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On the meaning of the chosen set-averaging method within Eshelby-Kröner self-consistent scale transition model: the geometric mean versus the classical arithmetic average.

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Abstract

Scale-transition models, such as Eshelby-Kröner self-consistent framework, which are often used for predicting the effective behavior of heterogeneous materials or estimating the distribution of local states from the knowledge of the corresponding macroscopic quantities, require the extensive use of set averages. In the present work, the fundamental formalism historically introduced by Kröner is, for the first time, considered from the point of view of both the geometric and the arithmetic set averages methods. It is demonstrated in this paper, that the polarization tensors describing the relations existing between the local and the macroscopic mechanical states do have a strong physical meaning when expressed using the geometric average, instead of the classical arithmetic mean.

1. Introduction

Scale transition models have a long history and rich literature. Among their applications to the field of mechanical engineering, their ability to predict the effective behavior and mechanical states of macroscopically homogeneous but microscopically heterogeneous materials is often valued. Numerous, still recent, papers have actually dealt with the question of estimating the effective stiffness of single-phase (Kocks et al., 1998) and two-phases (Fréour et al., 2003a) metallic bulk polycrystals, thin solid films (Welzel and Fréour, 2007), or even metal / organic matrix composites (Fréour et al., 2006a), for instance. Scale transition models are also often used for calculating the (XEC) X-Ray Elasticity Constants (Hauk, 1997; Koch et al., 2004), required for achieving internal stress determination from X-Ray Diffracting peak-shifting measurements, since XEC are otherwise rather uneasy to deduce from experiments, even if some valuable experimental investigations have already been published (Singh et al., 1998). The connected question of predicting the macroscopic Coefficients of Thermal Expansion or the Coefficients of Moisture Expansion of such heterogeneous materials has also (in most previously cited cases) been addressed. The interested reader can refer, as an example, to (Fréour et al., 2004; Jacquemin et al., 2005) for recent advances in the field of micro-mechanical modeling about this topic.
Another interesting aspect of scale transition models is their ability to provide links between local fields (such as the mechanical states, either strains or stresses, as an example), and their macroscopic counterparts. This feature is strongly exploited in order to manage to investigate, as an example, the micro-mechanical elastic-plastic behavior of materials (Masson and Zaoui,

1999), their time-dependent creep and relaxation (Weng, 1993) or even their durability through damage modeling (Chaboche et al., 2001).

The third driving force behind the extensive use of scale-transition models is for solving materials properties identification problems. The precise knowledge of the local properties of each constituent of a heterogeneous material is required in order to achieve the prediction of its effective behavior (and especially its mechanical states) through scale transition models. Actually, in the case that strongly heterogeneous industrial materials, often presenting various constituents and complex microstructures, are considered, it often happens that both the average (pseudo-macroscopic) elastic stiffness and coefficients of expansion of their constituents and the corresponding single-crystal (mesoscopic) quantities (if relevant) do remain unknown. As an example, the practical determination of the hygro-thermo-mechanical properties of fiber-reinforced organic matrix composite materials are, most of the time, achieved on unidirectionally reinforced composites, on the one hand, and on unreinforced resins, on the other hand (Bowles et al., 1981; Dyer et al., 1992; Ferreira et al., 2006a; Ferreira et al., 2006b; Herakovich, 1998; Sims et al., 1977). In spite of the existence of several papers dedicated to the experimental characterization of the properties of the isolated reinforcements (DiCarlo, 1986, Tsai and Chiang, 2000, Tsai and Daniel, 1994), the practical achieving of this task remains particularly difficult to handle. Thus, the available published data for typical reinforcements employed in composite design are still scarce. As a consequence, the properties of such single-reinforcements exhibiting so extreme morphologies (such as fibers), are not often known from experiments, but more usually, they are deduced from the knowledge of the properties of the pure organic matrices, and those of the composite ply, through appropriate identification procedures often involving inverse scale transition models. The question of determining the multi-scale properties of some constituents of heterogeneous materials has been extensively addressed in the field of materials science. Complex polycrystalline metallic alloys (like titanium alloys, cf. Fréour et al., 2002; Fréour et al., 2005; Fréour et al., 2006b), or metal matrix composites (typically, Aluminum-Silicon Carbide composites, cf. Fréour et al., 2003a; Fréour et al., 2004 or iron oxides from the inner core of the Earth, cf. Matthies et al., 2001, for instance) have been extensively studied. More recently, an application of inverse scale transition models devoted to the identification of the strength envelope of the organic matrix constituting fiber reinforced composite plies has been built (Jacquemin and Fréour, 2008).

In order to achieve any of the three previously cited main goals, one specific scale transition model (i.e. mathematical formalism), has to be chosen, among the numerous theoretical frameworks available in the literature, able to handle such problems: Voigt (Voigt, 1928), Reuss, (Reuss, 1929), Neerfeld-Hill (Neerfeld, 1942; Hill, 1952), Tsai-Hahn (Tsai and Hahn, 1980) Mori-Tanaka (Mori and Tanaka, 1973; Tanaka and Mori, 1970), Eshelby-Kröner self-consistent approach (Eshelby, 1957; Kröner, 1958), are classical alternate solutions often used for dealing with the cases of bulk materials. Besides, Vook-Witt (Vook and Witt, 1965) and inverse Vook-Witt models (Welzel et al., 2003) have shown their ability to manage to handle the strongly anisotropic elastic behaviour exhibited in practice by thin solid film or by the subsurface of bulk specimens. The interested reader can refer, as an example, to Welzel et al., 2009, where a relative agreement, as good as 89 %, between the lattice strains, measured on ultra-thin solid films made of Palladium and the corresponding values, predicted by Vook-Witt model, was obtained. In order to deal with such situations, a modified version of Eshelby-Kröner model, the so-called “self-consistent free-surface method”, was also recently proposed by Baczmanski and his co-workers (Baczmanski et al., 2006; Baczmanski et al., 2008a; Baczmanski et al., 2008b). Moreover, according to (Benveniste et al., 1987), most of

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the historical above-listed scale-transition approaches do fail, due to their constitutive mathematical framework, to handle materials exhibiting complex microstructures including various morphologies of their constituents, presented by many new industrial products (Baptiste, 2003; Le Pen et al., 2002; Boursier et al., 2006). Consequently, many recent works have been dedicated to the investigation of new scale-transition models enabling to provide a reliable answer to the question of dealing with the coexistence of several inclusions morphologies in the same Representative Volume Element. The interested reader can refer to the following related works: (Qiu and Weng 1991; Benveniste, et al., 1991; Chen et al., 1992; Pham, 2000; Lacoste et al., 2010).

