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THERMAL EXPANSION OF POLYCRYSTALS WITH GRAIN BOUNDARY SLIDING

Y. BENVENISTE
Department of Mechanics of Solids, Materials and Structures, Faculty of Engineering,
Tel-Aviv University, Ramat-Aviv, Tel-Aviv 69978, Israel

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Abstract—Anisotropic polycrystals in which the shear tractions vanish at several locations of the grain boundaries are considered. For three-dimensional polycrystals whose crystals belong to the tetragonal, hexagonal or trigonal class, it is shown that the effective thermal expansion tensor is given in terms of its effective elastic compliance and the properties of the constituent crystals. If the crystals are cubic, it is shown that the components of the effective compliance tensor obey a constraint condition whereas the effective thermal expansion tensor is equal to that of the constituent crystals. Polycrystals containing an inclusion phase and exhibiting grain boundary sliding at possible locations of the crystal–crystal and crystal–inclusion boundaries are also considered. For such polycrystals microstructure independent relations for the effective thermal expansion tensor are derived under the restriction that both the crystals and the inclusion phase are cubic. Corresponding results for planar polycrystals in plane stress or plane strain conditions are also presented. © 1997 Elsevier Science Ltd. All rights reserved.

1. INTRODUCTION

In a series of works Hashin (1984), and Schulgasser (1987, 1989) showed that the effective thermal expansion tensor of certain three-dimensional polycrystals can be expressed in terms of the effective polycrystal compliance and the properties of the constituent crystals. In this paper it is shown that a microstructure independent expression of the nature given in the above papers can also be derived for certain polycrystals which undergo grain boundary sliding. Grain boundary sliding in polycrystals is encountered in high temperature environments and has been extensively studied in several papers since the early work of Zener (1941); see, for example, Hart (1967), Crossman and Ashby (1975), Speight (1976), Chen and Argon (1979), Ghahremani (1979), and Anderson and Rice (1985). Grain boundaries which are weak in shear have been modeled in the literature by viscous heterogeneities, and self consistent approximations and finite element calculations have been used to study their effect on the effective behaviour of polycrystals. The problem is a highly complex one and may involve the nucleation and growth of cavities at grain boundaries. We do not aim in the present work at an elaborate and precise description of grain boundary sliding. Instead, our purpose is to adopt a simplified model which will allow the derivation of exact microstructure-independent relations for the effective thermal expansion tensor. An idealized representation of grain boundary sliding is achieved by assuming that the shear tractions at several locations of the grain boundaries are completely relaxed and vanish. Such a condition has been used by Zener (1945), Ghahremani (1979), and more recently by Rodin (1995), and is expected to describe the long time creep behaviour of some polycrystals. The present paper is thus concerned with polycrystalline aggregates in which the grain boundaries exhibit perfect bonding at some locations, but may freely slide at others in view of vanishing shear tractions at those places. The method of derivation here for the effective thermal expansion tensor is based on the creation of uniform fields in the polycrystal; for applications of this method in heterogeneous media, see Dvorak (1986, 1990), Benveniste and Dvorak (1990a, 1990b), and Benveniste (1994).

In the second section of the paper it is shown that in three-dimensional anisotropic polycrystals with grain boundary sliding of the nature described above, the thermal expansion tensor can be expressed in terms of the effective compliance of the polycrystal and the properties of the constituent crystals, provided that the polycrystal consists of a single type of crystals belonging to the tetragonal, hexagonal or trigonal classes. It turns out that the derived expression is identical to that given by Hashin (1984), and Schulgasser (1987, 1989), but yet accounts for grain boundary sliding through the fact that the effective compliance of the polycrystal exhibiting slip is different than that of the polycrystal with perfectly bonded crystals. Two-dimensional polycrystalline aggregates in plane stress or plane strain conditions are also considered, and a corresponding relation for the effective thermal expansion tensor is obtained for a planar polycrystal with orthotropic constituent crystals.

In the second section we consider also the case of three-dimensional anisotropic polycrystals made of cubic crystals and exhibiting free slip at some locations. We show that the components of the effective compliance tensor obey a constraint condition which turns out to be identical to that given by Walpole (1985) for the case of perfectly bonded cubic crystals. The effective thermal expansion tensor of this polycrystalline aggregate is equal to that of the cubic crystals.

