A variational principle for numerical homogenization of periodic magnetoelastic composites

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Résumé :

Cette texte porte sur l'étude du comportement des élastomères renforcés avec des particules ferritiques sous chargements mécanique et magnétique et spécifiquement sur la proposition d'un principe variationnel augmenté pour traiter le problème d'homogénéisation périodique. Ces matériaux montre de couplage magnéto-mécanique et ils peuvent se déformer dans de grandes proportions grâce à la présence de la matrice polymérique.

Abstract :

In this study, we propose an augmented variational principle that is able to simulate the magnetoelastic response of magnetorheological elastomers (MREs). These materials are ferromagnetic particle impregnated rubbers whose mechanical properties are altered by the application of external magnetic fields. In addition, these composite materials can deform at very large strains due to the presence of the soft polymeric matrix.

Mots clefs : Mots clefs Magnetoelasticity, homogenization, finite strains

1 Magnetostatics

We consider a magnetoelastic deformable solid that occupies a region $\mathcal{V}_0$ in the reference configuration (and $\mathcal{V}$) with boundary $\partial\mathcal{V}_0$ (and $\partial\mathcal{V}$) of outward normal $\boldsymbol{\mathcal{N}}$ (and $\mathbf{n}$) in the undeformed stress-free (current) configuration. Material points in the solid are identified by their initial position vector $\mathbf{X}$ in the undeformed configuration $\mathcal{V}_0$, while the current position vector of the same point in the deformed configuration $\mathcal{V}$ is given by $\mathbf{x} = \boldsymbol{\chi}(\mathbf{x})$. Motivated by the usual physical arguments, the mapping $\boldsymbol{\chi}$ is required to be continuous and one-to-one on $\mathcal{V}_0$. In addition, we assume that $\boldsymbol{\chi}$ is twice continuously differentiable, except possibly on existing interfaces (e.g., due to the presence of different phases) inside the material. The deformation gradient $\mathbf{F}$ at $\mathbf{X}$ is defined then by

$$\mathbf{F} = \mathrm{Grad}\boldsymbol{\chi}, \quad J = \det\mathbf{F} > 0, \qquad \forall\,\mathbf{X} \in \mathcal{V}_0 \cup \partial\mathcal{V}_0, \tag{1}$$

where Grad denotes the gradient operator with respect to $\mathbf{X}$ in the reference configuration. In addition, the reference density of the solid ρ_0 is related to the current density ρ by $\rho_0 = \rho J$. Time dependence in not considered here. In a general setting, the deformation gradient $\mathbf{F}$ maybe discontinuous across material interfaces (e.g., between consecutive layers in a laminate composite) or boundaries and thus is required to satisfy the jump conditions $[\![\mathbf{F}]\!] = \boldsymbol{\mathcal{G}} \otimes \mathbf{N}$. The vector $\boldsymbol{\mathcal{G}}$ should be determined from the solution of the problem.

In pure magnetics and in the absence of deformation ($\mathbf{F} = \mathbf{I}$), the magnetic field $\mathbf{b}$, the $h-$field $\mathbf{h}$ and the magnetization per unit current volume are related via

$$\mathbf{b} = \mu_0(\mathbf{h} + \mathbf{m}) \qquad \text{in} \quad \mathcal{V}, \qquad \mathbf{b} = \mu_0 \mathbf{h} \qquad \text{in} \quad R^3 \setminus \mathcal{V}, \tag{2}$$

where $\mathcal{V}$ is the volume in the current configuration and $R^3 \setminus \mathcal{V}$ is used to define the region occupied by the air/aether. This equation is used to identify one out of the three vector fields when one vector field is used as an independent variable and the other one is given by a constitutive equations, e.g., $\mathbf{h} = f(\mathbf{b})$. In general, and in pure mathematical terms, one could choose any of the above as an independent variable. Note, however, that $\mathbf{b}$ and $\mathbf{h}$ are $a\ priori$ Eulerian quantities that need to satisfy differential constraints and boundary conditions, i.e., the Maxwell field equations (with no current density) and interface/boundary conditions

$$\begin{aligned} &\text{div}\mathbf{b} = 0 \qquad \text{and} \qquad \text{curl}\mathbf{h} = 0, \qquad \text{in} \quad \mathcal{V}, \\ &[\![\mathbf{b}]\!] \cdot \mathbf{n} = 0 \qquad \text{and} \qquad [\![\mathbf{h}]\!] \times \mathbf{n} = 0, \qquad \text{in} \quad \partial\mathcal{V}, \end{aligned} \tag{3}$$

