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A three-dimensional phenomenological model for Magnetic Shape Memory Alloys

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We present a three-dimensional thermodynamically-consistent phenomenological model for the magneto-mechanical behavior of magnetic shape memory materials featuring a cubic-to-tetragonal martensitic transformation. Existence of *energetic solutions* for both the constitutive relation problem and the three-dimensional quasi-static evolution problem are proved. The proposed model reduces to some former one via parameter asymptotics by means of a rigorous Γ -convergence argument.

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Magnetic Shape Memory Alloys (MSMAs) present the usual superelastic and shape memory effects of SMAs combined with an impressive magnetostrictive behavior up to strains of 5-8%. This is the effect of the ferromagnetic nature of martensites in MSMAs which present the classical magnetic domain structure (domains with uniform magnetization). Local magnetization tends to align with external magnetic fields. Generally, this alignment corresponds to two mechanisms: the magnetic domain wall motion and the magnetization vector rotation. In MSMAs, a third phenomenon arises for martensitic variants rearrange in order to minimize the magnetic energy.

Our focus here is on the phenomenological description of MSMA behavior in three dimensions. We concentrate our attention on so-called *magnetically uniaxial* materials, namely those presenting a single *easy axis* (preferred magnetization axis) at the martensitic crystal level. This is the case for MSMAs featuring a cubic-to-tetragonal martensitic transformation as Ni_2MnGa , FePd , FePt . By applying a magnetic field, one variant may be favored with respect to the others. This results in a variant reorientation and a macroscopic strain.

Some alternative phenomenological modeling of MSMAs are proposed in [4] and [5]. The referred papers, albeit taking their origin from the same basic principles, differ from the present approach as they are essentially restricted to two dimensions (or two martensitic variants), and they feature a *scalar* internal variable (local proportion of one martensitic variant with respect to the others) and a different choice of the relevant potentials. On the contrary, the present model is three-dimensional and *tensorial* in nature.

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We formulate the model in the framework of irreversible thermodynamics in terms of the internal magnetic field \mathbf{H} , the total stress $\boldsymbol{\sigma}$, and the absolute temperature T of the MSMA specimen. The linearized (small) strain $\boldsymbol{\varepsilon}$ is additively decomposed into $\boldsymbol{\varepsilon} = \mathbb{C}^{-1}:\boldsymbol{\sigma} + \mathbf{z}$ where \mathbb{C} is the elasticity tensor and $\mathbf{z} \in \mathbb{R}_{\text{dev}}^{3 \times 3}$ is the deviatoric inelastic (or *transformation*) strain due to martensitic transformation. The latter is regarded as the indicator of the internal martensitic structure of the material. We introduce an affine relation associating with any transformation strain $\mathbf{z} \in \mathbb{R}_{\text{dev}}^{3 \times 3}$ a specific (signed) easy axis of magnetization in \mathbb{R}^3 as

$$\mathbf{z} \mapsto \mathbf{A}_0 + \mathbb{A}:\mathbf{z}$$

where $\mathbf{A}_0 := \frac{1}{3}(1, 1, 1)^\top$ and \mathbb{A} is a third order tensor of components

$$\mathbb{A}_{iii} = -\frac{2}{3}\sqrt{\frac{2}{3}}\frac{1}{\varepsilon_L}, \quad \mathbb{A}_{ijj} = \frac{1}{3}\sqrt{\frac{2}{3}}\frac{1}{\varepsilon_L}, \quad \mathbb{A}_{ijk} = 0 \quad \text{for } i \neq j \neq k \in \{1, 2, 3\}.$$

Here $\varepsilon_L > 0$ is the maximum strain modulus obtainable due to alignment of martensitic variants and \mathbf{A}_0 represents the *mean easy axis* vector related to the so-called *equivariant state* $\mathbf{z} = \mathbf{0}$ (equal proportion of the three martensitic variants).

Our main modeling choice consists of directly linking the magnetization \mathbf{M} with the transformation strain \mathbf{z} by means of the affine relation

$$\mathbf{M} := \alpha \mathcal{A}\mathbf{z} = \alpha m_{\text{sat}}(\mathbf{A}_0 + \mathbb{A}:\mathbf{z}).$$

Here, $\alpha \in [-1, 1]$ describes the local (signed) proportion of magnetic domains oriented in the direction of the easy axis and $m_{\text{sat}} > 0$ is the saturation magnetization. This specific choice relies on the assumption that the magnetic anisotropy of the material is sufficiently strong so that the magnetization stays rigidly attached to the easy axes of the martensitic variants and no magnetization rotation occurs [9].

