Equivalence of magnetoelastic, elastic, and mechanical work energies with stress-induced anisotropy

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ABSTRACT

This work investigates the equivalence of thermodynamic potentials utilizing stress-induced anisotropy energy and potentials using elastic, magnetoelastic, and mechanical work energies. The former is often used to model changes in magnetization and strain due to magnetic field and stress in magnetostrictive materials. The enthalpy of a ferromagnetic body with cubic symmetry is written with magnetization and strain as the internal states and the equilibrium strains are calculated by minimizing the enthalpy. Evaluating the enthalpy using the equilibrium strains, functions of the magnetization orientation, results in an enthalpy expression devoid of strain. By inspecting this expression, the magnetoelastic, elastic, and mechanical work energies are identified to be equivalent to the stress-induced anisotropy plus magnetostriction-induced fourth order anisotropy. It is shown that as long as the value of fourth order crystalline anisotropy constant K_1 includes the value of magnetostriction-induced fourth order anisotropy constant ΔK_1 , energy formulations involving magnetoelastic, elastic, and mechanical work energies are equivalent to those involving stress-induced anisotropy energy. Further, since the stress-induced anisotropy is only given for a uniaxial applied stress, an expression is developed for a general 3D stress.

Keywords: magnetostriction, magnetoelastic, magnetocrystalline, anisotropy, energy, delta K, 3-dimensional

1. INTRODUCTION

Magnetostrictive materials exhibit dimensional and magnetization changes in response to magnetic fields and stresses. The dimensional change due to the application of a magnetic field is exploited for actuation. The magnetization change due to stress is used for sensing. The development of new magnetostrictive materials like Iron-Gallium alloys (Galfenol) demonstrating moderate magnetostriction and steel-like structural properties enables these materials to be used in applications involving bending, torsion, etc. in 3D structures. Such applications require modeling tools that capture the nonlinear constitutive response of magnetostrictive materials.

Nonlinear modeling of magnetostriction often involves the calculation of the system's free energy, where the internal states are magnetization and strain and the applied work is due to mechanical stresses and magnetic fields. Alternative energy approaches^{2–4} use only the magnetization as the internal state and incorporate magnetomechanical coupling by including the anisotropy energy induced by applied stress in the system's free energy. The energy with only the magnetization as an internal state is

$$E_T = E_K + E_{\sigma}^{aniso} - W_{mag},\tag{1}$$

where the first, second, and third terms are magnetocrystalline anisotropy, stress-induced anisotropy, and magnetic work (Zeeman energy) energies respectively. Although the second term in the energy expression is sometimes

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referred to as magnetoelastic energy, the works of Kittel et al. and Chikazumi et al. show that it is actually the stress-induced anisotropy energy.^{5,6} The expression for the magnetoelastic energy involves strains as will be described in equation (6) while the expression for stress-induced anisotropy does not.

Jiles and Thoelke² used the energy expression (1) for modeling the effects of stress and anisotropy on the magnetization and magnetostriction of Terfenol-D. The approach calculates the bulk magnetization and magnetostriction as the sum of the contributions from the various equlibria without explicitly calculating the fractional occupancy of the material in each equilibrium. Armstrong³ used an empirical expression to explicitly calculate the energy distribution and subsequently the bulk material magnetization and magnetostriction of Terfenol-D. Evans and Dapino⁷ employed a thermodynamic framework to calculate the energy distribution and model the magnetization and magnetostriction of Galfenol. The Armstrong model has also been used to model actuation and sensing behavior of Iron-Gallium alloys.^{8–10}

The modeling approaches discussed here agree well with experiments despite their use of an energy potential lacking strain as an internal state. In this paper, the conditions are given for which (1) is equivalent to an energy potential which includes strain through the elastic, magnetoelastic, and mechanical work energies. Under these conditions, the accuracy of models utilizing (1) is not effected by the absence of strain. Further, the energy expression (1) is typically for 3-D magnetic fields and unidirectional stresses. Therefore, an expression suitable not only for 3-D magnetic fields but also for 3-D stresses is developed which is of importance for modeling 3-D Galfenol behavior.

