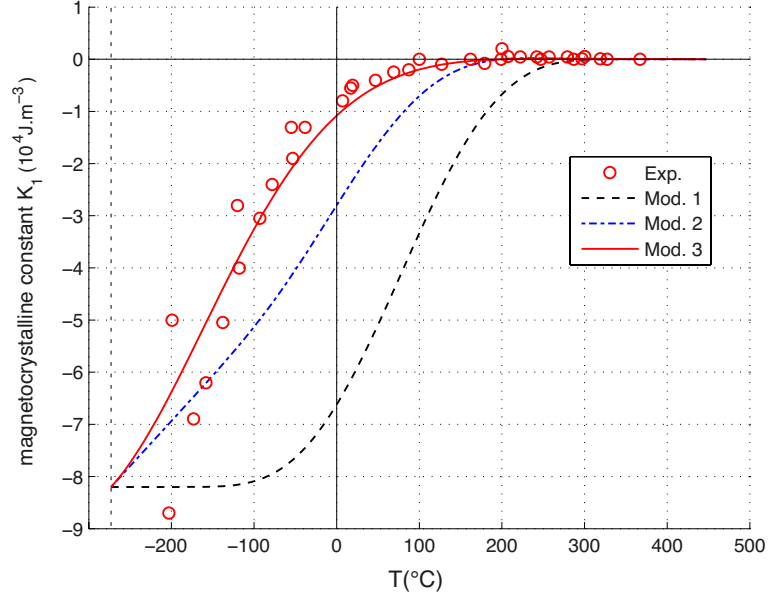


Figure 14: Comparison between experimental and modeled variation of K_1 with temperature.

with: $K_2^0 = \pm 28 \times 10^3 \text{ J/m}^3$, $k_2 = 2.78 \times 10^{-5} \text{ K}^{-2}$.

K_2^0 will be considered either positive or negative during the modeling since the sign of K_2 is controversial. Figure 16 gathers experimental points from various authors [6, 24] (including a negative estimation from [31]) and results of the model. The sensitivity of magnetostriction modulus to the K_2 sign has to be estimated to verify if this uncertainty is significant or not.

- Magnetostriction constants - No theoretical relation between magnetostriction and temperature is available in literature. A polynomial variation is chosen to model the saturation magnetization of isotropic polycrystal:

$$\lambda_s(T) = \lambda_s^i (1 - (T/T_C)^m) \quad (47)$$

with $\lambda_s^i = -32 \times 10^{-6}$ and $m = 3.4$. Extension of this function to λ_{100} and λ_{111} constants is considered, leading to:

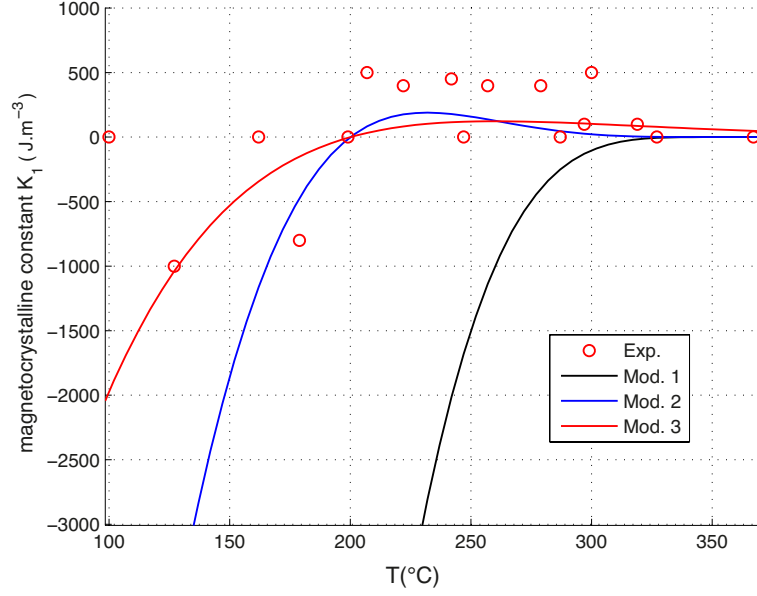


Figure 15: Comparison between experimental and modeled variation of K_1 with temperature - zoom of figure 14.

$$\lambda_{100}(T) = \lambda_{100}^i (1 - (T/T_C)^m) \quad (48)$$

$$\lambda_{111}(T) = \lambda_{111}^i (1 - (T/T_C)^m) \quad (49)$$

559 with $\lambda_{100}^i = -54 \times 10^{-6}$ and $\lambda_{111}^i = -27 \times 10^{-6}$ so that the values at RT cor-
 560 respond to classical values (-50×10^{-6} and -25×10^{-6} respectively). Re-
 561 sults are plotted in figure 17 showing a good ability of the function to
 562 model the experimental data.