It is worth pointing out that, for any $\mathbf{z} \in \mathbb{R}_{\text{dev}}^{3 \times 3}$, the vectors \mathbf{A}_0 and $\mathbb{A}:\mathbf{z}$ are orthogonal. Thus, along with this specific form of the operator \mathcal{A} , the magnetization \mathbf{M} satisfies the usual constraint $|\mathbf{M}| \leq m_{\text{sat}}$. Furthermore, for every $\mathbf{z} \in \mathbb{R}_{\text{dev}}^{3 \times 3}$, we get $\mathcal{A}\mathbf{z} \neq \mathbf{0}$ and $\mathbf{M} = \mathbf{0}$ will be possibly achieved for $\alpha = 0$. Eventually, it can be checked that the choice of \mathcal{A} is compatible with material symmetries, see [3] for additional modeling details and motivation.

The constitutive relations for the model are derived from the Gibbs free energy density of the material (assumed of a constant and normalized density) as a function of $\boldsymbol{\sigma}$, \mathbf{H} , T , and of the internal variables \mathbf{z} and α as

$$\begin{aligned} G_\delta(\boldsymbol{\sigma}, \mathbf{H}, T, \mathbf{z}, \alpha) := & -\frac{1}{2}\boldsymbol{\sigma}:\mathbb{C}^{-1}:\boldsymbol{\sigma} - \boldsymbol{\sigma}:\mathbf{z} + \beta(T - T_{\text{crit}})^+|\mathbf{z}| + \frac{h}{2}|\mathbf{z}|^2 + I_{\varepsilon_L}(\mathbf{z}) \\ & + \frac{1}{2\delta}\alpha^2 + I_{[-1,1]}(\alpha) - \mu_0\mathbf{H}\cdot\alpha\mathcal{A}\mathbf{z}. \end{aligned} \quad (1)$$

The first line in (1) is exactly the Gibbs energy density of the non-magnetic SMA model originally advanced by Souza, Mamiya, & Zouain [8] and developed in [1, 2]. In particular, $T_{\text{crit}} > 0$ is a critical stress-free martensite-austenite switching temperature, $\beta > 0$ is a material parameter, $h > 0$ is an isotropic hardening modulus, and $I_{\varepsilon_L}:\mathbb{R}^{3 \times 3} \rightarrow \{0, \infty\}$ is the *indicator function* of the set $Z := \{\mathbf{z} \in \mathbb{R}_{\text{dev}}^{3 \times 3} : |\mathbf{z}| \leq \varepsilon_L\}$ (namely $I_{\varepsilon_L}(\mathbf{z}) = 0$ if $\mathbf{z} \in Z$ and

$I_{\varepsilon_L}(\mathbf{z}) = \infty$ otherwise). We shall let

$$F_{\text{mech}}(T, \mathbf{z}) := \beta(T - T_{\text{crit}})^+ |\mathbf{z}| + \frac{h}{2} |\mathbf{z}|^2 + I_{\varepsilon_L}(\mathbf{z}).$$

The second line in the expression of the Gibbs energy (1) describes the magnetic behavior of the material. The term $-\mu_0 \mathbf{H} \cdot \alpha \mathcal{A} \mathbf{z}$ is nothing but the classical *Zeeman energy* term $-\mu_0 \mathbf{H} \cdot \mathbf{M}$. Note that \mathbf{H} stands here for the *internal* magnetic field. Namely, \mathbf{H} is the magnetic field which is actually experienced by the material when subjected to some (externally) applied field and corresponds to the sum of the applied external field and the corresponding induced demagnetization field. The indicator function $I_{[-1,1]}$ is constraining the scalar α to take values in $[-1, 1]$ and $1/\delta$ is a user-defined hardening parameter.