2. ENERGY DERIVATION

Most widely used magnetostrictive materials like Nickel, Terfenol-D and Galfenol have a cubic symmetry and hence all the energy expressions used or derived in this section are for materials with cubic symmetry. As discussed in the introduction, an energy expression⁵ commonly used in magnetomechanical models is the sum of the magnetocrystalline anisotropy energy

$$E_K = K_1 \left(\alpha_1^2 \alpha_2^2 + \alpha_2^2 \alpha_3^2 + \alpha_3^2 \alpha_1^2 \right) + K_2 \left(\alpha_1^2 \alpha_2^2 \alpha_3^2 \right), \tag{2}$$

stress-induced anisotropy energy

$$E_{\sigma}^{aniso} = -\frac{3}{2}\lambda_{100}\sigma \left\{ \alpha_1^2 \beta_1^2 + \alpha_2^2 \beta_2^2 + \alpha_3^2 \beta_3^2 - \frac{1}{3} \right\} - 3\lambda_{111}\sigma \left(\alpha_1 \alpha_2 \beta_1 \beta_2 + \alpha_2 \alpha_3 \beta_2 \beta_3 + \alpha_3 \alpha_1 \beta_3 \beta_1 \right), \tag{3}$$

and magnetic work or Zeeman energy

$$W_{mag} = \mu_0 \mathbf{M}^T \mathbf{H}. \tag{4}$$

In the above equations, K_1 and K_2 are fourth and sixth order cubic anisotropy constants respectively and λ_{100} and λ_{111} are the magnetostriction constants. The direction cosines α_i of the magnetization vector \mathbf{M} depend on the applied magnetic field \mathbf{H} and stress σ acting along a direction given by the direction cosines β_i . Equilibrium directions of the magnetization can be calculated by minimizing the total energy. However, this total energy, as discussed in the introduction, lacks magnetoelastic E_{magel} , elastic E_{el} , and mechanical work W_{mech} terms.

To investigate the thermodynamic accuracy of using E_{σ}^{aniso} in place of E_{magel} , E_{el} , and W_{mech} , the internal energy and work energy of a ferromagnetic system are expressed as the sum of the E_K , E_{magel} , and E_{el} and sum of the W_{mag} and W_{mech} respectively. The Gibbs free energy of the system is then formulated as the Legendre transformation of the internal energy. Assuming isothermal and isentropic processes, the Gibbs free energy is reduced to the enthalpy of the system

$$\mathcal{H} = E_K + E_{magel} + E_{el} - W_{mag} - W_{mech}. \tag{5}$$

The expression for E_K is given by equation (2) and the expression for the magnetoelastic energy, derived by Néel^{5,11} considering bond straining due to atomic magnetic moment rotation, is given by

$$E_{magel} = B_1 \left\{ \epsilon_{xx} \left(\alpha_1^2 - \frac{1}{3} \right) + \epsilon_{yy} \left(\alpha_2^2 - \frac{1}{3} \right) + \epsilon_{zz} \left(\alpha_3^2 - \frac{1}{3} \right) \right\} + B_2 \left(\epsilon_{xy} \alpha_1 \alpha_2 + \epsilon_{yz} \alpha_2 \alpha_3 + \epsilon_{zx} \alpha_3 \alpha_1 \right)$$
(6)
= $\mathbf{b} \boldsymbol{\epsilon}$,

where

$$\mathbf{b} = \begin{bmatrix} B_1 \left(\alpha_1^2 - \frac{1}{3} \right) & B_1 \left(\alpha_2^2 - \frac{1}{3} \right) & B_1 \left(\alpha_3^2 - \frac{1}{3} \right) & B_2 \alpha_1 \alpha_2 & B_2 \alpha_2 \alpha_3 & B_2 \alpha_3 \alpha_1 \end{bmatrix}$$
(8)

and

$$\boldsymbol{\epsilon} = \begin{bmatrix} \epsilon_{xx} & \epsilon_{yy} & \epsilon_{zz} & \epsilon_{xy} & \epsilon_{yz} & \epsilon_{zx} \end{bmatrix}^T. \tag{9}$$

Constants B_1 and B_2 are called magnetomechanical coupling constants^{6,12} and can be calculated from the values of magnetostriction and elastic constants of a ferromagnetic material as will be seen later. The axis directions x,y, and z correspond to the < 100 > crystallographic directions of the material.

The elastic energy can be written as

$$E_{el} = \frac{1}{2} \epsilon^T \tilde{\mathbf{C}} \epsilon, \tag{10}$$

where $\tilde{\mathbf{C}}$ is the stiffness matrix. For cubic materials, $\tilde{\mathbf{C}}$ is expressed using elastic constants c_{11} , c_{12} , and c_{44} as

$$\tilde{\mathbf{C}} = \begin{bmatrix}
c_{11} & c_{12} & c_{12} & 0 & 0 & 0 \\
c_{12} & c_{11} & c_{12} & 0 & 0 & 0 \\
c_{12} & c_{12} & c_{11} & 0 & 0 & 0 \\
0 & 0 & 0 & c_{44} & 0 & 0 \\
0 & 0 & 0 & 0 & c_{44} & 0 \\
0 & 0 & 0 & 0 & 0 & c_{44}
\end{bmatrix}.$$
(11)