563 These various functions are introduced in the multiscale model (Ap-
 564 pendix A). In order to estimate the magnetostriction modulus, the multi-
 565 scale model is employed to model the effect of a small stress magnitude (*i.e.*
 566 $\Delta\sigma_{33} = 0.1 \text{ MPa}$) on the magnitude of macroscopic magnetostriction $\Delta\epsilon_{33}^\mu$. It
 567 leads to:

$$\frac{1}{E_m} = \left. \frac{d\epsilon_{33}^\mu}{d\sigma} \right|_{\sigma=0} \approx \left. \frac{\Delta\epsilon_{33}^\mu}{\Delta\sigma_{33}} \right|_{\sigma_{33}=0} \quad (50)$$

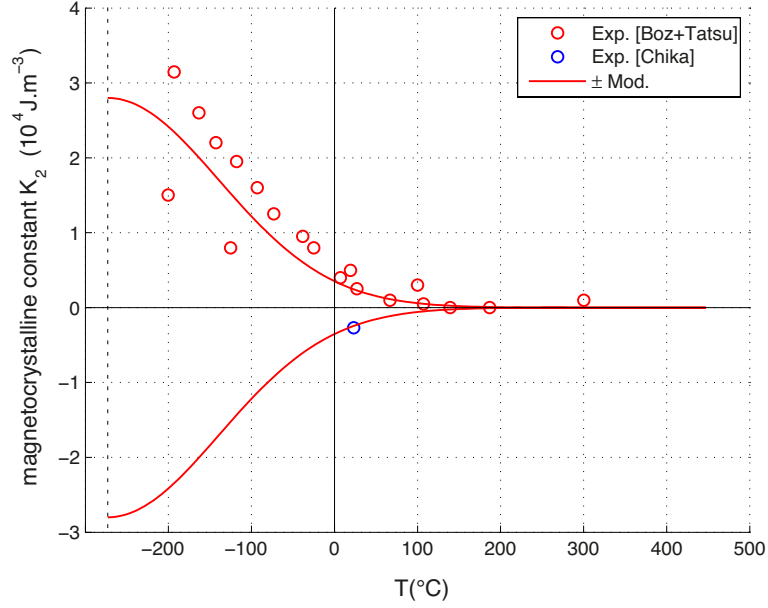


Figure 16: Comparison between experimental and modeled variation of K_2 with temperature.

The apparent Young's modulus E_a satisfies the rule of mixture:

$$\frac{1}{E_a} = \frac{1}{E} + \frac{1}{E_m} \quad (51)$$

The variation of apparent Young's modulus for isotropic polycrystalline nickel with temperature is finally plotted in figure 18 using a homogeneous stress assumption and in figure 19 for the self-consistent condition. Plotted curves correspond to multiscale model (MS), analytical model without rotation, and analytical model with free rotation. The results obtained using the MS model are qualitatively in good agreement with the experimental results with a first decrease with temperature followed by a strong increase up to the Curie temperature. The temperature corresponding to the minimum apparent Young's modulus is in accordance with experimental data. The global level of apparent Young's modulus is lower than expected from the room temperature up to 200°C, and the self-consistent approach leads to a clear underestimation of the Young's modulus variation. It can be observed by the way that the analytical model leads to a large (too large) frame

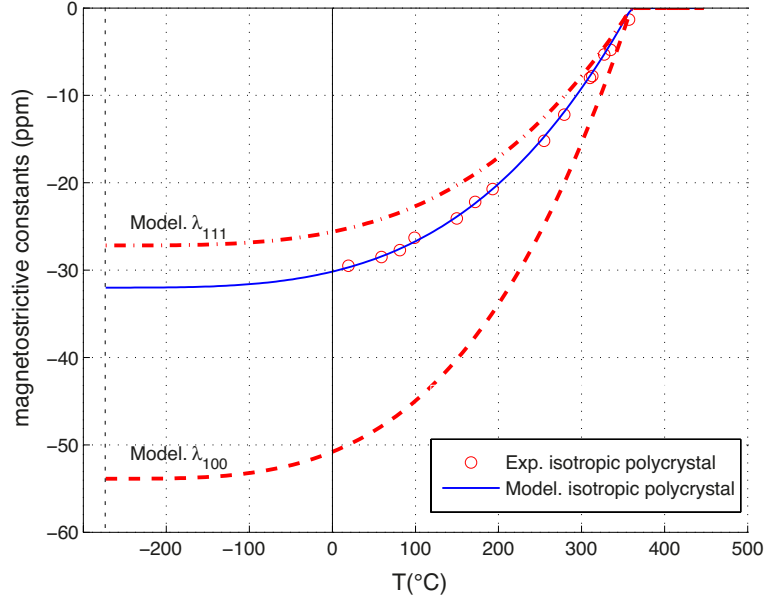


Figure 17: Comparison between experiment (circles) and modeling (full line) of the saturation magnetostriction with temperature. Representation of $\lambda_{100}(T)$ and $\lambda_{111}(T)$ functions.

of the MS solution in both cases for temperatures below 200°C. Above this temperature, analytical results do not frame the solution anymore (especially for the homogeneous stress estimation) indicating that the wall displacement mechanism hypothesis used to get the analytical modeling is not applicable any more. Since the homogeneous stress assumption gives results closer to experiments, it has been used for the next simulations.