Now, any of the scale-transition models presented in the previously cited articles do heavily rely upon the extensive use of set averages, in order to provide numerical results (see a more detailed presentation in section 2 below). Actually, except in (Matthies et al., 2001), the classical arithmetic mean has been used in each of these papers. Recently, the idea of using geometric averages instead of arithmetic averages was proposed by Morawiec (1989). Nevertheless, the consequences of replacing arithmetic sets averages by their geometric counterparts were neither extensively discussed by the author, nor the mathematical/physical considerations having driven such a modification of the traditional calculation framework. This new solution, historically introduced in particular cases by Aleksandrov and Aisenberg (1966), is based on the condition of the commutation of inversion and averaging operations. According to (Matthies and Humbert, 1993), if *"for a given single crystal property E^0, the inverse property* $\mathrm{H}^0 = \left[\mathrm{E}^0\right]^{-1}$ *generally exists, physically, the corresponding relation also holds for a polycrystalline sample,* $\overline{\mathrm{E}} = \left[\overline{\mathrm{H}}\right]^{-1} = \left[\overline{\mathrm{E}^{-1}}\right]^{-1}$. *Unfortunately, the arithmetic mean does not provide this important relation.* $\overline{\mathrm{E}}^{\mathrm{a}} = \left[\overline{\mathrm{E}^{-1}}^{\mathrm{a}}\right]^{-1}$ *may be quite different but constitute the extreme limits of the experimental data lying in between".* In order to address this apparent drawback of the arithmetic mean, one new scale transition model, the Geo model (also called Bulk Path Geo, or BPG, in the field of X-Ray crystallographic texture or stress analysis), was recently built upon this constitutive assumption (Matthies and Humbert, 1993; Baczmanski et al., 1993; Matthies et al., 1994; Matthies and Humbert, 1995; Matthies, 1996; Matthies et al., 2001).
Numerical computations of the effective elastic behaviour of metallic polycrystals were achieved. It was shown by the authors that Young's modulus (Morawiec, 1989) or Diffraction Elastic Constants (Baczmanski et al., 1993) predicted by the Geo approximation were very close to the corresponding numerical values provided by Eshelby-Kröner self-consistent model using arithmetic averages, classically considered as a reference for the rigorous modelling of macroscopic elastic properties in polycrystals. Nevertheless, the Geo framework remains independent from any other scale-transition model, even if it is very close to Reuss or Voigt rough-and-ready assumptions, from the standpoint of the mathematical simplicity. The closeness of the Geo approach predictions with those of others models in some specific cases does not prove, that geometric averages would, in any case, yield results similar to the prediction obtained through the more classical arithmetic averages, an extensive investigation involving one single scale-transition model (Eshelby-Kröner self-consistent model) and either arithmetic or geometric sets averages, was achieved (Fréour et al., 2007). Actually, until that

work, only the type of assumed interactions between microscopic constituents and the macroscopic structure, which generally depend on the fundamental hypotheses of each scale-transition model, was considered to play a role in such studies: the effect of the averaging method used in order to perform numerical computations was assumed negligible.
Nevertheless, the reader of (Fréour et al., 2007) could ask himself whether considering the geometrical average, instead of the traditional arithmetic average, within Eshelby-Kröner model, is just a purely mathematical approach, or if there exists a physical reasoning which justifies its use. In the case that the arithmetic sets average is considered for being employed in the context of the "traditional" Eshelby-Kröner model, such a physical reasoning does effectively clearly exist (see section 3 below). The purpose of the present work consists in demonstrating that the geometric average does have a strong physical meaning in Eshelby-Kröner model framework, as well. Section 2 of this article is dedicated to a definition of both geometric and arithmetic sets averages, from a purely mathematical standpoint. A clear definition of the various scales involved in the considered micro-mechanical approach is also given in the beginning of that very section. In section 3, the fundamental definitions introduced by Kröner (1958), especially those of the so-called "polarization tensors", that linearly relate the strain (or, respectively, the stress) experienced by a certain heterogeneous inclusion to the macroscopic mechanical stress (or, respectively the strain) experienced by the effective medium in which it is embedded, are carefully examined from the standpoint of the mathematical method envisaged for performing sets average operations. On the basis of the practical independence of physical properties from the mathematical method applied in order to proceed to their determination, analytical forms are determined for the polarization tensors expressed in the geometric average version of Eshelby-Kröner self-consistent framework. The obtained expressions are compared to their counterparts, satisfied within the traditional, arithmetic average version of the model. The conclusions deduced from this work are gathered in section 4, where some perspectives of many further investigations are provided as well.

2. Theoretical background

2.1 Multi-scale representation of an heterogeneous material

For the purpose of the modeling of heterogeneous polycrystalline materials, it is useful to distinguish various types (usually, one by scale of the representation) of averages of tensors (either materials properties, like the stiffness $\mathbf{L}$, or the states, such as the strain $\boldsymbol{\varepsilon}$). The real microstructure of a sample is thus generally considered at two different scales:

- The average of a tensor over a single crystallographic orientation Ω of the grains is denoted by the superscript ^{II}. This level of the representation exhibits the anisotropic properties of an elementary inclusion (Base Volume) at the so-called "mesoscopic" scale.
- Homogenisation operations performed over its aforementioned constituting grains are assumed to provide the effective behaviour of the polycrystalline aggregate, which defines the so-called "macroscopic" scale of the model, which are those calculated for the Homogeneous Effective Medium (HEM) in the standpoint of the scale-transition modeling. This average of a tensor over all crystallographic orientations of the grains constituting the polycrystalline aggregate is denoted by the superscript ^{I}.