The expression for W_{mag} is given by equation (4), while the expression for W_{mech} can be written as the product of an externally applied stress (σ) given in equation (12) and the resulting strain (ϵ).

$$\boldsymbol{\sigma}^T = \begin{bmatrix} \sigma_{xx} & \sigma_{yy} & \sigma_{zz} & \sigma_{xy} & \sigma_{yz} & \sigma_{zx} \end{bmatrix}. \tag{12}$$

$$W_{mech} = \boldsymbol{\sigma}^T \boldsymbol{\epsilon} \tag{13}$$

Magnetization can be expressed as $\mathbf{M} = M_s \left[\alpha_1 \ \alpha_2 \ \alpha_3\right]^T$, where M_s is the saturation magnetization, which is a material property. Using this, the enthalpy of the system can be written as a function of α_i and ϵ . Therefore, the variables α_i and ϵ can now be termed as the system's internal variables. Using equations (2), (4), (7), (10), and (13) the enthalpy can be expressed as

$$\mathcal{H}(\alpha_i, \boldsymbol{\epsilon}) = K_1 \left(\alpha_1^2 \alpha_2^2 + \alpha_2^2 \alpha_3^2 + \alpha_3^2 \alpha_1^2 \right) + K_2 \left(\alpha_1^2 \alpha_2^2 \alpha_3^2 \right) + \mathbf{b} \boldsymbol{\epsilon} + \frac{1}{2} \boldsymbol{\epsilon}^T \tilde{\mathbf{C}} \boldsymbol{\epsilon} - \mu_0 \mathbf{M}^T \mathbf{H} - \boldsymbol{\sigma}^T \boldsymbol{\epsilon}.$$
(14)

The equilibrium states of the system can be calculated by minimizing \mathcal{H} with respect to its internal variables α_i and ϵ . It is assumed that $\mathcal{H}(\alpha_i, \epsilon)$ is a continuous function of α_i and ϵ and has continuous second order partial derivatives.

2.1 Equilibrium strains

Some of the earlier works^{5, 6, 12, 13} that have derived the equilibrium strains did so under an assumption of a zero applied stress. In this work, the expression for the equilirium strains is derived assuming a constant 3-D stress. The enthalpy of the system, which is defined in equation (14) with α_i and ϵ as the internal variables, is minimized with respect to ϵ

$$\frac{\partial \mathcal{H}\left(\alpha_{i}, \epsilon\right)}{\partial \epsilon} = 0, \tag{15}$$

which gives

$$\mathbf{b}^T + \tilde{\mathbf{C}}\boldsymbol{\epsilon} - \boldsymbol{\sigma} = 0. \tag{16}$$

Solving for ϵ yields

$$\boldsymbol{\epsilon}^* = \tilde{\mathbf{C}}^{-1} \boldsymbol{\sigma} - \tilde{\mathbf{C}}^{-1} \mathbf{b}^T = \boldsymbol{\epsilon}_{mech} + \boldsymbol{\lambda}. \tag{17}$$

Taking a second partial derivative with respect to ϵ yields

$$\frac{\partial^2 \mathcal{H}\left(\alpha_i, \epsilon\right)}{\partial \epsilon^2} = \tilde{\mathbf{C}},\tag{18}$$

which is a positive value and hence ϵ^* corresponds to a relative minimum of \mathcal{H} . Therefore, ϵ^* is the equilibrium strain.

It is noted that the equilibrium strain derived earlier^{5,6,12,13} for zero stress included only the second part of the equation (17), which is the magnetostrictive $\lambda = -\tilde{\mathbf{C}}^{-1}\mathbf{b}^T$ strain. For the non-zero stress condition derived here, the equilibrium strain is a superposition of purely mechanical $\epsilon_{mech} = \tilde{\mathbf{C}}^{-1}\boldsymbol{\sigma}$ and magnetostrictive strains.

Using equations (8) and (11), the magnetostrictive strain can be calculated as

$$\lambda = \left[\frac{B_1}{c_{12} - c_{11}} \left(\alpha_1^2 - \frac{1}{3} \right) \quad \frac{B_1}{c_{12} - c_{11}} \left(\alpha_2^2 - \frac{1}{3} \right) \quad \frac{B_1}{c_{12} - c_{11}} \left(\alpha_3^2 - \frac{1}{3} \right) \quad -\frac{B_2}{c_{44}} \alpha_1 \alpha_2 \quad -\frac{B_2}{c_{44}} \alpha_2 \alpha_3 \quad -\frac{B_2}{c_{44}} \alpha_3 \alpha_1 \right]. \tag{19}$$