where "div" and "curl" are operators with respect to $\mathbf{x}$ and $\mathbf{n}$ is the unit normal to $\partial\mathcal{V}$ in the current configuration. In turn, magnetization $\mathbf{m}$, which is also a Eulerian quantity by definition through equation (2), does not need to satisfy any differential constraints or interface conditions. Therefore, depending on the problem at hand, the choice of $\mathbf{m}$ as an independent variable could be advantageous, especially when discontinuous magnetization fields are present inside the material (e.g., in the resolution of magnetic domain walls or in analytical homogenization since this could allow for piecewise constant approximations of the fields [1]). On the other hand, in the present context of magnetoelasticity where large strains are of interest, $\mathbf{m}$ does not have a unique Lagrangian counterpart, contrary to $\mathbf{b}$ and $\mathbf{h}$ and thus is less convenient, albeit perfectly valid (see for instance the works by [2] and [3]).

In this regard, at large strains where $\mathbf{F}$ is finite, the fields $\mathbf{b}$ and $\mathbf{h}$ can be pulled back from $\mathcal{V}$ to $\mathcal{V}_0$ to their Lagrangian forms, denoted by $\mathbf{B}$ and $\mathbf{H}$, respectively, such that

$$\mathbf{B} = J\mathbf{F}^{-1}\mathbf{b}, \qquad \text{and} \qquad \mathbf{H} = \mathbf{F}^T\mathbf{h}. \tag{4}$$

2 Local Constitutive behavior

In this section, we define constitutive laws for the coupled magnetomechanical response of the materials under study. The interest in this study is the modeling of composite materials which can be either magnetoelastic or purely elastic. In this regard, it is convenient to characterize their constitutive behaviors in a Lagrangian formulation by free energies $W(\mathbf{X}, \mathbf{F}, \mathbf{B})$. These functions are suitably amended in order to include the contribution of the Maxwell stress and read [4]

$$W(\mathbf{X}, \mathbf{F}, \mathbf{B}) = \rho_0 \Phi(\mathbf{X}, \mathbf{F}, \mathbf{B}) + \frac{1}{2\mu_0 J}\mathbf{F}\,\mathbf{B} \cdot \mathbf{F}\,\mathbf{B}, \tag{5}$$

where $\Phi(\mathbf{X}, \mathbf{F}, \mathbf{B})$ is a specific free-energy density to be defined below, while the second term in the above equation is considered so that the total first Piola-Kirchhoff stress $\mathbf{S}$ and the Lagrangian h-field $\mathbf{H}$ are simply given by

$$\mathbf{S} = \frac{\partial W}{\partial \mathbf{F}}(\mathbf{X}, \mathbf{F}, \mathbf{B}), \qquad \mathbf{H} = \frac{\partial W}{\partial \mathbf{B}}(\mathbf{X}, \mathbf{F}, \mathbf{B}). \tag{6}$$

Next, we consider that the composite material comprises $r = 1, ..., N$ (magneto)elastic phases occupying a subdomain $\mathcal{V}_0^{(r)}$ in the reference configuration so that the local potential W is re-written simply as

$$W(\mathbf{X}, \mathbf{F}, \mathbf{B}) = \sum_{r=1}^{N} \theta_0^{(r)}(\mathbf{X}) W^{(r)}(\mathbf{F}, \mathbf{B}). \tag{7}$$

In this expression, $\theta_0^{(r)}(\mathbf{X})$ denote characteristic functions occupied by phase r and take values $\theta_0^{(r)}(\mathbf{X}) = 1$ if $\mathbf{X} \in \mathcal{V}_0^{(r)}$ and zero otherwise.

In the case of periodic composites these functions are periodic and are fully determined by the unit cell occupying a domain $\mathcal{V}_0^{\#}$ by [5]

$$\theta_0^{(r)}(\mathbf{X}) = \sum_{q_1, q_2, q_3 \in \mathbb{Z}} \theta_0^{(r)}(\mathbf{X} + q_1 \mathbf{L}^1 + q_2 \mathbf{L}^2 + q_3 \mathbf{L}^3), \qquad \mathbf{X} \in \mathcal{V}_0^{\#}. \tag{8}$$

Here, the unit cell is assumed to be a parallelepiped defined via the lattice vectors $\mathbf{L}^i$ $(i = 1, 2, 3)$ in the reference configuration. Even though the scope of the present study does not involve the study of instabilities, it is relevant to mention that the solution of the problem could be periodic on a larger unit cell $\mathbf{q}\mathcal{V}_0^{\#}$ (with $\mathbf{q} = (q_1, q_2, q_3)$), especially if bifurcated solutions are present but such work is left for a future study. Nonetheless, in the present study, we focus on the evaluation of the effective response of magnetoelastic composites before bifurcation and thus the smallest unit cell $\mathcal{V}_0^{\#}$ suffices.