We focus here on the isothermal situation. Hence, we let $\beta^* := \beta(T^* - T_{\text{crit}})^+$ be fixed. The constitutive equations are classically derived as

$$\boldsymbol{\varepsilon} = -\frac{\partial G}{\partial \boldsymbol{\sigma}} = \mathbb{C}^{-1} \cdot \boldsymbol{\sigma} + \mathbf{z}, \quad (2)$$

$$\mathbf{M} = -\frac{1}{\mu_0} \frac{\partial G}{\partial \mathbf{H}} = \alpha \mathcal{A}^* \mathbf{z}, \quad (3)$$

$$\mathbf{g} \in -\frac{\partial G}{\partial \mathbf{z}} = \boldsymbol{\sigma} - \beta^* \partial |\mathbf{z}| - h \mathbf{z} - \partial I_{\varepsilon_L}(\mathbf{z}) + \mu_0 m_{\text{sat}} \alpha \mathbf{H} \cdot \mathbb{A}^*, \quad (4)$$

$$\gamma \in -\frac{\partial G}{\partial \alpha} = -\frac{1}{\delta} \alpha - \partial I_{[-1,1]}(\alpha) + \mu_0 \mathbf{H} \cdot \mathcal{A}^* \mathbf{z}, \quad (5)$$

where ∂ denotes subdifferentiation in the sense of Convex Analysis, \mathbb{A}^* is the symmetrized deviatoric part of \mathbb{A} , i.e., $\mathbb{A}_{ijk}^* := \frac{1}{2}(\mathbb{A}_{ijk} + \mathbb{A}_{ikj}) - \frac{1}{3} \mathbb{A}_{i\ell\ell} \delta_{jk}$ (summation convention), and $\mathcal{A}^* \mathbf{z} := m_{\text{sat}}(\mathbf{A}_0 + \mathbb{A}^* : \mathbf{z})$. Here, \mathbf{g} and γ represent the *thermodynamic forces* driving the evolution of the internal variables \mathbf{z} and α , respectively.

As for the flow rules for internal variables, we assume that the inelastic strain \mathbf{z} dissipates energy whereas the variable α is non-dissipative. This is of course disputable as the dissipation in α is, for instance, the basic dissipative mechanism in ferromagnetic materials. Still, experiments show that, at small strains, the dissipation in α is negligible with respect to that in \mathbf{z} . Eventually, the dissipation function associated with \mathbf{z} is given by

$$D(\dot{\mathbf{z}}) = \begin{cases} R |\dot{\mathbf{z}}| & \text{if } \dot{\mathbf{z}} \in \mathbb{R}_{\text{dev}}^{3 \times 3} \\ \infty & \text{else} \end{cases}$$

where $R > 0$ is the transformation radius. As the dissipation function D is independent of $\dot{\alpha}$, we have that $\gamma = 0$. Therefore, from relation (5) we obtain that the internal variable α can be directly obtained as a function of \mathbf{H} and \mathbf{z} as

$$\alpha = \text{proj}_{[-1,1]}(\delta \mu_0 \mathbf{H} \cdot \mathcal{A}^* \mathbf{z}) := \max \{ -1, \min \{ 1, \delta \mu_0 \mathbf{H} \cdot \mathcal{A}^* \mathbf{z} \} \}.$$

Let us introduce the function $F_{\text{magn}} : \mathbb{R} \rightarrow \mathbb{R}$ as

$$F_{\text{magn}}(r) := \frac{1}{2\delta} \min \left\{ (\delta \mu_0 r)^2, 2|\delta \mu_0 r| - 1 \right\} \text{ for all } r \in \mathbb{R},$$

in such a way that $\partial_z F_{\text{magn}}(\mathbf{H} \cdot \mathcal{A}^* \mathbf{z}) := \mu_0 \text{proj}_{[-1,1]}(\delta \mu_0 \mathbf{H} \cdot \mathcal{A}^* \mathbf{z}) \mathbf{H} \cdot \mathbb{A}^*$.