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Others aspects of the multi-scale representation of a heterogeneous sample are extensively discussed in (Macherauch et al., 1973; Sprauel and Castex, 1991; Sprauel, 1996).

2.2 Arithmetic and geometric averages

Macroscopic quantities can be obtained from scale transition model homogenisation procedures using volume weighted sets averages (that in fact replace volume integrals that would require Finite Elements Methods instead). This assertion was historically, rigorously demonstrated in (Hill, 1967). According to (Kocks et al., 1998), "*when the average is meant to represent a physical property of the aggregate* [i.e., of the macroscopic behaviour of the material], *it is crucial to decide which is the correct averaging procedure*". Unfortunately, this issue is not extensively developed in that book. Actually, if the classical arithmetic average is most of the time employed, in order to achieve such calculations, the geometric average was also considered as an alternate interesting procedure, after the publication of (Aleksandrov and Aisenberg, 1966). On the one hand, the geometric mean of a set of positive data is defined as the n^{th} root of the product of all the members of the set, where n is the number of members. On the other hand, in mathematics and statistics, the arithmetic mean (or simply the mean) of a list of numbers is the sum of all the members of the list divided by the number of items in the list.
In statistics, given a set of data, $X = \{x_1, x_2, ..., x_i, ..., x_n\}$ and corresponding weights, $W = \{w_1, w_2, ..., w_i, ..., w_n\}$, the weighted geometric (respectively, arithmetic) mean ${}_{GA}\langle X_\alpha \rangle_{\alpha=1,2,...,i,...,n}$ (respectively, ${}_{AA}\langle X_\alpha \rangle_{\alpha=1,2,...i,...n}$) is calculated as:

$$ {}_{GA}\langle X_\alpha \rangle_{\alpha=1,2,...,i,...,n} = \left(\prod_{\alpha=1}^{n} (x_\alpha)^{w_\alpha} \right)^{\left(\sum_{\alpha=1}^{n} w_\alpha \right)^{-1}} \quad (1) $$

$$ {}_{AA}\langle X_\alpha \rangle_{\alpha=1,2,...,i,...,n} = \left(\sum_{\alpha=1}^{n} x_\alpha \, w_\alpha \right) \left(\sum_{\alpha=1}^{n} w_\alpha \right)^{-1} \quad (2) $$

The geometric mean is actually useful for estimating averages in the context of a multiplicative situation, such as finding the average dimension of a box that would have the same volume as length x width x height. For example, let us assume a box with dimensions D = {30, 90, 100} cm. The geometric mean provides: ${}_{GA}\langle D \rangle = \left(\prod_{\alpha=1}^{3} (d_\alpha) \right)^{1/3} = \sqrt[3]{30.90.100} = 64.63 \text{cm}$, whereas the arithmetic mean would lead to ${}_{AA}\langle D \rangle = (30+90+100)/3 = 73.33 \text{cm}$. A cubic box with identical sides of 64,633 cm would enclose the same volume V = 30x90x100 = 0.27 m^3 as the initial parallelepiped. In the present case, $\left({}_{AA}\langle D \rangle \right)^3 = 0.394 \text{m}^3$, which does not correspond to the volume of the studied box.
The customary economic evaluation application is in determining "average" inflation or rate of return across several time periods. Suppose that your portfolio has these five annual

returns: R = {0.15, -0.20, -0.05, -0.10, 0.21}. The order does not matter if the portfolio has no contributions or withdrawals during the five years. The return arithmetic average is 0.002. However, a portfolio across five years with these annual returns would lose about 5% of its value. The geometric mean yields: $_{GA}\langle r\rangle = \left(\prod_{\alpha=1}^{5}(r_\alpha)\right)^{\frac{1}{5}} = \sqrt[5]{1.15*0.80*0.95*0.9*1.21} \approx 0.99$.

Thus, the average annual return would actually be 1 - 0.99 = - 0.01. Thus, contrarily to the predictions of the arithmetic mean, one portfolio of 100 $ would effectively lose 5 % in five years (100*1.15*0.80*0.95*0.9*1.21 = 95 $).

Both these examples demonstrate the relevance of the geometric mean for calculating averages of products of terms, whereas it is considered that the arithmetic mean better suits averaging operations performed on sums of terms. This link is also underlined by the property of commutativity for these operations, if the appropriate averaging method is used.

In statistics, achieving sets averages using either the geometric or the arithmetic mean often yields close outcome, if the terms do not have extremely different values. An illustration of such a closeness can be found in Morawiec (1989) where the results obtained for the elastic properties of polycrystals, through the geometric mixture law, were compared to others scale transition approaches involving the arithmetic mean. In the context of the present work, this statement suggests comparing the writing of a single scale transition model, from an arithmetic, sum based approach, or a geometric, product based formalism. The next section is devoted to the application of such an investigation, to the case of the classical Eshelby-Kröner self-consistent model in elasticity.

3. On the building of Eshelby-Kröner self-consistent model upon either arithmetic or geometric sets average

3.1 The historical description of the model: an arithmetic approach

Actually, Kröner's model is based on the constitutive assumption that, in a single-phase polycrystal composed of elastically anisotropic crystallites, the components of the mesoscopic stresses $\boldsymbol{\sigma}^{\mathbf{II}}(\Omega)$ and strains tensors $\boldsymbol{\varepsilon}^{\mathbf{II}}(\Omega)$ of a crystallite can be linked to the macroscopic strains $\boldsymbol{\varepsilon}^{\mathbf{I}}$ or stresses $\boldsymbol{\sigma}^{\mathbf{I}}$, respectively (Kröner, 1958; Welzel and Mittemeijer, 2003), through the following scale transition relations:

$$\boldsymbol{\sigma}^{\mathbf{II}}(\Omega) = \mathbf{p}^{\mathbf{II}}(\Omega) : \boldsymbol{\varepsilon}^{\mathbf{I}}, \tag{3}$$

$$\boldsymbol{\varepsilon}^{\mathbf{II}}(\Omega) = \mathbf{q}^{\mathbf{II}}(\Omega) : \boldsymbol{\sigma}^{\mathbf{I}}. \tag{4}$$

In (3, 4), $\mathbf{p}^{\mathbf{II}}(\boldsymbol{\Omega})$ and $\mathbf{q}^{\mathbf{II}}(\boldsymbol{\Omega})$ are the so-called "polarization tensors".

