Second Order Moments in Linear Smart Material Composites

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Homogenization is a mean field approach for the determination of the effective properties of heterogeneous materials. It can provide the average fields per phase but also some information about the field distribution such as second order moments. The use of second order moments of fields can notably improve the estimates of the macroscopic behavior in the nonlinear case. This has been studied mainly in the case of uncoupled behavior. We propose to define second order moments in the case of coupled elasto-magneto-electric behavior using homogenization tools. The results are compared to the field fluctuations obtained from a finite element model.

***Index Terms*—Field fluctuations, heterogeneous materials, homogenization, multiphysics.**

I. INTRODUCTION

HOMOGENIZATION is a modeling approach that enables to determine the effective behavior of heterogeneous materials [1]. It makes use of the properties of the material constituents and of a limited statistical description of its microstructure. In most cases, and particularly for linear behavior, the determination of mean fields per phase is sufficient to perform the homogenization process. Nevertheless, further information about the field distribution may be necessary in some cases, particularly when dealing with nonlinear constitutive laws.

Information on field fluctuations can be obtained by determining second order moments. They can be estimated with homogenization tools. This point has been deeply investigated in the case of uncoupled (mechanical, electric, magnetic) behavior (see for instance [2]–[5]). We propose to define second order moments in the case of coupled behavior. Elasto-magneto-electric couplings are considered. The model relies on a previous homogenization model based on a field decomposition into several contributions depending on their physical origin [6].

In the first part, elasto-magneto-electric constitutive laws are briefly presented. In the second part, the determination of second order moments of the elasto-magneto-electric fields is derived in the case of coupled behavior. In the last part, this homogenization approach is applied to a piezoelectric composite. The results for second order moments are compared to finite element (FE) simulations.

II. CONSTITUTIVE LAWS—HOMOGENIZATION

A. Elasto-Magneto-Electric Materials

The constitutive law of elasto-magneto-electric materials can be written in different ways, depending on the choice of the independent variables between $\mathbf{T}$ the stress tensor and $\mathbf{S}$ the strain tensor, between $\mathbf{B}$ the magnetic induction and $\mathbf{H}$ the magnetic field, and between $\mathbf{D}$ the electric induction and $\mathbf{E}$ the electric field. One possible choice is to regroup $\mathbf{T}$, $\mathbf{H}$, and $\mathbf{E}$ on one side (later referred to as $\mathbf{Y}$), and to regroup $\mathbf{S}$, $\mathbf{B}$, and $\mathbf{D}$ on the other side (later referred to as $\mathbf{X}$). The linear constitutive law reads:

$$\begin{pmatrix} \mathbf{T} \\ \mathbf{H} \\ \mathbf{E} \end{pmatrix} = \begin{pmatrix} \mathbb{C} & {}^t\mathbb{g} & {}^t\mathbb{h} \\ \mathbb{g} & \mathbb{v} & {}^t\mathbb{\lambda} \\ \mathbb{h} & \mathbb{\lambda} & \mathbb{k} \end{pmatrix} \cdot \begin{pmatrix} \mathbf{S} \\ \mathbf{B} \\ \mathbf{D} \end{pmatrix} \tag{1}$$

where $\mathbb{C}$ is the elastic stiffness tensor, $\mathbb{v}$ the magnetic reluctivity tensor, $\mathbb{k}$ the inverse permittivity tensor, $\mathbb{g}$ the piezomagnetic tensor, $\mathbb{h}$ the piezoelectric tensor and $\mathbb{\lambda}$ the magnetoelectric tensor. The constitutive law can be condensed into:

$$\mathbf{Y} = \mathbb{L} \cdot \mathbf{X} \tag{2}$$

It can be noticed that this choice of state variables leads to a symmetric positive-definite tensor $\mathbb{L}$.