The **constitutive relation problem** reads: given \mathbf{z}_0 , $t \mapsto \boldsymbol{\sigma}(t)$, and $t \mapsto \mathbf{H}(t)$, to find $t \mapsto \mathbf{z}(t) \in Z$ such that

$$\partial D(\dot{\mathbf{z}}) + \partial F_{\text{mech}}(\mathbf{z}) - \partial_z F_{\text{magn}}(\mathbf{H} \cdot \mathcal{A}^* \mathbf{z}) \ni \boldsymbol{\sigma} \quad \mathbf{z}(0) = \mathbf{z}_0. \tag{6}$$

We treat this problem within the framework of *energetic formulations* of rate-independent processes [6]. In particular, we impose the initial condition $\mathbf{z}(0) = \mathbf{z}_0$ and, for every t in $[0, T]$, the *global stability* (S) and the *energy equality* (E)

$$\begin{aligned} & F_{\text{mech}}(\mathbf{z}(t)) - F_{\text{magn}}(\mathbf{H}(t) \cdot \mathcal{A}^* \mathbf{z}(t)) - \boldsymbol{\sigma}(t) : \mathbf{z}(t) \\ & \leq F_{\text{mech}}(\hat{\mathbf{z}}) - F_{\text{magn}}(\mathbf{H}(t) \cdot \mathcal{A}^* \hat{\mathbf{z}}) - \boldsymbol{\sigma}(t) : \hat{\mathbf{z}} + D(\mathbf{z}(t) - \hat{\mathbf{z}}), \quad \forall \hat{\mathbf{z}} \in Z \quad \text{(S)} \\ & F_{\text{mech}}(\mathbf{z}(t)) - F_{\text{magn}}(\mathbf{H}(t) \cdot \mathcal{A}^* \mathbf{z}(t)) - \boldsymbol{\sigma}(t) : \mathbf{z}(t) + \text{Diss}_D(\mathbf{z}, [0, t]) \\ & = F_{\text{mech}}(\mathbf{z}_0) - F_{\text{magn}}(\mathbf{H}(0) \cdot \mathcal{A}^* \mathbf{z}_0) - \boldsymbol{\sigma}(0) : \mathbf{z}_0 \\ & + \int_0^t \left(-\dot{\boldsymbol{\sigma}}(s) : \mathbf{z}(s) - F'_{\text{magn}}(\mathbf{H} \cdot \mathcal{A}^* \mathbf{z}) \dot{\mathbf{H}}(s) \cdot \mathcal{A}^* \mathbf{z}(s) \right) ds \quad \text{(E)} \end{aligned}$$

where $\text{Diss}_D(\mathbf{z}, [0, T]) := \sup\{\sum_{i=1}^N D(\mathbf{z}(t^i) - \mathbf{z}(t^{i-1}))\}$ is the supremum taken over all partitions $\{0 = t^0 < t^1 < \dots < t^N = T\}$ of $[0, T]$.

Theorem 0.1 (Existence for the constitutive relation problem) *Assume to be given $\boldsymbol{\sigma} \in W^{1,1}(0, T; \mathbb{R}^{3 \times 3}_{\text{sym}})$, $\mathbf{H} \in W^{1,1}(0, T; \mathbb{R}^3)$, and a suitable initial condition \mathbf{z}_0 . Then, there exists an energetic solution of the constitutive relation (6), namely, a solution of the system (S)-(E).*

Let us now turn to the three-dimensional **quasi-static evolution problem**. Let $\Omega \subset \mathbb{R}^3$ be the reference configuration of the material and $\Gamma_0 \subset \partial\Omega$ with positive surface measure. The quasi-static evolution problem is obtained by coupling the constitutive relation and flow rule

$$\begin{pmatrix} \mathbf{0} \\ \partial D(\dot{\mathbf{z}}) \end{pmatrix} + \begin{pmatrix} \partial_{\boldsymbol{\sigma}} G(\boldsymbol{\sigma}, \mathbf{H}, \mathbf{z}) \\ \partial_z G(\boldsymbol{\sigma}, \mathbf{H}, \mathbf{z}) \end{pmatrix} \ni \begin{pmatrix} -\boldsymbol{\varepsilon}(\mathbf{U}) \\ \mathbf{0} \end{pmatrix} \tag{7}$$

with the equilibrium equation

$$\text{div } \boldsymbol{\sigma} + \mathbf{F} = \mathbf{0} \quad \text{in } \Omega, \tag{8}$$

for some given body force \mathbf{F} and some prescribed boundary conditions. Note that Maxwell's system is not considered here. In particular, the internal magnetic field \mathbf{H} is assumed to be given. We introduce the sets

$$\begin{aligned} \mathcal{U} & := \{ \mathbf{V} \in H^1(\Omega, \mathbb{R}^3) : \mathbf{V} = \mathbf{0} \text{ on } \Gamma_0 \} \\ \mathcal{Z} & := \{ \mathbf{z} \in BV(\Omega, \mathbb{R}^{3 \times 3}) \cap L^2(\Omega, \mathbb{R}^{3 \times 3}) : \mathbf{z} \in Z \text{ a.e. in } \Omega \}. \end{aligned}$$