The elongation due to magnetostriction along any direction $(\gamma_1, \gamma_2, \gamma_3)$ can be evaluated using the expression

$$\frac{\delta l}{l} = \lambda_{xx}\gamma_1^2 + \lambda_{yy}\gamma_2^2 + \lambda_{zz}\gamma_3^2 + \lambda_{xy}\gamma_1\gamma_2 + \lambda_{yz}\gamma_2\gamma_3 + \lambda_{zx}\gamma_3\gamma_1, \tag{20}$$

which becomes

$$\frac{\delta l}{l} = \frac{B_1}{c_{12} - c_{11}} \left(\gamma_1^2 \alpha_1^2 + \gamma_2^2 \alpha_2^2 + \gamma_3^2 \alpha_3^2 - \frac{1}{3} \right) - \frac{B_2}{c_{44}} \left(\gamma_1 \gamma_2 \alpha_1 \alpha_2 + \gamma_2 \gamma_3 \alpha_2 \alpha_3 + \gamma_3 \gamma_1 \alpha_3 \alpha_1 \right) \tag{21}$$

by substituting the expressions for λ_{ii} from equation (19).

The magnetostriction along the direction [100] occurs when the magnetization is along this direction. This can be calculated to be

$$\lambda_{100} = -\frac{2}{3} \frac{B_1}{c_{11} - c_{12}} \tag{22}$$

by using $\alpha_1 = \gamma_1 = 1$ and $\alpha_2 = \alpha_3 = \gamma_2 = \gamma_3 = 0$ in equation (21). Similarly, magnetostriction along [111] can be obtained to be

$$\lambda_{111} = -\frac{1}{3} \frac{B_2}{c_{44}} \tag{23}$$

by using $\alpha_i = \gamma_i = \frac{1}{\sqrt{3}}$ in equation (21).

Using equations (22) and (23), the magnetoelastic coupling constants can be expressed in terms of the magnetostriction constants and elastic constants as 5,6

$$B_1 = -\frac{3}{2}\lambda_{100} (c_{11} - c_{c12}); \quad B_2 = -3\lambda_{111}c_{44}$$
(24)

2.2 Expression for enthalpy

The equilibrium strain ϵ^* in equation (17) can be substituted back into equation (14) to obtain an expression for the enthalpy in terms of α_i . Minimizing this expression with respect to α_i will yield the equilibrium magnetization directions. As a result, any term that is not a function of α_i can be ignored.

$$\mathcal{H}(\alpha_i) = K_1 \left(\alpha_1^2 \alpha_2^2 + \alpha_2^2 \alpha_3^2 + \alpha_3^2 \alpha_1^2\right) + K_2 \left(\alpha_1^2 \alpha_2^2 \alpha_3^2\right) + E_{magel}\left(\boldsymbol{\epsilon}^*\right) + E_{el}\left(\boldsymbol{\epsilon}^*\right) - W_{mag} - W_{mech}\left(\boldsymbol{\epsilon}^*\right)$$
(25)

The expressions for $E_{magel}(\epsilon^*)$ and $E_{el}(\epsilon^*) - W_{mech}(\epsilon^*)$ will be individually evaluated and then summed up together to get an expression for the enthalpy.

2.2.1 Expression for magnetoelastic energy

Substituting the equilibrium strain (ϵ^*) in equation (6) and expanding gives the magnetoelastic energy as the sum of two terms:

$$E_{magel}(\epsilon^*) = \mathbf{b}(\epsilon_{mech} + \lambda) = \mathbf{b}\epsilon_{mech} + \mathbf{b}\lambda. \tag{26}$$

Supposing a stress (σ) acting on the ferromagnetic body along a direction $(\beta_1, \beta_2, \beta_3)$, the corresponding mechanical strain $\epsilon_{mech} = e_{ii}$ can be written as⁵

$$\epsilon_{mech} = \sigma \left[\frac{\beta_1^2}{c_{11} - c_{12}} + s_{12} \quad \frac{\beta_2^2}{c_{11} - c_{12}} + s_{12} \quad \frac{\beta_3^2}{c_{11} - c_{12}} + s_{12} \quad \frac{\beta_1 \beta_2}{c_{44}} \quad \frac{\beta_2 \beta_3}{c_{44}} \quad \frac{\beta_3 \beta_1}{c_{44}} \right]^T, \tag{27}$$

where s_{12} is a compliance constant.