B. Homogenization Model

Homogenization models have been mainly developed in the framework of uncoupled behavior (see for instance [7], [8], [9]). Some models rely on a mean field approach and are built from limited statistical information about the microstructure. This approach enables the analytical determination of the effective property tensor (for example the effective permeability tensor $\widetilde{\mathbb{\mu}}$ in magnetics) from the localization tensors $\mathbb{A}_i^{\mu}$ (or the concentration tensors $\mathbb{B}_i^{\mu}$). The localization tensors link the mean fields per phase to the macroscopic fields. Keeping the example of magnetics, the homogenization equations for a composite material made of n phases are:

$$\overline{\mathbf{B}} = \langle \mathbf{B} \rangle = \langle \mathbb{\mu} \cdot \mathbf{H} \rangle = \widetilde{\mathbb{\mu}} \cdot \langle \mathbf{H} \rangle = \widetilde{\mathbb{\mu}} \cdot \overline{\mathbf{H}} \tag{3}$$

$$\begin{aligned} \langle \mathbf{H} \rangle_i &= \mathbb{A}_i^{\mu} \cdot \overline{\mathbf{H}} \\ \langle \mathbf{B} \rangle_i &= \mathbb{B}_i^{\mu} \cdot \overline{\mathbf{B}} \end{aligned} \tag{4}$$

$$\widetilde{\mathbb{\mu}} = \sum_{i=1}^{n} f_i \mathbb{\mu}_i \cdot \mathbb{A}_i^{\mu} = \sum_{i=1}^{n} f_i \mathbb{\mu}_i^{-1} \cdot \mathbb{B}_i^{\mu} \tag{5}$$

where f_i is the volume fraction of phase i, $\mathbb{\mu}_i$ is the permeability tensor of phase i, $\overline{\mathbf{B}}$ the macroscopic magnetic induction and $\overline{\mathbf{H}}$ the macroscopic magnetic field. The operator $\langle . \rangle$ denotes an averaging operation over the whole volume of the material and the operator $\langle . \rangle_i$ denotes an averaging operation over the sole phase i. A possible homogenization scheme based on inclusion problems is to define the problem as n decorrelated problems [10]. The principle of this model is shown in Fig. 1. Each phase is assumed to behave "on average" as an inclusion embedded in an infinite medium. The choice of the infinite medium properties in the inclusion problems is a degree of freedom to describe particle interactions. It enables to determine several estimates (or bounds).

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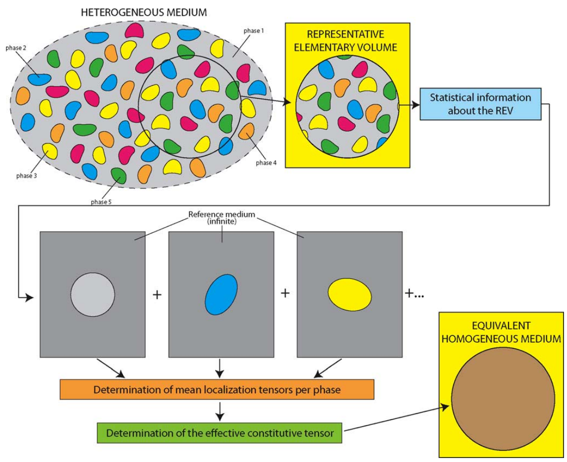

Fig. 1. Principle of the homogenization model based on inclusion problems.

A framework for the homogenization of coupled behavior has been recently proposed [6]. The coupled behavior is accounted for through an appropriate decomposition of the fields (6) coming from a similar method with viscoplatic materials [11]. The principle is to decompose the fields deriving from a potential ($\mathbf{S}$, $\mathbf{H}$ and $\mathbf{E}$) into several contributions, related to the physical origin of the field (see Fig. 2):

$$\left\{\begin{array}{l}\mathbf{S}=\mathbf{S}^{\mathcal{C}}+\mathbf{S}^{\mu}+\mathbf{S}^{\epsilon}\\ \mathbf{H}=\mathbf{H}^{\mathcal{C}}+\mathbf{H}^{\mu}+\mathbf{H}^{\epsilon}\\ \mathbf{E}=\mathbf{E}^{\mathcal{C}}+\mathbf{E}^{\mu}+\mathbf{E}^{\epsilon}\end{array}\right. \tag{6}$$