Then, the total energy of the MSMA body is given by the functional $\mathcal{W} : [0, T] \times \mathcal{U} \times \mathcal{Z} \rightarrow \mathbb{R}$

$$\begin{aligned} \mathcal{W}(t, \mathbf{U}, \mathbf{z}) & := \frac{1}{2} \int_{\Omega} (\boldsymbol{\varepsilon}(\mathbf{U}) - \mathbf{z}) : \mathbb{C} : (\boldsymbol{\varepsilon}(\mathbf{U}) - \mathbf{z}) dx + \int_{\Omega} F_{\text{mech}}(\mathbf{z}) dx + \text{Var}(\mathbf{z}) \\ & - \int_{\Omega} F_{\text{magn}}(\mathbf{H}(t) \cdot \mathcal{A}^* \mathbf{z}) dx - \langle \boldsymbol{\ell}(t), \mathbf{U} \rangle, \end{aligned}$$

where $\langle \ell(t), \mathbf{U} \rangle$ is the work of the external loading and $\text{Var}(\mathbf{z}) = \int_{\Omega} |\mathbf{D}\mathbf{z}|$ stands for the total variation of \mathbf{z} . Existence of a solution for the full quasi-static evolution problem is again obtained by means of the *energetic approach*. Being given ℓ , \mathbf{H} and a suitable initial datum $(\mathbf{U}_0, \mathbf{z}_0)$, an energetic solution of the quasi-static evolution problem is a function $t \in [0, T] \mapsto (\mathbf{U}(t), \mathbf{z}(t)) \in \mathcal{U} \times \mathcal{Z}$ such that $(\mathbf{U}(0), \mathbf{z}(0)) = (\mathbf{U}_0, \mathbf{z}_0)$ and, for every $t \in [0, T]$,

$$\mathcal{W}(t, \mathbf{U}(t), \mathbf{z}(t)) \leq \mathcal{W}(t, \hat{\mathbf{U}}, \hat{\mathbf{z}}) + \mathcal{D}(\mathbf{z}(t), \hat{\mathbf{z}}) \quad \forall (\hat{\mathbf{U}}, \hat{\mathbf{z}}) \in \mathcal{U} \times \mathcal{Z} \quad (\text{S}')$$

$$\mathcal{W}(t, \mathbf{U}(t), \mathbf{z}(t)) + \text{Diss}_{\mathcal{D}}(\mathbf{z}, [0, t]) = \mathcal{W}(0, \mathbf{U}_0, \mathbf{z}_0)$$

$$- \int_0^t \left(\langle \dot{\ell}(s), \mathbf{U}(s) \rangle + \int_{\Omega} F'_{\text{magn}}(\mathbf{H} \cdot \mathcal{A}^* \mathbf{z}) \dot{\mathbf{H}}(s) \cdot \mathcal{A}^* \mathbf{z}(s) \, dx \right) ds \quad (\text{E}')$$

where $\text{Diss}_{\mathcal{D}}(\mathbf{z}, [0, t])$ is defined as Diss_D , now starting from the distance $\mathcal{D}(\mathbf{a}, \mathbf{b}) := \int_{\Omega} D(\mathbf{a} - \mathbf{b}) \, dx$.

Theorem 0.2 (Existence for the quasi-static evolution) *Let be given $\ell \in W^{1,1}(0, T; \mathcal{U}')$, $\mathbf{H} \in W^{1,1}(0, T; L^1(\Omega, \mathbb{R}^3))$, and a suitable initial datum $(\mathbf{U}_0, \mathbf{z}_0)$. Then, there exists an energetic solution for the quasi-static evolution problem.*

Theorems 0.1-0.2 are proved by means of the classical existence proof for rate-independent systems [6] via an implicit time discretization. Note however that the specific form of the magnetic part of the energy requires some slight modification of the usual argument [3].