Mesoscopic and macroscopic Hooke's laws respectively write, in pure elasticity:

$$\boldsymbol{\sigma}^{\mathbf{II}}(\Omega) = \ell^{\mathbf{II}}(\Omega) : \boldsymbol{\varepsilon}^{\mathbf{II}}(\Omega) \tag{5}$$

$$\boldsymbol{\sigma}^{\mathbf{I}} = \mathbf{L}^{\mathbf{I}} : \boldsymbol{\varepsilon}^{\mathbf{I}} \tag{6}$$

where $\ell^{\mathbf{II}}(\Omega)$ is the single crystal elastic stiffness tensor and $\mathbf{L}^{\mathbf{I}}$ is the elastic stiffness tensor of the polycrystal.

As a consequence, the polarization tensors are linked together through:

$$\mathbf{p}^{\mathbf{II}}(\Omega) = \ell^{\mathbf{II}}(\Omega) : \mathbf{q}^{\mathbf{II}}(\Omega) : \mathbf{L}^{\mathbf{I}}, \tag{7}$$

In order to achieve the determination of the macroscopic stiffness of a polycrystal, from the knowledge of the stiffness tensor of its constitutive single-crystals, the historical proposal (Kröner; 1958) consists in writing the tensors $\mathbf{p}^{\mathbf{II}}(\Omega)$ (3) and $\mathbf{q}^{\mathbf{II}}(\Omega)$ (4) as sums of terms. Following this line of reasoning provides what we will call the "arithmetic" A-subscripted polarization tensors:

$$\mathbf{p}_{\mathbf{A}}^{\mathbf{II}}(\Omega) = \mathbf{L}^{\mathbf{I}} + \mathbf{r}_{\mathbf{A}}^{\mathbf{II}}(\Omega) \tag{8}$$

$$\mathbf{q}_{\mathbf{A}}^{\mathbf{II}}(\Omega) = \mathbf{L}^{\mathbf{I}^{-1}} + \mathbf{t}_{\mathbf{A}}^{\mathbf{II}}(\Omega) \tag{9}$$

The fourth-order tensors $\mathbf{r}_{\mathbf{A}}^{\mathbf{II}}(\Omega)$ and $\mathbf{t}_{\mathbf{A}}^{\mathbf{II}}(\Omega)$ stand for the arithmetic deviation of the elastic stiffness or compliance (respectively) of a single crystallite from the corresponding macroscopic quantity. As a consequence, the product $\mathbf{r}_{\mathbf{A}}^{\mathbf{II}}(\Omega) : \boldsymbol{\varepsilon}^{\mathbf{I}}$ (3-8) represents the arithmetic deviation between the macroscopic stress state (6) and that experienced by the considered crystallite. The same line of reasoning can be followed about the physical meaning of the product $\mathbf{t}_{\mathbf{A}}^{\mathbf{II}}(\Omega) : \boldsymbol{\sigma}^{\mathbf{II}}$ (4, 9), which obviously corresponds to the arithmetic deviation between the mesoscopic and macroscopic strains.

Taking into account the replacement rules (8) and (9), respectively for $\mathbf{p}_{\mathbf{A}}^{\mathbf{II}}(\Omega)$ and $\mathbf{q}_{\mathbf{A}}^{\mathbf{II}}(\Omega)$, enables to rewrite (3) and (4) as follows:

$$\boldsymbol{\sigma}^{\mathbf{II}}(\Omega) = \left[\mathbf{L}^{\mathbf{I}} + \mathbf{r}_{\mathbf{A}}^{\mathbf{II}}(\Omega)\right] : \boldsymbol{\varepsilon}^{\mathbf{I}} \tag{10}$$

$$\boldsymbol{\varepsilon}^{\mathbf{II}}(\Omega) = \left[\mathbf{L}^{\mathbf{I}^{-1}} + \mathbf{t}_{\mathbf{A}}^{\mathbf{II}}(\Omega)\right] : \boldsymbol{\sigma}^{\mathbf{I}} \tag{11}$$

In practice, the average over the mesoscopic strains should be identical to the strain experienced by the polycrystal, and a similar statement should obviously be satisfied regarding the stresses. As a consequence, the so-called "Hill's average principles" should be fulfilled (Hill, 1967):

$$\boldsymbol{\varepsilon}^{\mathbf{I}} = \left\langle \boldsymbol{\varepsilon}^{\mathbf{II}}(\Omega) \right\rangle \tag{12}$$

$$\boldsymbol{\sigma}^{\mathbf{I}} = \left\langle \boldsymbol{\sigma}^{\mathbf{II}}(\Omega) \right\rangle \tag{13}$$