For example, the total strain tensor $\mathbf{S}$ can be decomposed into an elastic strain $\mathbf{S}^{\mathcal{C}}$ caused by the stress $\mathbf{T}$, superimposed to a magnetic field induced strain $\mathbf{S}^{\mu}$ (also called magnetostriction strain), and to an electric field induced strain $\mathbf{S}^{\epsilon}$ (also called electrostriction strain). It has been shown that the use of this decomposition allows the use of the uncoupled homogenization tools ($\mathbb{A}_i^{\mathcal{C}}$ and $\mathbb{B}_i^{\mathcal{C}}$ for mechanics, $\mathbb{A}_i^{\mu}$ and $\mathbb{B}_i^{\mu}$ for magnetics, $\mathbb{A}_i^{\epsilon}$ and $\mathbb{B}_i^{\epsilon}$ for electricity) [6]. This scheme enables to define the effective property tensor $\widetilde{\mathbb{L}}$:

$$\overline{\mathbf{Y}}=\langle\mathbf{Y}\rangle=\langle\mathbb{L}\cdot\mathbf{X}\rangle=\widetilde{\mathbb{L}}\cdot\langle\mathbf{X}\rangle=\widetilde{\mathbb{L}}\cdot\overline{\mathbf{X}} \tag{7}$$

III. Second Order Moments

The effective property tensor $\widetilde{\mathbb{L}}$ of a composite material is usually defined as the link between the macroscopic fields $\overline{\mathbf{Y}}$ and $\overline{\mathbf{X}}$ ((7)). But an energetic definition of $\widetilde{\mathbb{L}}$ can also be given, noting that, thanks to the proposed choice of independent variables, the quantity $\mathbf{Y}\cdot\delta\mathbf{X}$ represents the energy variation. Equation (8) expresses the macroscopic energy in the composite as the average of the local energy over the volume.

$$\langle\mathbf{X}\cdot\mathbb{L}\cdot\mathbf{X}\rangle=\overline{\mathbf{X}}\cdot\widetilde{\mathbb{L}}\cdot\overline{\mathbf{X}} \tag{8}$$

Let now consider a small variation of the properties of the constituents, while maintaining constant the macroscopic field $\overline{\mathbf{X}}$. (8) becomes:

$$\langle(\mathbf{X}+\delta\mathbf{X})\cdot(\mathbb{L}+\delta\mathbb{L})\cdot(\mathbf{X}+\delta\mathbf{X})\rangle=\overline{\mathbf{X}}\cdot\left(\widetilde{\mathbb{L}}+\delta\widetilde{\mathbb{L}}\right)\cdot\overline{\mathbf{X}} \tag{9}$$

Restraining (9) to first order terms leads to:

$$\langle\mathbf{X}\cdot\mathbb{L}\cdot\delta\mathbf{X}\rangle+\langle\delta\mathbf{X}\cdot\mathbb{L}\cdot\mathbf{X}\rangle+\langle\mathbf{X}\cdot\delta\mathbb{L}\cdot\mathbf{X}\rangle=\overline{\mathbf{X}}\cdot\delta\widetilde{\mathbb{L}}\cdot\overline{\mathbf{X}} \tag{10}$$

By noticing that the property tensor $\mathbb{L}$ is symmetric, the two first terms in the left-hand side member can be regrouped:

$$2\langle\mathbf{X}\cdot\mathbb{L}\cdot\delta\mathbf{X}\rangle+\langle\mathbf{X}\cdot\delta\mathbb{L}\cdot\mathbf{X}\rangle=\overline{\mathbf{X}}\cdot\delta\widetilde{\mathbb{L}}\cdot\overline{\mathbf{X}} \tag{11}$$