Polycrystals often contain inclusions in the form of impurities or porosities. The effective thermal expansion of polycrystalline aggregates consisting of elongated crystals which are in a generalized plane strain condition, and which contain an inclusion phase has been recently studied by the author, Benveniste (1996). In the third section of this paper we consider a polycrystal containing an inclusion phase, and undergoing slip at possible locations of the crystal–crystal and crystal–inclusion boundaries. We show that for such a three-dimensional anisotropic polycrystal a microstructure independent relation for the effective thermal expansion tensor can be derived if the constituent crystals are cubic; the inclusion phase may be cubic, porous, or may even consist of a different cubic crystal with arbitrary orientations. For a two-dimensional polycrystal with plane stress or plane strain conditions (to be distinguished from the generalized plane strain case studied in Benveniste (1996)), it is shown that the effective thermal expansion tensor can be expressed in terms of the effective plane compliance and the properties of the constituents, provided that the crystals and the inclusion phase are square symmetric.

2. POLYCRYSTALS CONTAINING FRICTIONLESS GRAIN BOUNDARIES

Consider a polycrystalline aggregate consisting of a single type of crystals whose constitutive law is given by

$$\varepsilon^c_{ij} = S^c_{ijkl}\sigma^c_{kl} + \alpha^c_{ij}\theta_0, \tag{1}$$

where ε^c_{ij} and σ^c_{ij} denote, respectively, the strains and stresses in the crystals, S^c_{ijkl} and α^c_{ij} are the compliance and thermal expansion tensors of the crystals, and θ_0 is an increase in the temperature from a reference state.

At some locations of the polycrystal, the grain boundaries exhibit perfect bonding, whereas at others they are frictionless. At locations where there is perfect bonding, the traction and displacement vector are continuous. At the frictionless grain boundaries the shear tractions vanish; a jump in the tangential component of the displacement vector at these locations may thus be allowed. The normal components of the traction and displacement vectors, on the other hand, remain to be continuous at the frictionless grain boundaries as well. Clearly, the polycrystal may have perfect bonding or frictionless grain boundaries throughout. In this section we intend to show that the effective thermal expansion of the described polycrystal may be expressed in terms of the effective compliance tensor and the properties of the constituent crystals, provided that the crystals belong to the tetragonal, hexagonal or trigonal class.

The first step in the derivation is the search for a specific loading $(\hat{\sigma}_{ij}, \theta_0)$:

$$t_i(S) = \hat{\sigma}_{ij}n_j, \quad \theta(S) = \theta_0, \tag{2}$$

which generates a uniform stress and strain field in the polycrystal; in (2), t_i is the traction vector on the outside surface S of the polycrystal, n_i is the normal to that surface, and $\hat{\sigma}_{ij}$ denotes a constant stress. Let us choose $\hat{\sigma}_{ij}$ to be hydrostatic

$$\hat{\sigma}_{ij} = \hat{\sigma}\,\delta_{ij}, \tag{3}$$

where δ_{ij} denotes the Kronecker delta, and look for conditions under which this loading induces a uniform hydrostatic stress and strain in every crystal. Assume that the stress field in each crystal is given by (3). The corresponding strain field results as:

$$\varepsilon^c_{ij}(\mathbf{x}) = S^c_{ijkk}\hat{\sigma} + \alpha^c_{ij}\theta_0. \tag{4}$$

If the crystals possess a symmetry class which is tetragonal, hexagonal or trigonal, then

$$\begin{aligned}
\varepsilon^c_{11}(\mathbf{x}) &= \varepsilon^c_{22}(\mathbf{x}) = (S^c_{1111}+S^c_{1122}+S^c_{1133})\hat{\sigma}+\alpha^c_{11}\theta_0,\\
\varepsilon^c_{33}(\mathbf{x}) &= (2S^c_{1133}+S^c_{3333})\hat{\sigma}+\alpha^c_{33}\theta_0,\\
\varepsilon^c_{31}(\mathbf{x}) &= \varepsilon^c_{32}(\mathbf{x}) = \varepsilon^c_{12}(\mathbf{x}) = 0,
\end{aligned} \tag{5}$$

so that a hydrostatic state of strain in each crystal is achievable by demanding

$$\varepsilon^c_{11}(\mathbf{x}) = \varepsilon^c_{33}(\mathbf{x}). \tag{6}$$

This yields

$$\hat{\sigma} = (\alpha^c_{33}-\alpha^c_{11})\theta_0/(S^c_1-S^c_3), \tag{7}$$

where

$$S^c_1 = S^c_{1111}+S^c_{1122}+S^c_{1133}, \quad S^c_3 = 2S^c_{1133}+S^c_{3333}. \tag{8}$$