Substituting equation (27) in the first term of equation (26) and using equation (7) yields

$$\mathbf{b}\boldsymbol{\epsilon}_{mech} = B_1 \left\{ e_{xx} \left(\alpha_1^2 - \frac{1}{3} \right) + e_{yy} \left(\alpha_2^2 - \frac{1}{3} \right) + e_{zz} \left(\alpha_3^2 - \frac{1}{3} \right) \right\} + B_2 \left(e_{xy} \alpha_1 \alpha_2 + e_{yz} \alpha_2 \alpha_3 + e_{zx} \alpha_3 \alpha_1 \right)$$

$$= \frac{B_1}{c_{11} - c_{12}} \sigma \left\{ \alpha_1^2 \beta_1^2 + \alpha_2^2 \beta_2^2 + \alpha_3^2 \beta_3^2 - \frac{1}{3} \right\} + \frac{B_2}{c_{44}} \sigma \left(\alpha_1 \alpha_2 \beta_1 \beta_2 + \alpha_2 \alpha_3 \beta_2 \beta_3 + \alpha_3 \alpha_1 \beta_3 \beta_1 \right), \tag{28}$$

which can be simplified using the expressions for B_1 and B_2 from equation (24) to obtain

$$\mathbf{b}\boldsymbol{\epsilon}_{mech} = -\frac{3}{2}\lambda_{100}\sigma \left\{ \alpha_1^2 \beta_1^2 + \alpha_2^2 \beta_2^2 + \alpha_3^2 \beta_3^2 - \frac{1}{3} \right\} - 3\lambda_{111}\sigma \left(\alpha_1 \alpha_2 \beta_1 \beta_2 + \alpha_2 \alpha_3 \beta_2 \beta_3 + \alpha_3 \alpha_1 \beta_3 \beta_1 \right). \tag{29}$$

The above expression is the same as the expression for the stress-induced anisotropy energy given in equation (3). Hence, the first term of equation (26) can be replaced with

$$\mathbf{b}\epsilon_{mech} = E_{\sigma}^{aniso}.\tag{30}$$

The second term in equation (26) can be evaluated by substituting from equations (8) and (19) to obtain

$$\mathbf{b}\lambda = B_{1} \left\{ \lambda_{xx} \left(\alpha_{1}^{2} - \frac{1}{3} \right) + \lambda_{yy} \left(\alpha_{2}^{2} - \frac{1}{3} \right) + \lambda_{zz} \left(\alpha_{3}^{2} - \frac{1}{3} \right) \right\} + B_{2} \left(\lambda_{xy} \alpha_{1} \alpha_{2} + \lambda_{yz} \alpha_{2} \alpha_{3} + \lambda_{zx} \alpha_{3} \alpha_{1} \right)$$

$$= -\frac{B_{1}^{2}}{c_{11} - c_{12}} \left\{ \left(\alpha_{1}^{2} - \frac{1}{3} \right)^{2} + \left(\alpha_{2}^{2} - \frac{1}{3} \right)^{2} + \left(\alpha_{3}^{2} - \frac{1}{3} \right)^{2} \right\} - \frac{B_{2}}{c_{44}} \left(\alpha_{1}^{2} \alpha_{2}^{2} + \alpha_{2}^{2} \alpha_{3}^{2} + \alpha_{3}^{2} \alpha_{1}^{2} \right)$$

$$= \left(\frac{2B_{1}^{2}}{c_{11} - c_{12}} - \frac{B_{2}^{2}}{c_{44}} \right) \left(\alpha_{1}^{2} \alpha_{2}^{2} + \alpha_{2}^{2} \alpha_{3}^{2} + \alpha_{3}^{2} \alpha_{1}^{2} \right), \tag{31}$$

which can be simplified by utilizing the expressions for B_1 and B_2 from equation (24) to

$$\mathbf{b}\lambda = \frac{9}{2} \left[\lambda_{100}^2 (c_{11} - c_{12}) - 2\lambda_{111}^2 c_{44} \right] \left(\alpha_1^2 \alpha_2^2 + \alpha_2^2 \alpha_3^2 + \alpha_3^2 \alpha_1^2 \right). \tag{32}$$

Adding equations (30) and (32) gives the expression for the magnetoelastic energy

$$E_{magel}\left(\boldsymbol{\epsilon}^{*}\right) = \frac{9}{2} \left[\lambda_{100}^{2}(c_{11} - c_{12}) - 2\lambda_{111}^{2}c_{44}\right] \left(\alpha_{1}^{2}\alpha_{2}^{2} + \alpha_{2}^{2}\alpha_{3}^{2} + \alpha_{3}^{2}\alpha_{1}^{2}\right) + E_{\sigma}^{aniso}.$$
 (33)

It is noted that the magnetoelastic energy equals the stress-induced anisotropy energy plus an additional fourth order anisotropy energy term.