Achieving the volume weighted set average over (10) and (11), while accounting for both Hill's average principle (12-13) and the macroscopic Hooke's law (6), yields:

$$\left\langle \boldsymbol{\sigma}^{\mathbf{II}}(\Omega) \right\rangle = \left\langle \mathbf{L}^{\mathbf{I}} + \mathbf{r}_{\mathbf{A}}^{\mathbf{II}}(\Omega) \right\rangle : \boldsymbol{\varepsilon}^{\mathbf{I}} = \mathbf{L}^{\mathbf{I}} : \boldsymbol{\varepsilon}^{\mathbf{I}} + \left\langle \mathbf{r}_{\mathbf{A}}^{\mathbf{II}}(\Omega) \right\rangle : \boldsymbol{\varepsilon}^{\mathbf{I}} = \mathbf{L}^{\mathbf{I}} : \boldsymbol{\varepsilon}^{\mathbf{I}} \tag{14}$$

$$\left\langle \boldsymbol{\varepsilon}^{\mathbf{II}}(\Omega) \right\rangle = \left\langle \mathbf{L}^{\mathbf{I}^{-1}} + \mathbf{t}_{\mathbf{A}}^{\mathbf{II}}(\Omega) \right\rangle : \boldsymbol{\sigma}^{\mathbf{I}} = \mathbf{L}^{\mathbf{I}^{-1}} : \boldsymbol{\sigma}^{\mathbf{I}} + \left\langle \mathbf{t}_{\mathbf{A}}^{\mathbf{II}}(\Omega) \right\rangle : \boldsymbol{\sigma}^{\mathbf{I}} = \mathbf{L}^{\mathbf{I}^{-1}} : \boldsymbol{\sigma}^{\mathbf{I}} \tag{15}$$

Equations (14-15) respectively yield the following classical relations:

$$\left\langle \mathbf{r}_{\mathbf{A}}^{\mathbf{II}}(\Omega) \right\rangle = \mathbf{0} \tag{16}$$

$$\left\langle \mathbf{t}_{\mathbf{A}}^{\mathbf{II}}(\Omega) \right\rangle = \mathbf{0} \tag{17}$$

(16) and (17) are essential, because they are closely related to the name attributed to Kröner's model. This model is actually self-consistent, because the simultaneous fulfilling of fundamental relations (16) and (17) ensures that the average over the mesoscopic stresses (respectively the strains) are equal to the corresponding macroscopic quantity.

In the traditional, above-described, version of Kröner's self-consistent model, it would be legitimate to have the feeling that using arithmetic averages instead of geometric averages is more appropriate because (8-11) are based on arithmetic deviations between the single heterogeneity elastic behaviour and the macroscopic elastic behaviour of the considered Representative Volume Element.

3.2 Towards a product-based writing of Eshelby-Kröner self-consistent model, involving geometric averages

3.2.1 Rewriting the polarization tensors as geometric values

Now, (8) and (9) could have been written as products of factors instead of as sums. Following this line of reasoning provides what we will below call the "geometric" G-subscripted polarization tensors:

$$\mathbf{p}_{\mathbf{G}}^{\mathbf{II}}(\Omega) = \mathbf{r}_{\mathbf{G}}^{\mathbf{II}}(\Omega) : \mathbf{L}^{\mathbf{I}} = \mathbf{p}_{\mathbf{A}}^{\mathbf{II}}(\Omega) = \mathbf{p}^{\mathbf{II}}(\Omega) \tag{18}$$

$$\mathbf{q}_{\mathbf{G}}^{\mathbf{II}}(\Omega) = \mathbf{t}_{\mathbf{G}}^{\mathbf{II}}(\Omega) : \mathbf{L}^{\mathbf{I}^{-1}} = \mathbf{q}_{\mathbf{A}}^{\mathbf{II}}(\Omega) = \mathbf{q}^{\mathbf{II}}(\Omega) \tag{19}$$

Obviously, in practice, both the mechanical states of a given Ω crystallographically oriented grains family and those experienced by the whole polycrystal must not change in the real

specimen. As a consequence, the geometric polarization tensors must be numerically identical to their traditional arithmetic counterparts, as indicated in (18-19). In this context, the following relations should be satisfied for the "geometric" influence tensors $\mathbf{r}_{\mathbf{G}}^{\mathbf{II}}(\Omega)$ and $\mathbf{t}_{\mathbf{G}}^{\mathbf{II}}(\Omega)$:

$$\mathbf{r}_{\mathbf{G}}^{\mathbf{II}}(\Omega) = \mathbf{I} + \mathbf{r}_{\mathbf{A}}^{\mathbf{II}}(\Omega) : \mathbf{L}^{\mathbf{I}^{-1}} \tag{20}$$

$$\mathbf{t}_{\mathbf{G}}^{\mathbf{II}}(\Omega) = \mathbf{I} + \mathbf{t}_{\mathbf{A}}^{\mathbf{II}}(\Omega) : \mathbf{L}^{\mathbf{I}} \tag{21}$$

These relations also show that the geometrical deviation tensors are non-dimensional, which is not the case for the arithmetical tensors.

3.2.2 On the physical meaning of the fundamental relations of Eshelby-Kröner self-consistent geometric model

By replacing $\mathbf{p}^{\mathbf{II}}(\boldsymbol{\Omega})$ and $\mathbf{q}^{\mathbf{II}}(\boldsymbol{\Omega})$ in (3) and (4) by their product-based expressions (18) and (19), respectively, one establishes the following especially relevant result:

$$\boldsymbol{\sigma}^{\mathbf{II}}(\Omega) = \mathbf{r}_{\mathbf{G}}^{\mathbf{II}}(\Omega) : \mathbf{L}^{\mathbf{I}} : \boldsymbol{\varepsilon}^{\mathbf{I}} = \mathbf{r}_{\mathbf{G}}^{\mathbf{II}}(\Omega) : \boldsymbol{\sigma}^{\mathbf{I}} \tag{22}$$

$$\boldsymbol{\varepsilon}^{\mathbf{II}}(\Omega) = \mathbf{t}_{\mathbf{G}}^{\mathbf{II}}(\Omega) : \mathbf{L}^{\mathbf{I}^{-1}} : \boldsymbol{\sigma}^{\mathbf{I}} = \mathbf{t}_{\mathbf{G}}^{\mathbf{II}}(\Omega) : \boldsymbol{\varepsilon}^{\mathbf{I}} \tag{23}$$