3 Local Constitutive behavior

In this section, we define the homogenization problem insisting on the following important points. In order to be able to understand the underlying micro-mechanisms leading to the deformation of a composite material lying inside a uniform magnetic field and of course neglecting any boundary layer/corner effects present in a standard BVP, one needs to consider the following steps in the context of periodic homogenization:

- First, we need to write down the Lagrangian magnetic field $\mathbf{B}$ as

$$\mathbf{B} = \overline{\mathbf{B}} + \widetilde{\mathbf{B}} \tag{9}$$

  Here, $\overline{\mathbf{B}}$ denotes the average magnetic field and $\widetilde{\mathbf{B}}$ a perturbation field due to the presence of a magnetizable body.

- Next, we subtract from the total energy the effective energy term:

$$\overline{W}_{maxw} = \frac{\overline{\mathbf{F}}\,\overline{\mathbf{B}} \cdot \overline{\mathbf{F}}\,\overline{\mathbf{B}}}{2\mu_0 \overline{J}}. \tag{10}$$

  where $\overline{\mathbf{F}}$ corresponds to the average deformation gradient and and $\overline{J} = \det \overline{\mathbf{F}}$. The last equation corresponds to the effective magnetic energy in the air (ether medium). This energy results in a Maxwell stress term which serves to model the attraction forces between the two magnetic poles. Since in a realistic situation the two magnetic poles are unmovable and fixed while at the same time are not in contact with the boundary of the solid, the corresponding traction does not contribute to the deformation of the magnetizable body lying between the magnets. While in a standard BVP such geometric configuration is readily taken into account by standard boundary conditions and by the presence of the air between the magnets and the body, in the present case of periodic homogenization we have to take this term out beforehand. In any other case, this would lead to a fictitious stressing of the magnetizable (or any non-magnetizable) body as if the magnets were attached on the boundary of the solid exerting an additional stressing to the body due to their mutual attraction[1]. While the homogenization problem itself is well-posed and one could homogenize and subtract this energy afterwards, this would not allow for a correct interpretation of the micro-deformation mechanisms observed during the numerical simulation.

- Finally, considering again a realistic experimental configuration, one has to apply the Eulerian part of the magnetic field $\overline{\mathbf{b}}$ instead of the Lagrangian one, $\overline{\mathbf{B}}$. The reason is well explained by Brown and Eriksen in the sense that the macroscopic average magnetic field $\overline{\mathbf{b}}$ is the one created by the magnets and is present ab initio without the presence of the magnetizable body. Then, the periodic magnetizable body will induce a perturbation field $\widetilde{\mathbf{B}}$ which will be periodic with zero average. In other words, if one is sitting in a given point the average (background) field does not change with the deformation of the magnetizable body and thus constitutes (by nature) a Eulerian measure. This has significant implications in the resulting deformation of the periodic medium as well as the relevant periodic boundary conditions since one has to apply

$$\overline{\mathbf{b}} = \frac{1}{\overline{J}} \overline{\mathbf{F}}\,\overline{\mathbf{B}} = const \tag{11}$$

  and not $\overline{\mathbf{B}} \neq const$. This last expression constitutes a nonlinear constraint on the average variables $\overline{\mathbf{F}}$ and $\overline{\mathbf{B}}$. Of course this last constraint is convenient to be applied during the homogenization process since it leads to a non-proportional loading in the $\overline{\mathbf{F}}$-$\overline{\mathbf{B}}$ space. Again, if this is not done during the numerical simulation, one could scan the entire $\overline{\mathbf{F}}$-$\overline{\mathbf{B}}$ space and then pick only the points that satisfy equation (11). Nonetheless, in this case, one will not be able to directly observe the underlying micro-deformation mechanisms that lead to the overall magnetostriction of the composite.

[1] It is interesting to note in this case, that in the context of electro-active polymers, this term needs not be taken out of the energy if the deformation results due to electrodes attached on the body since they deform with its boundary while the attractive forces between the electrodes contribute to the deformation of the body itself.

Considering the above three conditions, one could write the the variational formulation (neglecting the body forces)

$$\widetilde{W}(\overline{\mathbf{F}},\overline{\mathbf{B}}) = \min_{\widetilde{\mathbf{u}},\widetilde{\mathbf{A}}} \frac{1}{|\mathbf{q}\mathcal{V}_0^{\#}|}\int_{\mathbf{q}\mathcal{V}_0^{\#}} W\left(\overline{\mathbf{F}}+\mathrm{Grad}\widetilde{\mathbf{u}},\overline{\mathbf{B}}+\mathrm{Curl}\widetilde{\mathbf{A}}\right)\mathrm{d}V - \frac{1}{2\mu_0\overline{J}}\overline{\mathbf{F}}\,\overline{\mathbf{B}}\cdot\overline{\mathbf{F}}\,\overline{\mathbf{B}} + \frac{1}{2\mu_0\xi}\left|\overline{\mathbf{F}}\,\overline{\mathbf{B}}-\overline{J}\,\overline{\mathbf{b}}\right|^2, \tag{12}$$