Because of uncertainties concerning the K_2 anisotropy constant, it has been decided to simulate the situation where $K_2(T)$ is the exact opposite of previous function and the situation where $K_2(T) = 0$. Behaviors are plotted in figure 20 (using homogeneous stress condition). A very small change is observed meaning that K_2 is a second order parameter. It has been kept positive for the next simulations.

Reasons that explain the discrepancy between experiment and modeling are numerous: representativity of RVE, various uncertainties on physical values,.... The main drawback is associated to the high uncertainty on the variation of initial anhysteretic susceptibility with temperature and a possible anisotropic initial distribution of domains. It must finally be kept in mind

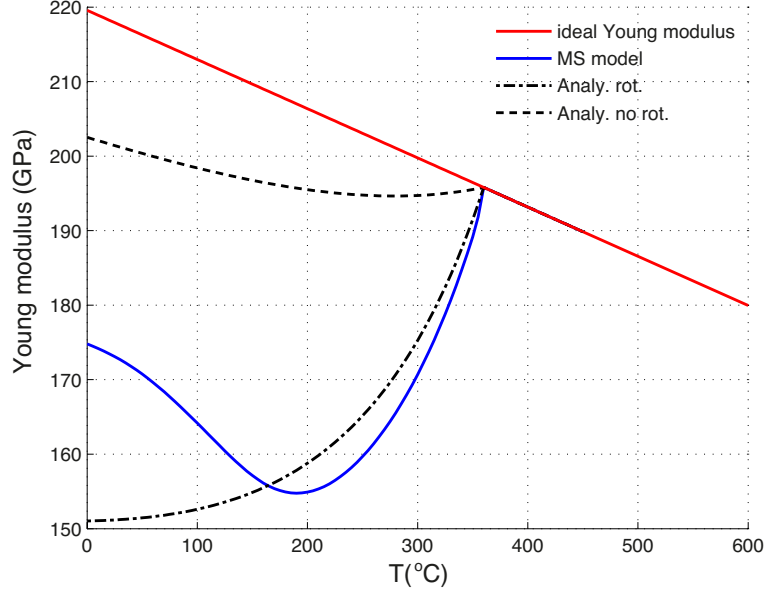


Figure 18: Change of nickel Young's modulus with temperature - ideal and apparent Young's modulus - homogeneous stress estimation.

that the mechanical loading used to measure the apparent Young's modulus cannot be considered as an *anhysteretic* loading, meaning that comparisons between modeling and experiments should be considered at this step as mainly qualitative comparisons, waiting for a hysteretic version of the modeling (see [33, 34] for propositions of extension to hysteretic modeling).

4.3. Simulation of NiO coating effects

The experimental measurements reported in figure 3 show that the "stiffening" effect magnitude below T_C highly varies depending on the sample state (as-received, two sides oxidized, single side oxidized, peeled-off oxide) to another. To highlight and explain that effect, the following points have to be considered:

- nickel has a larger dilatation coefficient than the oxide.
- oxide is formed at high temperature ($T_{Ox}=1100^\circ\text{C}$).
- for any temperature below T_{Ox} , the oxide layer is in compression on the nickel.

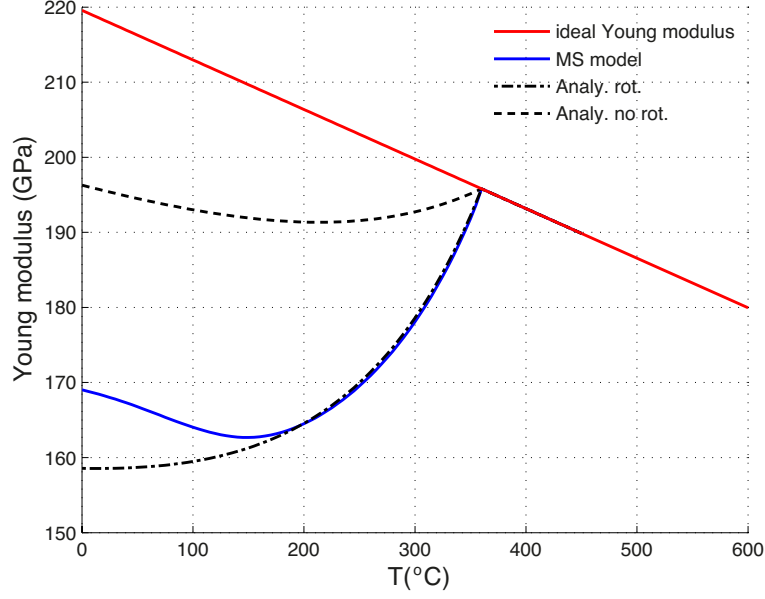


Figure 19: Change of nickel Young's modulus with temperature - ideal and apparent Young's modulus - self-consistent estimation.