Thus, according to (22), while its arithmetic historical counterpart $\mathbf{r}_{\mathbf{A}}^{\mathbf{II}}(\Omega)$ does neither have a very strong physical meaning nor practical use in the field of meso-macro modelling, $\mathbf{r}_{\mathbf{G}}^{\mathbf{II}}(\Omega)$ provides the scale transition relation linking the macroscopic stress $\boldsymbol{\sigma}^{\mathbf{I}}$ to those experienced by an Ω crystallographically oriented inclusions family. Thus $\mathbf{r}_{\mathbf{G}}^{\mathbf{II}}(\Omega)$ actually corresponds to the so-called "stress concentration tensor", usually denoted by $\mathbf{B}^{\mathbf{II}}(\Omega)$ in the literature (Freour et al., 2006a; Lacoste et al., 2010). Following the same line of reasoning, but applied on (23), $\mathbf{t}_{\mathbf{G}}^{\mathbf{II}}(\Omega)$ provides the scale transition relation linking the macroscopic strain $\boldsymbol{\varepsilon}^{\mathbf{I}}$ to the corresponding quantities, at mesoscopic scale: $\boldsymbol{\varepsilon}^{\mathbf{II}}(\Omega)$. This actually precisely corresponds to the definition of the "strain localization tensor", often denoted by $\mathbf{A}^{\mathbf{II}}(\Omega)$, even more widely used in the field of scale transition modelling (see, as an example, El Mouden and Molinari, 1996; Freour et al., 2003a; Freour et al., 2004; Welzel et al., 2005; Lacoste et al., 2010).

Averaging (22) and (23) over the entire specimen results in:

$$\left\langle \boldsymbol{\sigma}^{\mathbf{II}}(\Omega) \right\rangle = \left\langle \mathbf{r}_{\mathbf{G}}^{\mathbf{II}}(\Omega) \right\rangle : \boldsymbol{\sigma}^{\mathbf{I}} = \boldsymbol{\sigma}^{\mathbf{I}} \tag{24}$$

$$\left\langle \boldsymbol{\varepsilon}^{\mathbf{II}}(\Omega) \right\rangle = \left\langle \mathbf{t}_{\mathbf{G}}^{\mathbf{II}}(\Omega) \right\rangle : \boldsymbol{\varepsilon}^{\mathbf{I}} = \boldsymbol{\varepsilon}^{\mathbf{I}} \tag{25}$$

(24) and (25) respectively yield the following relations:

$$\left\langle \mathbf{r}_{\mathbf{G}}^{\mathbf{II}}(\Omega) \right\rangle = \mathbf{I} \tag{26}$$

$$\left\langle \mathbf{t}_{\mathbf{G}}^{\mathbf{II}}(\Omega) \right\rangle = \mathbf{I} \tag{27}$$

These relations are the expected results for both the volume fraction weighted averages over the mesoscopic stress/strains localization tensors within Eshelby-Kröner self-consistent framework. Actually, (26) and (27) mean that the average of the mesoscopic strains or stresses is respectively identical to their macroscopic counterparts, which satisfy both the previously introduced Hill's average principles (12-13), that are expected to be valid within any scale transition mathematical model.

While the product-based description of the behaviour of a single-heterogeneity embedded in a homogeneous material is considered, it is reasonable to regard the geometric mean as an appropriate manner to perform the volume-weighted averaging operation involved in, for instance, (24-25). Here, it is justified, because the geometric average is appropriate for calculating averages of products, whereas the arithmetic average is usually better for the statistical analysis of sums of terms.

3.3 Checking the compatibility of the geometric version of Eshelby-Kröner self-consistent model with its historical arithmetic counterpart

Moreover, one can show that (the interested reader can refer to Kocks et al., 1998, where an extensive demonstration is provided):

$$\boldsymbol{\sigma}^{\mathbf{II}}(\Omega) - \boldsymbol{\sigma}^{\mathbf{I}} = -\mathbf{L}^{\mathbf{I}} : \mathbf{R}^{\mathbf{I}} : \left(\boldsymbol{\varepsilon}^{\mathbf{II}}(\Omega) - \boldsymbol{\varepsilon}^{\mathbf{I}} \right) \tag{28}$$

Introducing (4) and (10) in (28), one obtains:

$$\left[\mathbf{L}^{\mathbf{I}} + \mathbf{r}_{\mathbf{A}}^{\mathbf{II}}(\Omega) \right] : \boldsymbol{\varepsilon}^{\mathbf{I}} - \boldsymbol{\sigma}^{\mathbf{I}} = -\mathbf{L}^{\mathbf{I}} : \mathbf{R}^{\mathbf{I}} : \left(\mathbf{q}_{\mathbf{A}}^{\mathbf{II}}(\Omega) : \boldsymbol{\sigma}^{\mathbf{I}} - \boldsymbol{\varepsilon}^{\mathbf{I}} \right) \tag{29}$$

Taking into account (6-7), the following relation can be written:

$$\left[\mathbf{L}^{\mathbf{I}} + \mathbf{r}_{\mathbf{A}}^{\mathbf{II}}(\Omega) - \mathbf{L}^{\mathbf{I}} \right] : \boldsymbol{\varepsilon}^{\mathbf{I}} = -\mathbf{L}^{\mathbf{I}} : \mathbf{R}^{\mathbf{I}} : \left(\ell^{\mathbf{II}^{-\mathbf{1}}}(\Omega) : \mathbf{p}_{\mathbf{A}}^{\mathbf{II}}(\Omega) - \mathbf{I} \right) : \boldsymbol{\varepsilon}^{\mathbf{I}} \tag{30}$$

Thus, after some obvious simplifications and use of the replacement rule given by (8), one obtains:

$$\mathbf{r}_{\mathbf{A}}^{\mathbf{II}}(\Omega) = -\mathbf{L}^{\mathbf{I}} : \mathbf{R}^{\mathbf{I}} : \left(\ell^{\mathbf{II}^{-1}}(\Omega) : \left[\mathbf{L}^{\mathbf{I}} + \mathbf{r}_{\mathbf{A}}^{\mathbf{II}}(\Omega) \right] - \mathbf{I} \right) \tag{31}$$