where $\widetilde{\mathbf{u}}$ and $\widetilde{\mathbf{B}} = \mathrm{Curl}\widetilde{\mathbf{A}}$ are $\mathbf{q}\mathcal{V}_0^{\#}$-periodic fields such that the deformation gradient and magnetic fields are given by $\mathbf{F} = \overline{\mathbf{F}} + \mathrm{Grad}\widetilde{\mathbf{u}}$ and $\mathbf{B} = \overline{\mathbf{B}} + \mathrm{Curl}\widetilde{\mathbf{A}}$. In addition, $\xi \to 0$ is simply penalizing the constraint (11). The addition of μ_0 in the last term is done in order for this term to be in the same order of magnitude as the other terms in the variational principle.

4 Results

Figure 1 shows representative results for the average response of a rectangular periodic unit-cell with external aspect ratio $w_d = L_2/L_1 = 0.5$ comprising circular rigid magnetizable inclusions forming chains along the x_2 direction (see inset in the same figure). The composite is subjected to a magnetic field in the x_2 direction together with $\overline{F}_{12} = \overline{F}_{21}$ and $\overline{\sigma}_{11}^{mech} = \overline{\sigma}_{22}^{mech} = 0$ (where the superscript $mech$ serves to denote the purely mechanical part). In the context of Figure 1a, we observe a monotonic increase of the average magnetization $\overline{m}_2/m_s$ with increase of the volume fraction c. On the other hand,

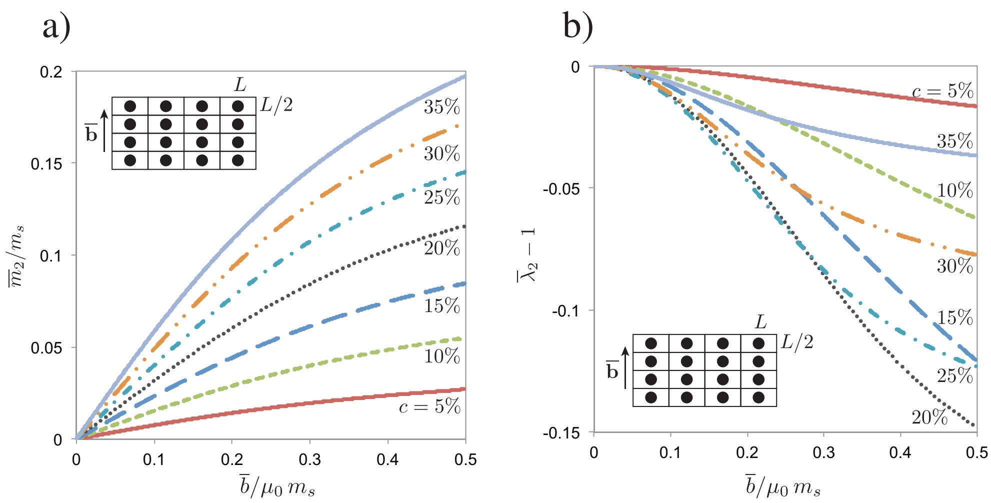

Figure 1: Macroscopic response of a rectangular periodic unit-cell with external aspect ratio $w_d = 0.5$ comprising circular rigid magnetizable inclusions forming chains along the x_2 direction. The composite is subjected to a magnetic field in the x_2 direction, zero overall mechanical traction. (a) Average magnetization and (b) average magnetostriction as a function of the normalized average Eulerian magnetic field $\overline{b}/\mu_0 m_s$ for various particle volume fractions $c = 5, 10, 15, 20, 25, 30, 35\text{vol}\%$.

in Fig. 1b, the corresponding average magnetostriction exhibits a markedly non-monotonic response with increase of the volume fraction c. For instance, we observe that $c = 25\%$ leads to a maximum attained straining at $\overline{b}/\rho_0 m_s = 0.5$. In contrast, as we increase further the volume fraction to $c = 35\%$ the overall magnetostriction reduces dramatically lying between the curves for $c = 5\%$ and $c = 10\%$. This can be explained by the fact that increase of c leads to a substantially stiffer mechanical response of the composite which dominates over the stronger magnetic interaction of the particles in that case. It should be noted that if the additional terms were not considered in the above described variational principle, the resulting magnetostriction would be monotonic with respect to the volume fraction c (which is consistent with an experiment of a dielectric elastomeric composite covered with electrodes at the top and bottom surface).

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