Two points should be emphasized at this stage: (a) a hydrostatic uniform state of stress and strain is not achievable, under (2), for three dimensional polycrystals whose crystals have a higher anisotropy than that of the tetragonal class, (b) the derived uniform field solution, summarized by

$$\begin{aligned}
\sigma^c_{ij}(\mathbf{x}) &= (\alpha^c_{33}-\alpha^c_{11})\theta_0/(S^c_1-S^c_3)\,\delta_{ij},\\
\varepsilon^c_{ij}(\mathbf{x}) &= (\alpha^c_{33}S^c_1-\alpha^c_{11}S^c_3)\theta_0/(S^c_1-S^c_3)\,\delta_{ij},
\end{aligned} \tag{9}$$

is valid *not only* for a polycrystal with perfectly bonded crystals, but *also* for polycrystals which possess frictionless grain boundaries at several locations; the applied loading (2) and (3), with $\hat{\sigma}$ given by (7), does not induce any sliding at these locations even if, potentially, it may take place there.

Let us now subject the external surface of the polycrystal to the boundary conditions:

$$t_i(S) = 0, \quad \theta(S) = \theta_0. \tag{10}$$

The average stresses $\bar{\sigma}^{pc}_{ij}$, and strains $\bar{\varepsilon}^{pc}_{ij}$ in the polycrystal are then given by

$$\bar{\sigma}^{pc}_{ij} = 0, \quad \bar{\varepsilon}^{pc}_{ij} = \alpha^*_{ij}\theta_0, \tag{11}$$

where α^*_{ij} is the effective thermal expansion tensor of the polycrystal. The determination of α^*_{ij} hinges thus upon the knowledge of the average strain in the polycrystal under the loading (10). Note that this loading may induce slip at the frictionless grain boundaries. To determine the average strain we decompose the loading (10) into two different components:

$$t_i^{(I)}(S) = \hat{\sigma} n_i, \quad \theta^{(I)}(S) = \theta_0,$$
$$t_i^{(II)}(S) = -\hat{\sigma} n_i, \quad \theta^{(II)}(S) = 0, \tag{12}$$

where $\hat{\sigma}$ is given in (7). Under the boundary condition $(12)_1$, the solution is the uniform field solution (9), whereas under $(12)_2$ the average strain is given by

$$\bar{\varepsilon}_{ij}^{(II)} = -S_{ijkl}^{*} \hat{\sigma}\, \delta_{kl}, \tag{13}$$

where S_{ijkl}^{*} is the effective compliance tensor of the polycrystal. Thus, by superposition and use of (11)–(13) together with (9), we obtain:

$$\alpha_{ij}^{*} = [(S_1^c \alpha_{33}^c - S_3^c \alpha_{11}^c)/(S_1^c - S_3^c)]\, \delta_{ij} - S_{ijkk}^{*} (\alpha_{33}^c - \alpha_{11}^c)/(S_1^c - S_3^c). \tag{14}$$

It is thus remarkable that this result is valid *both* for polycrystals with perfectly bonded crystals, and for polycrystals with grain boundary sliding. It should be noted however that the effective compliance of the polycrystal in each case is different, and leads therefore through (14) to a different effective thermal expansion tensor as well.