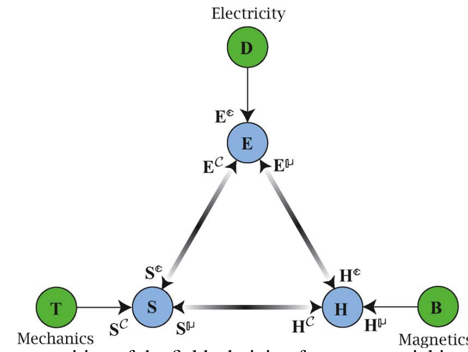

Fig. 2. Decomposition of the fields deriving from a potential into several contributions, related to their physical origin.

The first term in the left-hand side member is equal to zero. Indeed $\mathbf{X}\cdot\mathbb{L}\cdot\delta\mathbf{X}$ is equal to $\mathbf{Y}\cdot\delta\mathbf{X}$ that is the local variation of energy. The field distribution verifies the minimum energy principle, so that the corresponding macroscopic variation of energy is equal to zero. Finally (11) becomes:

$$\langle\mathbf{X}\cdot\delta\mathbb{L}\cdot\mathbf{X}\rangle=\overline{\mathbf{X}}\cdot\delta\widetilde{\mathbb{L}}\cdot\overline{\mathbf{X}} \tag{12}$$

The properties being uniform per phase, the averaging operation can be decomposed as follows:

$$\sum_{i=1}^{n} f_i\,\langle\mathbf{X}\cdot\delta\mathbb{L}_i\cdot\mathbf{X}\rangle_i=\overline{\mathbf{X}}\cdot\delta\widetilde{\mathbb{L}}\cdot\overline{\mathbf{X}} \tag{13}$$

Thus, the second order moments per phase $\langle\mathbf{X}\otimes\mathbf{X}\rangle_i$ (second order tensor) are obtained by derivation of the effective property tensor $\widetilde{\mathbb{L}}$ with respect to the phase properties.

$$\langle\mathbf{X}\otimes\mathbf{X}\rangle_i=\frac{1}{f_i}\overline{\mathbf{X}}\cdot\frac{\partial\widetilde{\mathbb{L}}}{\partial\mathbb{L}_i}\cdot\overline{\mathbf{X}} \tag{14}$$

Second order moments of $\mathbf{Y}$ can be obtained in a similar way:

$$\langle\mathbf{Y}\otimes\mathbf{Y}\rangle_i=\frac{1}{f_i}\overline{\mathbf{Y}}\cdot\frac{\partial\widetilde{\mathbb{L}}^{-1}}{\partial\mathbb{L}_i^{-1}}\cdot\overline{\mathbf{Y}} \tag{15}$$

IV. Application to Piezoelectric Composites

In order to validate the proposed approach, the homogenization results are compared to the second order moments extracted from a FE model. The derivatives of the effective tensor in (14) have been processed numerically in the model. The composite structure studied in the FE model is a periodic cell of randomly distributed fibers aligned along the z-axis and embedded in a matrix (see Fig. 3). Fibers can neither overlap nor touch each other. Several realizations of the microstructure (random position of the fibers) have been simulated and the results have been averaged, the variation in the results between the different realizations are so small that it is not reported in the result figures. The matrix material (phase 1) is PZT-2 and the fibers (phase 2) are made of Baryum Titanate. Both phases are polarized along the z-axis (see Table I).

This composite is submitted to a null macroscopic electric field $\overline{\mathbf{E}}$ and the macroscopic strain $\overline{\mathbf{S}}$ is also imposed to zero except the $\overline{S_{xx}}$ strain. This loading leads to a macroscopic stress $\overline{\mathbf{T}}$ and a macroscopic electric induction $\overline{\mathbf{D}}$. Several volume fractions of the fibers are studied. The homogenization model is performed using the piezoelectric material 1 as reference medium in the elementary inclusion problems (Mori-Tanaka estimate).