2.2.2 Expressions for elastic and mechanical work energies

The expression for $E_{el}(\epsilon^*)-W_{mech}(\epsilon^*)$ is evaluated by substituting the equilibrium strain (ϵ^*) from equation (17) into equations (10) and (13) to obtain

$$E_{el}(\boldsymbol{\epsilon}^*) - W_{mech}(\boldsymbol{\epsilon}^*) = \frac{1}{2} (\boldsymbol{\epsilon}_{mech} + \boldsymbol{\lambda})^T \tilde{\mathbf{C}} (\boldsymbol{\epsilon}_{mech} + \boldsymbol{\lambda}), \qquad (34)$$

which can be expanded and simplified to

$$E_{el}(\epsilon^*) - W_{mech}(\epsilon^*) = \frac{1}{2} \lambda^T \tilde{\mathbf{C}} \lambda - \frac{1}{2} \epsilon_{mech}^T \tilde{\mathbf{C}} \epsilon_{mech}.$$
(35)

The second term in the equation (35) is devoid of α_i . Therefore, as mentioned before, the equilibrium α_i do not depend on this term and can be ignored.

The first term in equation (35) can be expanded by using equation (11) to obtain

$$\frac{1}{2}\boldsymbol{\lambda}^{T}\tilde{\mathbf{C}}\boldsymbol{\lambda} = \frac{1}{2}\left[c_{11}\left(\lambda_{xx}^{2} + \lambda_{yy}^{2} + \lambda_{zz}^{2}\right) + c_{44}\left(\lambda_{xy}^{2} + \lambda_{yz}^{2} + \lambda_{zx}^{2}\right) + 2c_{12}\left(\lambda_{xx}\lambda_{yy} + \lambda_{yy}\lambda_{zz} + \lambda_{zz}\lambda_{xx}\right)\right].$$
 (36)

Substituting the values of λ_{ii} from equation (19) gives

$$\frac{1}{2} \boldsymbol{\lambda}^{T} \tilde{\mathbf{C}} \boldsymbol{\lambda} = \frac{1}{2} c_{11} \frac{B_{1}^{2}}{(c_{11} - c_{12})^{2}} \left(\left(\alpha_{1}^{2} - \frac{1}{3} \right)^{2} + \left(\alpha_{2}^{2} - \frac{1}{3} \right)^{2} + \left(\alpha_{3}^{2} - \frac{1}{3} \right)^{2} \right) + \cdots$$

$$c_{12} \frac{B_{1}^{2}}{(c_{11} - c_{12})^{2}} \left(\left(\alpha_{1}^{2} - \frac{1}{3} \right) \left(\alpha_{2}^{2} - \frac{1}{3} \right) + \left(\alpha_{2}^{2} - \frac{1}{3} \right) \left(\alpha_{3}^{2} - \frac{1}{3} \right) + \left(\alpha_{3}^{2} - \frac{1$$

which can be simplified by utilizing the expressions for B_1 and B_2 from equation (24) to yield

$$\frac{1}{2} \boldsymbol{\lambda}^T \tilde{\mathbf{C}} \boldsymbol{\lambda} = -\frac{9}{4} \left[\lambda_{100}^2 (c_{11} - c_{12}) - 2\lambda_{111}^2 c_{44} \right] \left(\alpha_1^2 \alpha_2^2 + \alpha_2^2 \alpha_3^2 + \alpha_3^2 \alpha_1^2 \right). \tag{38}$$

Therefore,

$$E_{el}(\epsilon^*) - W_{mech}(\epsilon^*) = -\frac{9}{4} \left[\lambda_{100}^2(c_{11} - c_{12}) - 2\lambda_{111}^2 c_{44} \right] \left(\alpha_1^2 \alpha_2^2 + \alpha_2^2 \alpha_3^2 + \alpha_3^2 \alpha_1^2 \right)$$
(39)

ignoring the energy term that is independent of α_i .

Adding equations (33) and (39) gives

$$E_{magel}(\epsilon^*) + E_{el}(\epsilon^*) - W_{mech}(\epsilon^*) = \frac{9}{4} \left[\lambda_{100}^2(c_{11} - c_{12}) - 2\lambda_{111}^2 c_{44} \right] \left(\alpha_1^2 \alpha_2^2 + \alpha_2^2 \alpha_3^2 + \alpha_3^2 \alpha_1^2 \right) + E_{\sigma}^{aniso}. \tag{40}$$