- the mechanical balance states that the nickel layer is submitted to an equibitension residual stress of amplitude σ_0 .

$$\boldsymbol{\sigma}_r = \begin{pmatrix} 0 & & \\ & \sigma_0 & \\ & & \sigma_0 \end{pmatrix}$$

Experimental XRD measurements reported in section 2.3 and provided at RT enable the estimation of σ_0 magnitude for the 1-side oxidized and the 2-sides oxidized situations. For NiO-Ni-NiO system, σ_0 is homogeneous in the nickel layer and has been estimated to +9 MPa. For Ni-NiO, stress is heterogeneous across the thickness. Overall the average value in the nickel layer has been estimated to +3 MPa. For a more accurate modeling, it must be taken into account that σ_0 depends on temperature since it decreases theoretically to zero at T_{Ox} . The following parametric formula can be used:

$$\sigma_0(T) = \sigma_0^0 - qT \quad (52)$$

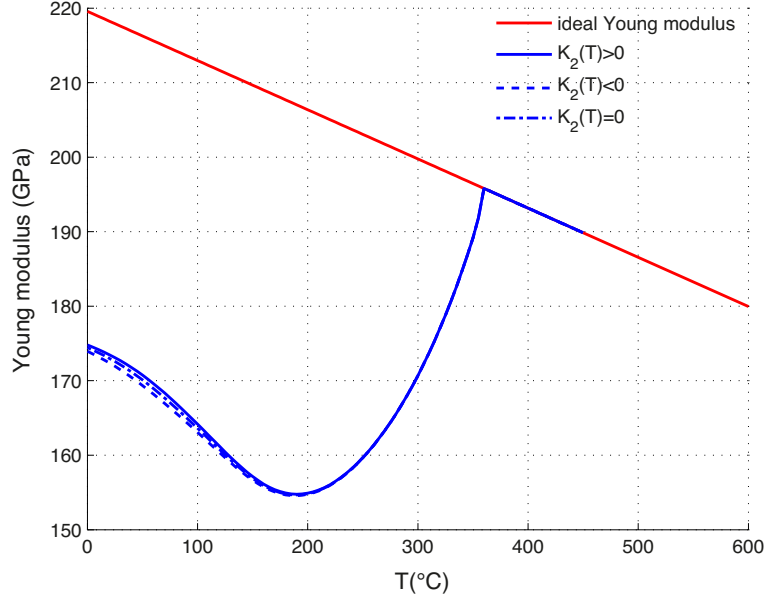


Figure 20: Change of nickel Young's modulus with temperature - effect of K_2 magneto crystalline constant - homogeneous stress estimation.

621 with $\sigma_0^0 = \{11.42, 3.81\}$ MPa and $q = \{8.25, 2.75\} \times 10^{-3}$ MPa/K for the {2-sides
 622 oxidized , 1-side oxidized} situations respectively. $\sigma_0(T)$ functions are plot-
 623 ted in figure 21 in the temperature range of experiments.

624

625 The residual stress tensor is introduced in the multiscale model as a con-
 626 stant external loading (the relaxation of this stress with the magnetostriction
 627 strain of the sample is not considered). The procedure explained above is
 628 used to extract the magnetostriction modulus variations with temperature.
 629 Results are plotted in figure 22. The expected saturation effect is observed.
 630 The amplitude reduction is lower than observed experimentally. Uncertain-
 631 ties on the residual stress level and other approximations are probably at the
 632 origin of these discrepancies.

633 In order to estimate the sensitivity to higher stress, the model has been
 634 tested for a superimposed constant uniaxial applied stress $\sigma_{33} = \sigma_a$. Results
 635 are illustrated in figure 23 where σ_a varies from 5 MPa to 50 MPa exhibiting
 636 the mechanical saturation phenomenon already discussed in literature [6] and
 637 reported in figures 3 (as received material) and 4b (cold rolled sample).