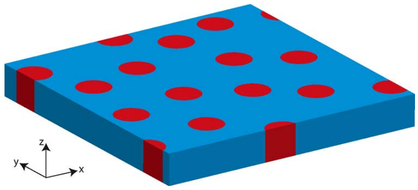

Fig. 3. Studied composite microstructure, fibers (phase 2: Baryum Titanate) randomly distributed in a matrix (phase 1: PZT-2).

TABLE I
MATERIAL PROPERTIES[1]

		PZT-2	Baryum Titanate
$C^{\mathbf{E}}_{11} = C^{\mathbf{E}}_{22}$	(GPa)	134.868	275.121
$C^{\mathbf{E}}_{33}$		113.297	164.860
$C^{\mathbf{E}}_{12}$		67.8883	178.967
$C^{\mathbf{E}}_{13} = C^{\mathbf{E}}_{23}$		68.0876	151.555
$C^{\mathbf{E}}_{44} = C^{\mathbf{E}}_{55}$		22.2222	54.3478
$C^{\mathbf{E}}_{66}$		33.4448	113.122
$\epsilon^{\mathbf{S}}_{11} = \epsilon^{\mathbf{S}}_{22}$	(no unit)[2]	504.1	1976.8
$\epsilon^{\mathbf{S}}_{33}$		270	111.7
$e_{31} = e_{32}$	(C/m^2)	-1.81603	-2.69289
e_{33}		9.05058	3.65468
$e_{15} = e_{24}$		9.77778	21.3043

[1] The material properties are given in a different formulation than the one presented in (1), see [12] for the different formulations.
These material parameters correspond to the following formulation for piezoelectric behavior:
$$\begin{pmatrix} \mathbf{T} \\ \mathbf{D} \end{pmatrix} = \begin{pmatrix} \mathbb{C}^{\mathbf{E}} & -{}^t\mathbb{e} \\ \mathbb{e} & \epsilon^{\mathbf{S}} \end{pmatrix} \cdot \begin{pmatrix} \mathbf{S} \\ \mathbf{E} \end{pmatrix}.$$
[2] Permittivity coefficients are relative ones.

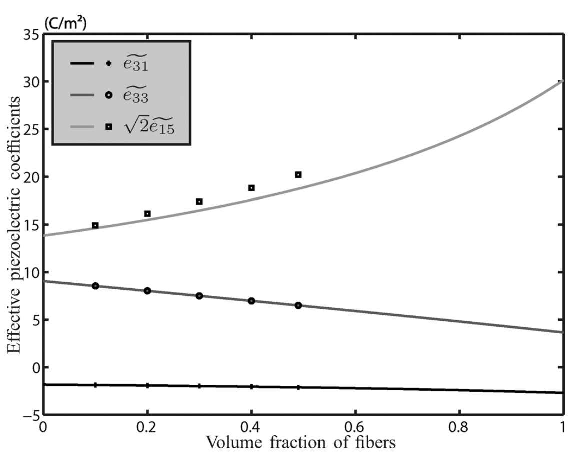

Fig. 4. Effective piezoelectric coefficients as a function of volume fraction of fibers. Different macroscopic loadings have been applied to the composite in order to identify the coefficients. Lines: homogenization, Symbols: FE.

Macroscopic piezoelectric coefficients (Fig. 4) are correctly predicted by the model. The error on the $\widetilde{e_{15}}$ coefficient grows with the volume fraction of fibers. This may be due to the choice of the matrix properties for the infinite medium in the inclusion problems. This choice neglects the interactions between fibers, these interactions grow with the volume fraction.

The mean fields per phase (strain (Fig. 5) and electric induction (Fig. 6)) are very accurately predicted.

Second order moments (Figs. 7, 8 and 9) are also accurately predicted.