The first term in equation (40) is a contribution to the anisotropy energy due to the equilibrium magnetostrictive strains. A fourth-order magnetostrictive anisotropy constant

$$\Delta K_1 = \frac{9}{4} \left[\lambda_{100}^2 (c_{11} - c_{12}) - 2\lambda_{111}^2 c_{44} \right] \tag{41}$$

is defined 5,6,13 and equation (40) becomes

$$E_{magel}\left(\boldsymbol{\epsilon}^{*}\right) + E_{el}\left(\boldsymbol{\epsilon}^{*}\right) - W_{mech}\left(\boldsymbol{\epsilon}^{*}\right) = \Delta K_{1}\left(\alpha_{1}^{2}\alpha_{2}^{2} + \alpha_{2}^{2}\alpha_{3}^{2} + \alpha_{3}^{2}\alpha_{1}^{2}\right) + E_{\sigma}^{aniso}.$$

$$(42)$$

Substituting equation (42) in equation (25) yields the expression for the enthalpy of the system

$$\mathcal{H}(\alpha_i) = (K_1 + \Delta K_1) \left(\alpha_1^2 \alpha_2^2 + \alpha_2^2 \alpha_3^2 + \alpha_3^2 \alpha_1^2 \right) + K_2 \left(\alpha_1^2 \alpha_2^2 \alpha_3^2 \right) + E_{\sigma}^{aniso} - W_{mag}. \tag{43}$$

2.3 Discussion

Comparing equation (43) to the total energy expression in equation (1), it can be seen that the only difference between the two is the fourth order anisotropy constant K_1 . The total energy in equation (1) uses the magnetocrystalline anisotropy energy with fourth order anisotropy constant as K_1 whereas the enthalpy expression derived here shows that it is in fact K_1 plus the magnetostriction-induced fourth order anisotropy constant ΔK_1 . Kittel et al.⁶ described that an experimental determination of K_1 can be made only if the ferromagnetic body is held at a constant strain. If the ferromagnetic body is allowed to strain, then the value observed for K_1 would in fact be $K_1 + \Delta K_1$. Since it is experimentally difficult to maintain a constant strain, the value of theoretical K_1 is usually obtained by subtracting the calculated value of ΔK_1 from the experimentally observed K_1 value.

The values of the fourth order cubic anisotropy constant K_1 for FeGa alloys reported by Rafique et al.¹⁴ do not include the corrective ΔK_1 term. Therefore, the reported values are actually the values of $K_1 + \Delta K_1$. The appropriate values for K_1 can be calculated by subtracting ΔK_1 calculated using equation (41) with values of the magnetostriction and elastic constants.

Figure 1 shows the corrected or theoretical K_1 values for different compositions of FeGa along with the reported values from Rafique et al.¹⁴ and calculated values of ΔK_1 . For the calculation of ΔK_1 , magnetostrictive values reported by Clark et al.¹⁵ and stiffness constant values reported by Wuttig et al.¹⁶ were used.

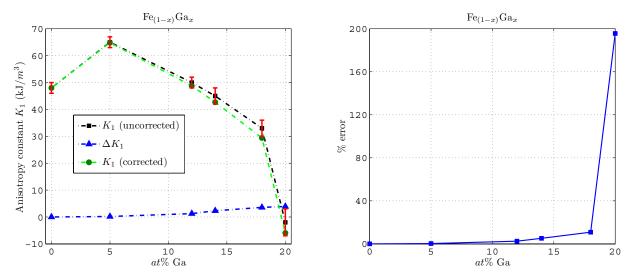


Figure 1. Experimentally determined (uncorrected) K_1 and Corrected K_1 for different at% Ga FeGa alloys

Figure 2. Percent deviation of uncorrected $(K_1 + \Delta K_1)$ values from corrected values (K_1)

In figures 1 and 2 the deviation of corrected from uncorrected values of K_1 for FeGa alloys with less than 18% Ga content, is less than 10%, while close to 20% Ga content, where K_1 becomes very small, it can be as high as 200%. However, since K_1 for FeGa alloys around 20 at% Ga is very small, crystalline anisotropy energy is dominated by the other energy terms and as a result, the usage of K_1 instead of $K_1 + \Delta K_1$ will only affect very low magnetic field or mechanical stress conditions. Moreover, the percentage deviations are within the error bounds of measured K_1 values (uncorrected) reported by Rafique et al. Therefore, it is concluded that no changes are required for the reported values of K_1 for FeGa alloys. In magnetostrictive materials other than FeGa, ΔK_1 may be more significant. For thermodynamic consistency, when E_{magel} , E_{el} , and W_{mech} is replaced with E_{σ}^{aniso} in the total energy, the total anisotropy constant $K_1 + \Delta K_1$ should be used.

2.4 Energy expression for 3D stresses

For 3-D modeling, the energy expression in equation (43) needs slight modification. While equation (43) describes the free energy expression for 3-D magnetic fields, it is valid only for unidirectional stresses. Equation (43) can be easily extended to incorporate 3-D stresses.