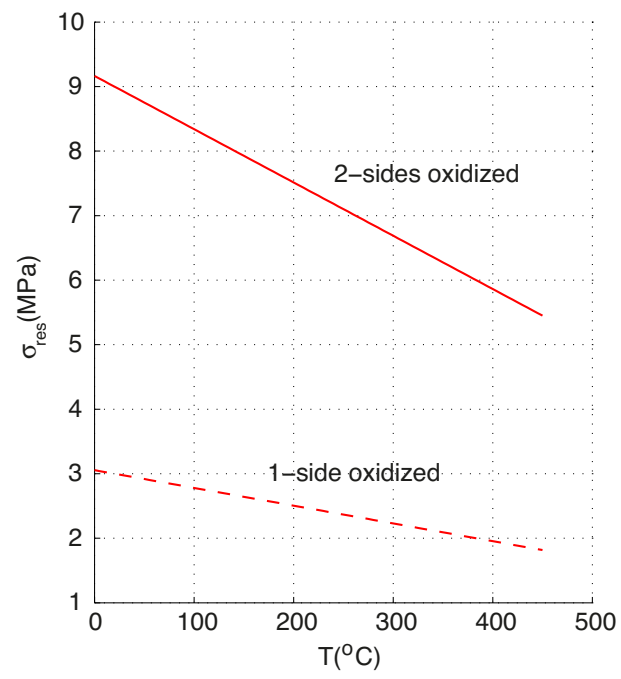


Figure 21: Evolution of residual stress associated to oxide layers with temperature.

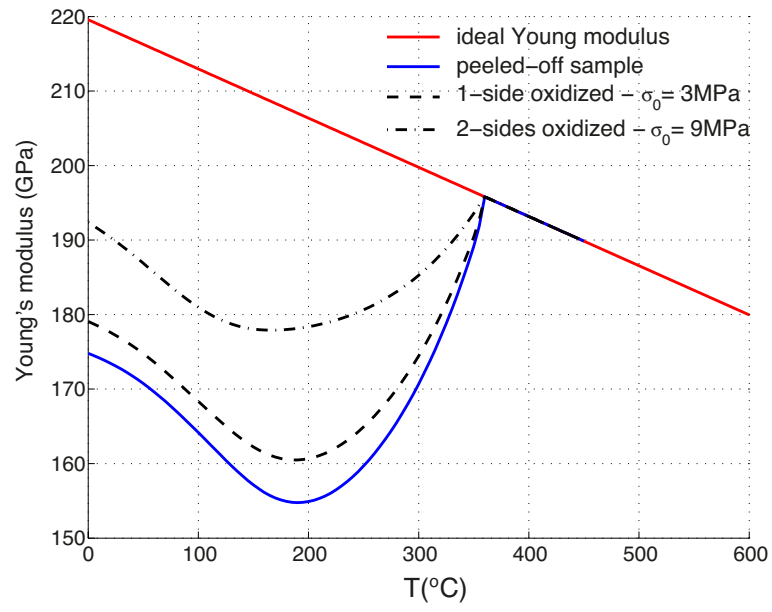


Figure 22: Influence of residual stress associated to oxide layers on the apparent nickel Young's modulus - homogeneous stress estimation.

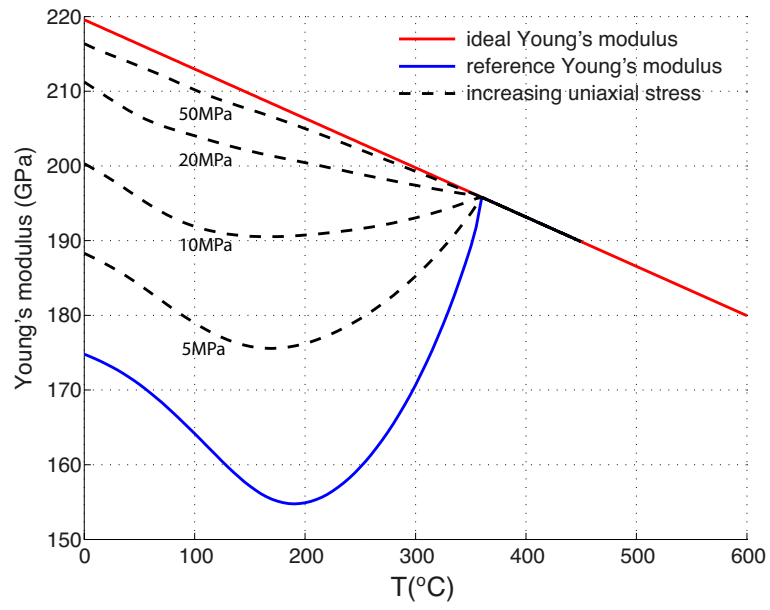


Figure 23: Change of nickel Young's modulus with temperature - effect of uniaxial applied stress - homogeneous stress estimation.

638 The model gives also the opportunity to test the influence of a magnetic
639 field on the apparent Young's modulus of nickel. The effect of a superim-
640 posed constant magnetic field $H_3 = H_a$ is illustrated in figure 24. H_a varies
641 from 1000A/m to 10000A/m exhibiting the magnetic saturation phenomenon
642 already discussed in literature [6] and reported in figure 4a.