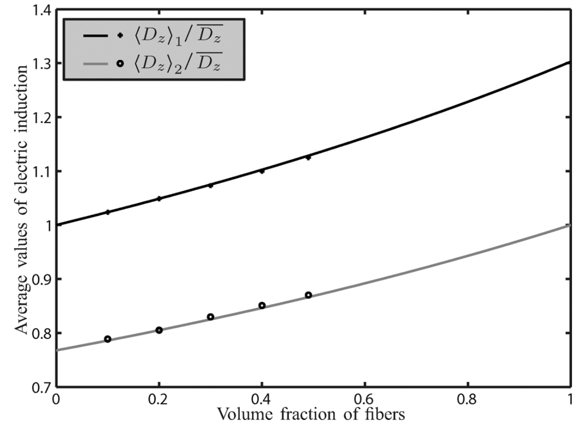

Fig. 5. Normalized mean induction field along z-axis in matrix and fibers as a function of volume fraction of fibers when the composite is subjected to the following macroscopic loading: null electric field and null strain except $\overline{S_{xx}}$ component. Lines: homogenization, Symbols: FE.

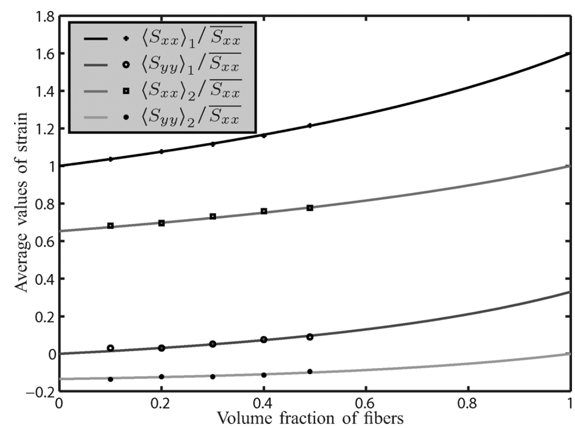

Fig. 6. Normalized average strain in matrix and fibers as a function of volume fraction of fibers when the composite is subjected to the same macroscopic loading. Lines: homogenization, Symbols: FE.

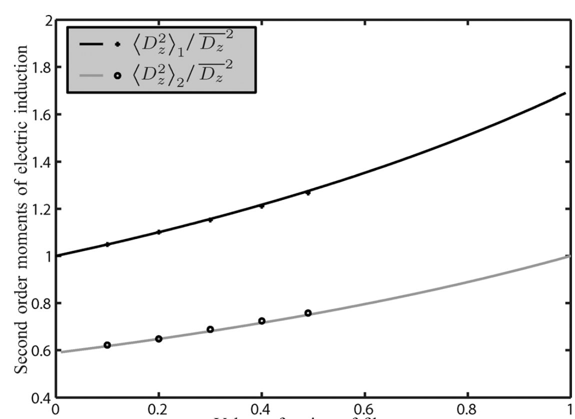

Fig. 7. Normalized second order moments of electric induction in matrix and fibers as a function of volume fraction of fibers when the composite is subjected to the same macroscopic loading. Lines: homogenization, Symbols: FE.

Another parameter to highlight the field fluctuations is the variance per phase $\mathbb{V}_i$:

$$\mathbb{V}_i = \langle \mathbf{X} \otimes \mathbf{X} \rangle_i - \langle \mathbf{X} \rangle_i \otimes \langle \mathbf{X} \rangle_i \qquad (16)$$

Fig. 10 plots the variance of the product between strain and induction field. Homogenization and FE results are very close. The homogenization model predicts a null variance in phase 2 (fibers). This is due to the choice of Mori-Tanaka estimate

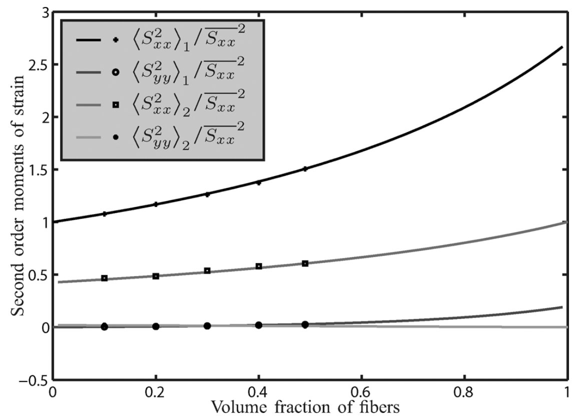

Fig. 8. Normalized second order moments of strain in matrix and fibers as a function of volume fraction of fibers when the composite is subjected to the same macroscopic loading. Lines: homogenization, Symbols: FE.