It is well known that any 3-D stress tensor acting on a body can be decomposed into principle stresses and principle directions by solving the eigenvalue problem

$$\begin{bmatrix} \sigma_{xx} & \sigma_{xy} & \sigma_{zx} \\ \sigma_{xy} & \sigma_{yy} & \sigma_{yz} \\ \sigma_{zx} & \sigma_{yz} & \sigma_{zz} \end{bmatrix} \begin{pmatrix} \beta_1 \\ \beta_2 \\ \beta_3 \end{pmatrix} = \sigma \begin{pmatrix} \beta_1 \\ \beta_2 \\ \beta_3 \end{pmatrix}, \tag{44}$$

which results in three principle stresses (eigenvalues), σ_j acting along three principle directions (eigenvectors), $(\beta_{1j}, \beta_{2j}, \beta_{3j})$.

The mechanical strain resulting from all the three principle stresses can be evaluated by the principle of superposition

$$\epsilon_{mech} = \sum_{j=1}^{3} \sigma \left[\frac{\beta_{1j}^{2}}{c_{11} - c_{12}} + s_{12} \quad \frac{\beta_{2j}^{2}}{c_{11} - c_{12}} + s_{12} \quad \frac{\beta_{3j}^{2}}{c_{11} - c_{12}} + s_{12} \quad \frac{\beta_{1j}\beta_{2j}}{c_{44}} \quad \frac{\beta_{2j}\beta_{3j}}{c_{44}} \quad \frac{\beta_{3j}\beta_{1j}}{c_{44}} \right]^{T}. \tag{45}$$

From equations (30) and (45), it directly follows that the net stress-induced anisotropy energy is sum of the stress induced anisotropy energies due to each principle stress

$$E_{\sigma_{3D}}^{aniso} = \sum_{j=1}^{3} -\frac{3}{2} \lambda_{100} \sigma \left\{ \alpha_{1}^{2} \beta_{1j}^{2} + \alpha_{2}^{2} \beta_{2j}^{2} + \alpha_{3}^{2} \beta_{3j}^{2} - \frac{1}{3} \right\} - 3 \lambda_{111} \sigma \left(\alpha_{1} \alpha_{2} \beta_{1j} \beta_{2j} + \alpha_{2} \alpha_{3} \beta_{2j} \beta_{3j} + \alpha_{3} \alpha_{1} \beta_{3j} \beta_{1j} \right)$$

$$= \sum_{j=1}^{3} E_{\sigma}^{aniso} \left(\sigma_{j}, \beta_{ij} \right), \tag{46}$$

Therefore, the enthalpy expression that must be used to model the response of ferromagnetic materials subjected to 3-D magnetic fields and mechanical stresses is given by

$$\mathcal{H}(\alpha_i) = (K_1 + \Delta K_1) \left(\alpha_1^2 \alpha_2^2 + \alpha_2^2 \alpha_3^2 + \alpha_3^2 \alpha_1^2 \right) + K_2 \left(\alpha_1^2 \alpha_2^2 \alpha_3^2 \right) + \sum_{i=1}^3 E_{\sigma}^{aniso} \left(\sigma_j, \beta_{ij} \right) - W_{mag}. \tag{47}$$

3. CONCLUSIONS

An expression for the enthalpy of a ferromagnetic body has been derived. Starting from the enthalpy expression, which includes the energy density due to magnetocrystalline anisotropy, magnetoelastic coupling, and elastic strain and work energy densities due to magnetic fields and mechanical stresses, the equilibrium strains were derived. It has been shown that, as expected, the equilibrium strain is the superposition of pure mechanical strain and pure magnetostrictive strain. Evaluating the enthalpy expression with the equilibrium strains yields an expression which has only the magnetization orientation as the internal state. This expression is interpreted as the sum of the magnetocrystalline anisotropy, the stress-induced anisotropy, and the magnetic work energies where the fourth-order magnetocrystalline anisotropy constant is the sum of the intrinsic magnetic constant K_1 and an anisotropy change ΔK_1 due to magnetoelastic coupling. Since the experimental determination of the crystalline anisotropy constant is usually done at constant stress, reported values include ΔK_1 . It was shown that the difference in K_1 and $K_1 + \Delta K_1$ is within the experimental error of measurement for reported values of FeGa. It was concluded that modeling approaches that use stress-induced anisotropy energy in place of elastic, magnetoelastic, and mechanical work energies are thermodynamically consistent as long the magnetocrystalline anisotropy coefficients include ΔK_1 due to magnetoelastic coupling. Further, an expression for enthalpy suitable for modeling the response of ferromagnetic materials subjected to 3-D magnetic fields as well as 3-D mechanical stresses was provided.

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