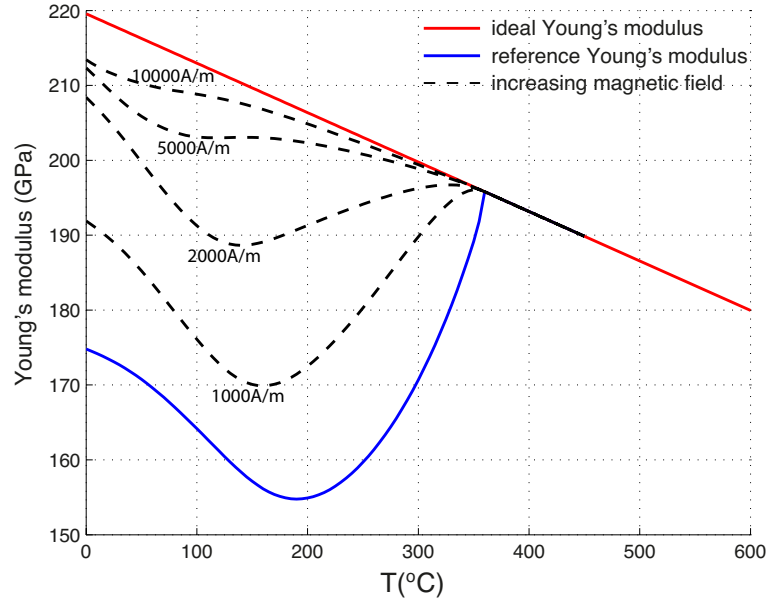


Figure 24: Change of nickel Young's modulus with temperature - effect of constant applied magnetic field - homogeneous stress estimation.

643 5. Conclusion

644 In this work a modeling of the variation of Young's modulus with temper-
645 ature of Ni and Ni-NiO layers has been proposed. The magnetic origin of this
646 behavior has first been underlined, justifying the use of a magneto mechanical
647 approach for the modeling. A first analytical modeling includes the change
648 of the saturation magnetization, of the initial anhysteretic susceptibility and
649 of the maximal magnetostriction with a relaxation of magneto-crystalline
650 anisotropy concomitant to increasing temperature. The second modeling is
651 a numerical modeling giving the average behavior of a representative volume
652 element composed of 546 regularly distributed grains. This modeling requires

653 to define the temperature dependence of many magnetic and magnetostric-
 654 tive parameters. It allows a continuous description of the change of Young's
 655 modulus with temperature.
 656 The discrepancies observed with experiments concern the lower level of Young's
 657 modulus at room temperature up to 200°C (as observed for peeled-off, 1-side
 658 oxidized or 2-sides oxidized sample). Discrepancies can be explained mainly
 659 by the fact that the modeling is reversible although the physical phenomenon
 660 is irreversible (hysteresis effect) and that the variation of initial anhysteretic
 661 susceptibility with temperature remains unknown. Other uncertainties and
 662 approximations (infinite medium) are additive reasons.
 663 It has also been shown that even if crystallographic texture remains roughly
 664 isotropic after oxidizing at 1100°C, the grain size increases drastically for
 665 high duration heat treatments [4]. This size may reach the thickness of the
 666 layer leading to a surface effect whose magnetic and magnetostrictive conse-
 667 quences have been extensively discussed in [36]. This surface effect may have
 668 important consequences on the global response of apparent elastic behavior
 669 because the domain structure is strongly modified by free surface conditions.
 670 The analysis proposed in this paper remains nevertheless sufficient to under-
 671 stand now clearly how the Ni-NiO system behaves. An extension to another
 672 *Ni / coating* system or more generally another *ferromagnetic substrate / coat-*
 673 *ing* system is possible, opening to a wide range of applications. It could be
 674 for example applied to the measurement of thickness deposits and/or to the
 675 inverse identification of internal stress levels inside a substrate.

676 6. acknowledgements

677 The authors wish to thank Jocelyne Balmain, LaSIE UMR 7356 CNRS,
 678 Université de La Rochelle, for her careful preparation of oxidized samples.

679 Appendix A. Multiscale modeling

680 The multiscale model involves three scales: domain scale, grain scale and
 681 polycrystalline scale (representative volume element - RVE). It is especially
 682 dedicated to estimate the macroscopic magnetization and magnetostrictive
 683 responses to macroscopic magnetic field and/or stress loadings of polycrys-
 684 talline anisotropic media. Initially proposed by [26] at the grain scale, it was
 685 extended to polycrystals by [13] and [27]. In the present study, it is used to
 686 model the variation of magnetostriction with respect to stress ($d\epsilon^u/d\sigma - \Delta E$
 687 effect) considering:

- 688 • free specimen (peeled-off sample)
- 689 • 1-side oxidized sample (biaxial stress - $\sigma_0=3\text{MPa}$)
- 690 • 2-sides oxidized sample (biaxial stress - $\sigma_0=9\text{MPa}$)
- 691 • increasing uniaxial stress on a sample
- 692 • increasing magnetic field on a sample

693 An isotropic grain distribution has been used. Since this model always
 694 refers to equilibrium, modeling results must be compared to anhysteretic
 695 (reversible) experimental measurements.