The present model reduces to the referred original non-magnetic SMA model from [1, 2, 8] as $\mathbf{H} \equiv \mathbf{0}$. Moreover, by letting $\delta \rightarrow 0$, one can rigorously check this asymptotics by Γ -convergence. Note that $\delta = 0$ corresponds to assume infinite hardening on the magnetic domain proportion α . Let G_0 be defined by

$$G_0(\boldsymbol{\sigma}, \mathbf{H}, T, \mathbf{z}, \alpha) := \begin{cases} -\frac{1}{2} \boldsymbol{\sigma} : \mathbb{C}^{-1} : \boldsymbol{\sigma} - \boldsymbol{\sigma} : \mathbf{z} + F_{\text{mech}}(T^*, \mathbf{z}) & \text{if } \alpha = 0 \\ \infty & \text{else.} \end{cases}$$

Theorem 0.3 (Convergence as $\delta \rightarrow 0$ for the constitutive relation) *Assume to be given $\boldsymbol{\sigma} \in W^{1,1}(0, T; \mathbb{R}_{\text{sym}}^{3 \times 3})$, $\mathbf{H} \in W^{1,1}(0, T; \mathbb{R}^3)$, and a suitable initial condition \mathbf{z}_0 . For all $\delta > 0$, let $t \mapsto (\boldsymbol{\varepsilon}_{\delta}(t), \mathbf{z}_{\delta}(t), \alpha_{\delta}(t)) \in \mathbb{R}_{\text{sym}}^{3 \times 3} \times \mathbb{R}_{\text{dev}}^{3 \times 3} \times \mathbb{R}$ be an energetic solution associated with the constitutive relation problem corresponding to the pair (G_{δ}, D) . Then, up to a not relabeled subsequence, we have that $(\boldsymbol{\varepsilon}_{\delta}(t), \mathbf{z}_{\delta}(t), \alpha_{\delta}(t)) \rightarrow (\boldsymbol{\varepsilon}(t), \mathbf{z}(t), \alpha(t))$ for all $t \in [0, T]$, where $(\boldsymbol{\varepsilon}, \mathbf{z}, \alpha)$ is an energetic solution of the constitutive relation problem associated with (G_0, D) , i.e. the non-magnetic model.*

The latter convergence result is obtained within the general Γ -limiting scheme for rate-independent processes developed in [7] and can be obtained for quasi-static evolution problem as well.

Let us conclude this discussion by presenting the outcome of some numerical experiment on the MSMA model. To this aim, let us specify the material parameters of our model as $E = 800$ MPa (Young's modulus), $\nu = 0.3$ (Poisson's ratio), $\beta = 3$ MPa/K, $T_{\text{crit}} = 313$ K, $T^* = 315$ K, $h = 7.9$ MPa, $\varepsilon_L = 6.2$ %, $m_{\text{sat}} = 5.14 \cdot 10^4$ A/m, $1/\delta = 1$ MPa. A first experimental test case consists of applying a compressive stress in such a way to bias a certain structure (single variant state), and then to apply a competing variable magnetic field to induce the reorientation. Figure 1 below reports the predicted curves in 2D for two different and

fixed compressions along the $(1, 0, 0)$ -axis and a variable $(0, 1, 0)$ -directed magnetic field. A second classical experimental benchmark is to reproduce the so-called super-elastic stress-strain hysteretic behavior under different choices for the magnetic field, see Figure 2.

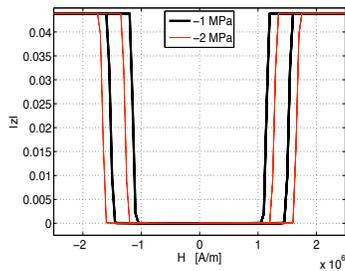


Fig. 1 (online colour at: wileyonlinelibrary.com) Magnetically-induced transformation strain under fixed compression: transformation strain vs. magnetic field

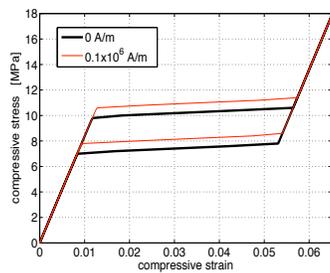


Fig. 2 (online colour at: wileyonlinelibrary.com) Stress-induced transformation strain under fixed magnetic field: compressive stress vs. compressive strain

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