Finally, tensor $\mathbf{r}_{\mathbf{A}}^{\mathbf{II}}(\Omega)$ satisfies:

$$\mathbf{r}_{\mathbf{A}}^{\mathbf{II}}(\Omega) = -\left(\mathbf{I} + \mathbf{L}^{\mathbf{I}} : \mathbf{R}^{\mathbf{I}} : \ell^{\mathbf{II}^{-1}}(\Omega) \right)^{-1} : \mathbf{L}^{\mathbf{I}} : \mathbf{R}^{\mathbf{I}} : \left(\ell^{\mathbf{II}^{-1}}(\Omega) : \mathbf{L}^{\mathbf{I}} - \mathbf{I} \right) \tag{32}$$

Now, this formalism will be used in order to express the scale-transition relation required for finding the macroscopic stiffness $\mathbf{L}^{\mathbf{I}}$. Introducing (9), and the macroscopic Hooke's law (6), (11) transforms as:

$$\boldsymbol{\varepsilon}^{\mathbf{II}}(\Omega) = \left[\mathbf{L}^{\mathbf{I}^{-1}} + \mathbf{q}_{\mathbf{A}}^{\mathbf{II}}(\Omega) - \mathbf{L}^{\mathbf{I}^{-1}} \right] : \mathbf{L}^{\mathbf{I}} : \boldsymbol{\varepsilon}^{\mathbf{I}} = \mathbf{q}_{\mathbf{A}}^{\mathbf{II}}(\Omega) : \mathbf{L}^{\mathbf{I}} : \boldsymbol{\varepsilon}^{\mathbf{I}} \tag{33}$$

Whereas $\mathbf{q}_{\mathbf{A}}^{\mathbf{II}}(\Omega)$ can be rewritten according to (7) and the right-hand side of (8), yielding:

$$\boldsymbol{\varepsilon}^{\mathbf{II}}(\Omega) = \ell^{\mathbf{II}^{-1}}(\Omega) : \left[\mathbf{L}^{\mathbf{I}} + \mathbf{r}_{\mathbf{A}}^{\mathbf{II}}(\Omega) \right] : \boldsymbol{\varepsilon}^{\mathbf{I}} \tag{34}$$

Combining (32) to (34) enables to achieve the following development:

$$\begin{aligned}
\boldsymbol{\varepsilon}^{\mathbf{II}}(\Omega) &= \ell^{\mathbf{II}^{-1}}(\Omega) : \left[\mathbf{L}^{\mathbf{I}} + \mathbf{r}_{\mathbf{A}}^{\mathbf{II}}(\Omega) \right] : \boldsymbol{\varepsilon}^{\mathbf{I}} \\
&= \ell^{\mathbf{II}^{-1}}(\Omega) : \left[\mathbf{L}^{\mathbf{I}} - \left(\mathbf{I} + \mathbf{L}^{\mathbf{I}} : \mathbf{R}^{\mathbf{I}} : \ell^{\mathbf{II}^{-1}}(\Omega) \right)^{-1} : \mathbf{L}^{\mathbf{I}} : \mathbf{R}^{\mathbf{I}} : \left(\ell^{\mathbf{II}^{-1}}(\Omega) : \mathbf{L}^{\mathbf{I}} - \mathbf{I} \right) \right] : \boldsymbol{\varepsilon}^{\mathbf{I}} \\
&= \left[\ell^{\mathbf{II}^{-1}}(\Omega) : \mathbf{L}^{\mathbf{I}} - \left(\ell^{\mathbf{II}}(\Omega) + \mathbf{L}^{\mathbf{I}} : \mathbf{R}^{\mathbf{I}} \right)^{-1} : \mathbf{L}^{\mathbf{I}} : \mathbf{R}^{\mathbf{I}} : \left(\ell^{\mathbf{II}^{-1}}(\Omega) : \mathbf{L}^{\mathbf{I}} - \mathbf{I} \right) \right] : \boldsymbol{\varepsilon}^{\mathbf{I}} \\
&= \left(\ell^{\mathbf{II}}(\Omega) + \mathbf{L}^{\mathbf{I}} : \mathbf{R}^{\mathbf{I}} \right)^{-1} : \left[\left(\ell^{\mathbf{II}}(\Omega) + \mathbf{L}^{\mathbf{I}} : \mathbf{R}^{\mathbf{I}} \right) : \ell^{\mathbf{II}^{-1}}(\Omega) : \mathbf{L}^{\mathbf{I}} - \mathbf{L}^{\mathbf{I}} : \mathbf{R}^{\mathbf{I}} : \left(\ell^{\mathbf{II}^{-1}}(\Omega) : \mathbf{L}^{\mathbf{I}} - \mathbf{I} \right) \right] : \boldsymbol{\varepsilon}^{\mathbf{I}}
\end{aligned} \tag{35}$$

Some terms cancel together, so that one finally obtains:

$$\boldsymbol{\varepsilon}^{\mathbf{II}}(\Omega) = \left(\ell^{\mathbf{II}}(\Omega) + \mathbf{L}^{\mathbf{I}} : \mathbf{R}^{\mathbf{I}} \right)^{-1} : \left[\mathbf{L}^{\mathbf{I}} + \mathbf{L}^{\mathbf{I}} : \mathbf{R}^{\mathbf{I}} \right] : \boldsymbol{\varepsilon}^{\mathbf{I}} \tag{36}$$

From (36), the classical line of reasoning, widely reported in the literature (Kocks et al., 1998), can be followed:

$$\ell^{\mathbf{II}}(\Omega) : \boldsymbol{\sigma}^{\mathbf{II}}(\Omega) = \left(\ell^{\mathbf{II}}(\Omega) + \mathbf{L}^{\mathbf{I}} : \mathbf{R}^{\mathbf{I}} \right)^{-1} : \left[\mathbf{L}^{\mathbf{I}} + \mathbf{L}^{\mathbf{I}} : \mathbf{R}^{\mathbf{I}} \right] : \boldsymbol{\varepsilon}^{\mathbf{I}} \tag{37}$$