696 Appendix A.1. Micromagnetic model (grain scale)

697 A polycrystalline ferromagnetic media can be considered as an aggregate
 698 of single crystals assembled following the orientation data. The microscopic
 699 model proposed by [26] is written using the volumetric fraction f_α of each
 700 domain family α (six $\langle 100 \rangle$ or height $\langle 111 \rangle$ families depending on
 701 easy directions), and magnetization rotation (two angles θ_α and ϕ_α per do-
 702 main family) as internal variables. The potential energy (A.1) is defined for
 703 each magnetic domain family α as the sum of the magneto-crystalline (A.2),
 704 magnetostatic (A.3) and elastic (A.4) energies, detailed hereafter.

$$W^\alpha = W_K^\alpha + W_H^\alpha + W_\sigma^\alpha \quad (\text{A.1})$$

$$W_K^\alpha = K_1(\gamma_1^2\gamma_2^2 + \gamma_2^2\gamma_3^2 + \gamma_3^2\gamma_1^2) + K_2(\gamma_1^2\gamma_2^2\gamma_3^2) \quad (\text{A.2})$$

$$W_H^\alpha = -\mu_0 \vec{H}^\alpha \cdot \vec{M}^\alpha \quad (\text{A.3})$$

$$W_\sigma^\alpha = \frac{1}{2} \boldsymbol{\sigma}^\alpha : \mathbb{C}^{\alpha-1} : \boldsymbol{\sigma}^\alpha \quad (\text{A.4})$$

705 where $\vec{M}^\alpha = M_s \vec{\gamma}^\alpha$ is the magnetization vector of the domain family α
 706 (M_s : saturation magnetization), $\vec{\gamma}^\alpha$ denotes the direction of magnetization
 707 (γ_i^α : direction cosines) in the crystal frame. K_1 and K_2 are the magnetocrystalline
 708 energy constants. \vec{H}^α is the magnetic field at the domain scale. $\boldsymbol{\sigma}^\alpha$
 709 is the stress tensor at the domain scale. \mathbb{C}^α denotes the stiffness tensor of a
 710 domain family (or grain $\mathbb{C}^g = \mathbb{C}^\alpha$). Homogeneous field and deformation assumptions
 711 lead to a definition of magneto static and elastic energies involving
 712 magnetic and mechanical loadings at the grain scale:

$$W_H^\alpha = -\mu_0 \vec{H}^g \cdot \vec{M}^\alpha \quad (\text{A.5})$$

$$W_\sigma^\alpha = -\boldsymbol{\sigma}^g : \boldsymbol{\epsilon}_\mu^\alpha \quad (\text{A.6})$$

713 where $\boldsymbol{\epsilon}_\mu^\alpha$ denotes the magnetostriction strain tensor of a domain family
 714 α , where λ_{100} and λ_{111} are the magneto-elastic constants:

$$\boldsymbol{\epsilon}_\mu^\alpha = \frac{3}{2} \begin{pmatrix} \lambda_{100}(\gamma_1^2 - \frac{1}{3}) & \lambda_{111}\gamma_1\gamma_2 & \lambda_{111}\gamma_1\gamma_3 \\ \lambda_{111}\gamma_1\gamma_2 & \lambda_{100}(\gamma_2^2 - \frac{1}{3}) & \lambda_{111}\gamma_2\gamma_3 \\ \lambda_{111}\gamma_1\gamma_3 & \lambda_{111}\gamma_2\gamma_3 & \lambda_{100}(\gamma_3^2 - \frac{1}{3}) \end{pmatrix}_{CF} \quad (\text{A.7})$$

715 At the grain scale, the volume fraction f_α of a family domain α is calculated
 716 using a statistical approach (Boltzmann function - A.8) [37] assuming
 717 that a magnetic domain is much smaller than a representative volume element
 718 (considered as a small body immersed into a large closed thermodynamic system).
 719 θ_α and ϕ_α are the results of a minimization of the potential energy of
 720 a domain family (A.10).

$$f_\alpha = \frac{\exp(-A_s \cdot W^\alpha)}{\sum_\alpha \exp(-A_s \cdot W^\alpha)} \quad (\text{A.8})$$

721 with

$$A_s = \frac{3\chi_0}{\mu_0 M_s^2} \quad (\text{A.9})$$

$$\{\theta_\alpha, \phi_\alpha\} = \min(W^\alpha) \quad (\text{A.10})$$

722 χ_0 , M_s and μ_0 are the initial anhysteretic susceptibility (model expressed
 723 in reversible condition), the saturation magnetization and the vacuum per-
 724 meability respectively. This formulation uses the assumption that initial
 725 magnetization process is due to magnetic wall displacement and that rota-
 726 tion mechanism is neglected. This assumption is true for nickel at RT. An
 727 increasing temperature may compromise this hypothesis (especially when K_1
 728 is reduced, that enhances the rotation mechanism).