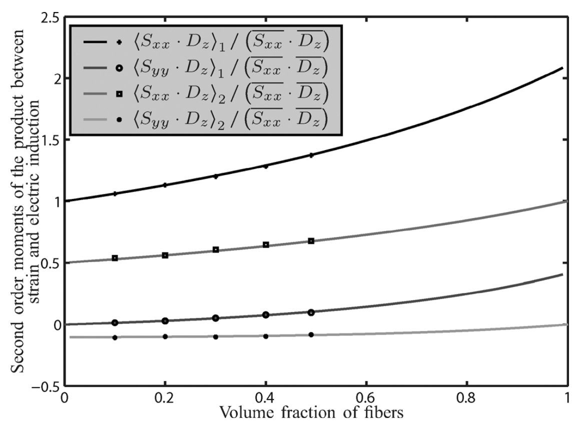

Fig. 9. Normalized second order moments of the product between strain and electric induction in matrix and fibers as a function of volume fraction of fibers when the composite is subjected to the same macroscopic loading. Lines: homogenization, Symbols: FE.

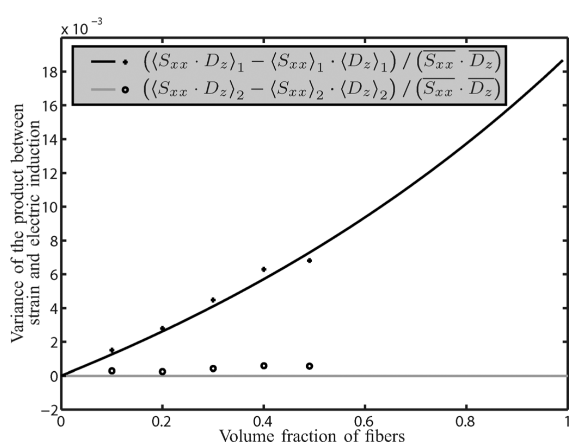

Fig. 10. Normalized variance of the product between strain and electric induction in matrix and fibers as a function of volume fraction of fibers when the composite is subjected to the same macroscopic loading. Lines: homogenization, Symbols: FE.

that neglects interactions between fibers. It then leads to uniform fields in the fibers. Other choices of the infinite reference medium (such as self-constitent estimate) would lead to field fluctuations in the fibers.

The larger discrepancies in this figure is connected to the order of magnitude of the variance (10^{-3}) compared with the order of magnitude of the second order moments (10^0) plotted in Fig. 9. This result is then more sensitive to numerical noise.

V. Conclusion

Homogenization tools have been used to determine second order moments in linear smart material composites. The main advantage of such an approach is its computational time compared to full field models such as FE methods (ratio: 10^3). The comparison to a finite element model for a piezoelectric composite with matrix/inclusion microstructure shows a satisfying agreement. The model can also deal with piezomagnetic materials and is able to catch the extrinsic magnetoelectric effect exhibited in piezoelectric/piezomagnetic composites [6].

The main purpose of the determination of second order moments with this approach is dedicated to the homogenization of composites when dealing with nonlinear behavior. It has been shown in mechanics that nonlinear homogenization, where linearization schemes are used, give better results using the second order moments of fields instead of mean fields. It is the case for the so-called "modified secant" nonlinear homogenization model [13]. The use of this model in a nonlinear homogenization model is currently a work in progress.

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