$$\boldsymbol{\sigma}^{\mathbf{II}}(\Omega) = \ell^{\mathbf{II}^{-1}}(\Omega) : \left(\ell^{\mathbf{II}}(\Omega) + \mathbf{L}^{\mathbf{I}} : \mathbf{R}^{\mathbf{I}} \right)^{-1} : \left[\mathbf{L}^{\mathbf{I}} + \mathbf{L}^{\mathbf{I}} : \mathbf{R}^{\mathbf{I}} \right] : \boldsymbol{\varepsilon}^{\mathbf{I}} \tag{38}$$

$$\left\langle \boldsymbol{\sigma}^{\mathbf{II}}(\Omega) \right\rangle = \left\langle \ell^{\mathbf{II}^{-1}}(\Omega) : \left(\ell^{\mathbf{II}}(\Omega) + \mathbf{L}^{\mathbf{I}} : \mathbf{R}^{\mathbf{I}} \right)^{-1} : \left[\mathbf{L}^{\mathbf{I}} + \mathbf{L}^{\mathbf{I}} : \mathbf{R}^{\mathbf{I}} \right] \right\rangle : \boldsymbol{\varepsilon}^{\mathbf{I}} = \boldsymbol{\sigma}^{\mathbf{I}} = \mathbf{L}^{\mathbf{I}} : \boldsymbol{\varepsilon}^{\mathbf{I}} \tag{39}$$

Thus, the macroscopic stiffness tensor satisfies:

$$\mathbf{L}^{\mathbf{I}} = \left\langle \ell^{\mathbf{II}^{-1}}(\Omega) : \left(\ell^{\mathbf{II}}(\Omega) + \mathbf{L}^{\mathbf{I}} : \mathbf{R}^{\mathbf{I}} \right)^{-1} : \left[\mathbf{L}^{\mathbf{I}} + \mathbf{L}^{\mathbf{I}} : \mathbf{R}^{\mathbf{I}} \right] \right\rangle \tag{40}$$

Combination of (32) and (20) provides the following expression for $\mathbf{r}_{\mathbf{G}}^{\mathbf{II}}(\Omega)$:

$$\mathbf{r}_{\mathbf{G}}^{\mathbf{II}}(\Omega) = \mathbf{I} + \mathbf{r}_{\mathbf{A}}^{\mathbf{II}}(\Omega) : \mathbf{L}^{\mathbf{I}^{-1}} = \mathbf{I} - \left(\mathbf{I} + \mathbf{L}^{\mathbf{I}} : \mathbf{R}^{\mathbf{I}} : \ell^{\mathbf{II}^{-1}}(\Omega) \right)^{-1} : \mathbf{R}^{\mathbf{I}} : \left(\ell^{\mathbf{II}^{-1}}(\Omega) : \mathbf{L}^{\mathbf{I}} - \mathbf{I} \right) \tag{41}$$

Moreover, introducing (19) in (23) gives:

$$\boldsymbol{\varepsilon}^{\mathbf{II}}(\Omega) = \mathbf{q}_{\mathbf{A}}^{\mathbf{II}}(\Omega) : \mathbf{L}^{\mathbf{I}} : \boldsymbol{\varepsilon}^{\mathbf{I}} \tag{42}$$

We have already demonstrated that: $\mathbf{q}_{\mathbf{A}}^{\mathbf{II}}(\Omega) : \mathbf{L}^{\mathbf{I}} : \boldsymbol{\varepsilon}^{\mathbf{I}} = \ell^{\mathbf{II}^{-1}}(\Omega) : \left[\mathbf{L}^{\mathbf{I}} + \mathbf{r}_{\mathbf{A}}^{\mathbf{II}}(\Omega) \right] : \boldsymbol{\varepsilon}^{\mathbf{I}}$ (see (33) and (34)). The satisfaction of that equation was demonstrated to be compatible with the traditional expression (40) employed for achieving the macroscopic stiffness determination. As a consequence, the geometric (product-based) rewriting of the fundamental relations of Eshelby-Kröner self-consistent model (cf. (18) and (19)) yields the same homogenization relation for estimating the macroscopic stiffness tensor $\mathbf{L}^{\mathbf{I}}$ than the traditional arithmetic description (cf. (8) and (9)). Actually, the above investigated product-based description of Eshelby-Kröner self-consistent model does not lead to a strongly different mathematical framework, since the final equations (those that are employed in practice by the user), are, as expected, rigorously the same. The main interest of such a description is to clarify the physical meaning justifying the use of geometric averages instead of the more classical arithmetic approach.

4. Conclusions and perspectives

In the present work, the fundamental equations of Eshelby-Kröner self-consistent model have been investigated from the standpoint of either the historical, classical arithmetic framework or, for the first time, the product-based, "geometric", deviation of the mechanical states experienced by a single crystallite from the corresponding macroscopic quantities. The first formulation results in a sum of terms, whereas the second involves products of factors. This fact yields a privileged (but not exclusive) link between each formulation and the corresponding averaging operation. It was demonstrated that the geometric polarization tensors are proportional to either the strain localization tensor or the stress concentration tensor, two quantities on which many scale transition models are based upon, for practical applications, but also because of their strong physical meaning. On the contrary, the classical arithmetic polarization tensors did hold very little appeal on the scientific community working on this field of research. Since the arithmetic mean is considered as better suited for achieving averages over sets of sums of terms, it was historically clearly the most appropriate solution,

in the mathematical framework of Eshelby-Kröner model. The present work underlines however, that the geometric set average-type, which is, in statistics, considered as better suited for performing such mathematical operations over products of factors, would also be relevant, since the corresponding analytical writing of Eshelby-Kröner model involves more physically meaningful intermediate quantities. Thus, according to the results obtained in the present study, either the arithmetic, or the geometric mean, could be employed at the discretion of the user in order to perform calculation according to Eshelby-Kröner self-consistent model.
In further works, extensive comparisons between the numerical results provided by Eshelby-Kröner self-consistent model, as a function on the chosen mathematical way for realizing sets averages, will be achieved in the many fields of applications of that very model (pure elasticity, thermoelasticity, viscoelasticity, elastoplasticity, and so on). A specific care will be put upon the consequence, induced by the chosen sets averages method, on the critical applications of this model, which consist in the identification of some materials properties.

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