729 A_s , through its relation with χ_0 , is a parameter that accounts for ener-
 730 getic terms not considered in the final expression (exchange energy, magneto-
 731 static phenomena). Its expression evolves with temperature since saturation
 732 magnetization and initial anhysteretic susceptibility are temperature depen-
 733 dent. Moreover, a global inverse proportionality dependence to temperature
 734 should be considered for A_s following the reference statistical approach [37],
 735 leading to the final expression:

$$A_s = \frac{3\chi_0(T)}{\mu_0 M_s(T)^2} \frac{T^{RT}}{T} \quad (\text{A.11})$$

736 with T^{RT} the room temperature.

737

738 Assuming that the elastic behavior is homogeneous within a grain, the
 739 magnetostriction strain of a single crystal is written as the mean magne-
 740 tostriction over the domains (A.12). The magnetization in a grain is defined
 741 as well (A.13).

$$\epsilon_\mu^g = \langle \epsilon_\mu^\alpha \rangle = \sum_\alpha f_\alpha \epsilon_\mu^\alpha \quad (\text{A.12})$$

$$\vec{M}^g = \langle \vec{M}^\alpha \rangle = \sum_\alpha f_\alpha \vec{M}^\alpha \quad (\text{A.13})$$

742 The discrete approach has been modernized by [27]. In this new version,
 743 the easy directions are not defined *a priori*. The possible directions $\vec{\gamma}^\alpha$ are
 744 described through the mesh of a unit radius sphere (N unit vectors \vec{x}_n). A

34635 points mesh has been used in the present study. This new approach avoids the minimization operation A.10 and is less time consuming.

Appendix A.2. Localization and homogenization

Previous calculations are made for each grain of the polycrystalline aggregate. The polycrystalline aggregate considered in the study is a regularly distributed orientation data file made of 546 orientations [13]. The magnetic behavior at the polycrystalline scale is defined as the average value of magnetization (A.14). A local demagnetizing field in each grain due to the magnetization of the surrounding grains can be introduced [13, 36]: the magnetic field at the grain scale \vec{H}^g is defined as a function of the external field, the mean secant equivalent susceptibility of the material χ_m , ($\chi_m = M/H$) and the difference between the mean magnetization \vec{M} and the magnetization at the grain scale \vec{M}^g (A.15). The elastic behavior is obtained using a self-consistent homogenization scheme. The macroscopic magnetostriction strain (A.16) is estimated using the Eshelby's solution and considering the local magnetostriction as a free strain; \mathbb{B}^g denotes the fourth order stress concentration tensor.

$$\vec{M} = \langle \vec{M}^g \rangle \quad (\text{A.14})$$

$$\vec{H}^g = \vec{H} + \frac{1}{3 + 2\chi_m}(\vec{M} - \vec{M}^g) \quad (\text{A.15})$$

$$\epsilon_\mu = \langle {}^t \mathbb{B}^g : \epsilon_\mu^g \rangle \quad (\text{A.16})$$

The magnetostriction strain at the grain scale is elastically incompatible and creates a stress that changes the magneto-elastic energy term (self-stress). The stress at the grain scale σ^g is derived from the implicit equation (A.17).

$$\sigma^g = \mathbb{B}^g : \sigma + \mathbb{C}^{acc} : (\epsilon_\mu - \epsilon_\mu^g) \quad (\text{A.17})$$

with the accommodation stiffness tensor:

$$\mathbb{C}^{acc} = ((\mathbb{C}^g)^{-1} + (\mathbb{C}^*)^{-1})^{-1} \quad (\text{A.18})$$

and the stress concentration tensor:

$$\mathbb{B}^g = \mathbb{C}^g : (\mathbb{C}^g + \mathbb{C}^\star)^{-1} : (\mathbb{C}^0 + \mathbb{C}^\star) : (\mathbb{C}^0)^{-1} \quad (\text{A.19})$$

768 $\mathbb{C}^\star = \mathbb{C}^0 : ((\mathbb{S}^{Esh})^{-1} - \mathbb{I})$ is the Hill's constraint tensor. \mathbb{C}^0 is the stiffness
769 tensor of the effective medium. If a self-consistent scheme is chosen, \mathbb{C}^0 refers
770 to the self-consistent stiffness tensor. $\boldsymbol{\sigma}$ is the macroscopic stress. \mathbb{S}^{Esh} is the
771 so-called Eshelby tensor, calculated following Mura [35].

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