Next, let us consider a two-dimensional polycrystal, say a polycrystalline thin film, approximated by plane stress conditions

$$\sigma_{i3}^c(\mathbf{x}) = 0, \quad i = 1, 2, 3. \tag{15}$$

Let the crystals be orthotropic with the planar constitutive law being given by:

$$\varepsilon_{11}^c = S_{1111}^c \sigma_{11}^c + S_{1122}^c \sigma_{22}^c + \alpha_{11}^c \theta_0,$$
$$\varepsilon_{22}^c = S_{1122}^c \sigma_{11}^c + S_{2222}^c \sigma_{22}^c + \alpha_{22}^c \theta_0,$$
$$\varepsilon_{12}^c = S_{1212}^c \sigma_{12}^c. \tag{16}$$

The planar effective constitutive law of the polycrystal is represented by

$$\bar{\varepsilon}_{\alpha\beta}^{pc} = S_{\alpha\beta\gamma\delta}^{*} \bar{\sigma}_{\gamma\delta}^{pc} + \alpha_{\alpha\beta}^{*} \theta_0, \tag{17}$$

where the Greek indices assume the values of 1 or 2. This two-dimensional representation may also refer to a generalized plane stress condition of the thin film in which case $\sigma_{\alpha\beta}$ and $\varepsilon_{\alpha\beta}$ stand for average values over the thickness of the film. Alternatively, eqns (16) and (17) may also describe the planar deformation of a polycrystal which is infinitely thick in the x_3 direction, and with plane strain conditions $\varepsilon_{i3} = 0$, $i = 1, 2, 3$. In this latter case the components $S_{\alpha\beta\gamma\delta}$ in (16) and (17) are not identical to those of the $\mathbf{S}$ tensor in its three-dimensional representation, but are obtained through an elimination procedure of the non-vanishing stress σ_{33}. Both of these two-dimensional configurations are to be distinguished from a polycrystal with elongated crystals and stress free ends which is under a generalized plane strain condition, and exhibits an axial displacement in the form $u_3 = \varepsilon_{33}^0 x_3$. A comprehensive study of the bulk and shear modulus of effectively isotropic planar polycrystals with perfect bonding at crystal boundaries has been recently given by Avellaneda *et al.* (1996).

We now consider the polycrystal described by (16), and assume planar slip at some locations of crystal boundaries and perfect bonding at other places. Following the procedure employed in the above three-dimensional case, it is easily proved that the effective planar thermal expansion tensor of the two-dimensional polycrystal, described by (16) and (17), and which exhibits free slip at some of the crystal interfaces, is given by:

$$\alpha^*_{\alpha\beta} = \frac{(S^c_{1111}+S^c_{1122})\alpha^c_{22}-(S^c_{2222}+S^c_{1122})\alpha^c_{11}}{(S^c_{1111}-S^c_{2222})}\delta_{\alpha\beta}-S^*_{\alpha\beta\gamma\gamma}\frac{(\alpha^c_{22}-\alpha^c_{11})}{(S^c_{1111}-S^c_{2222})}. \tag{18}$$

In the derivation of (18), we have first looked for an in-plane loading

$$t_\alpha(S) = \sigma' n_\alpha, \quad t_3(S) = 0, \quad \theta(S) = \theta_0, \tag{19}$$

which result in uniform dilatational planar stress and strain field throughout. Assuming

$$\sigma^c_{\alpha\beta}(\mathbf{x}) = \sigma'\,\delta_{\alpha\beta}, \tag{20}$$

and demanding

$$\varepsilon^c_{11}(\mathbf{x}) = (S^c_{1111}+S^c_{1122})\sigma'+\alpha^c_{11}\theta_0 = \varepsilon^c_{22}(\mathbf{x}) = (S^c_{1122}+S^c_{2222})\sigma'+\alpha^c_{22}\theta_0, \tag{21}$$

readily provides the sought value of σ'. Using the superposition scheme in (12) with this value of σ' leads to eqn (18).

This section is concluded by considering a result obtained by Walpole (1985) for anisotropic polycrystals with cubic crystals, and previously established by Hill (1952) for the case of overall isotropy, and showing that it is *also* valid for polycrystals with frictionless grain boundaries as well. A cubic crystal is characterized by:

$$\mathbf{S}^c = \begin{bmatrix} S_{1111} & S_{1122} & S_{1122} & 0 & 0 & 0 \\ S_{1122} & S_{1111} & S_{1122} & 0 & 0 & 0 \\ S_{1122} & S_{1122} & S_{1111} & 0 & 0 & 0 \\ 0 & 0 & 0 & S_{1212} & 0 & 0 \\ 0 & 0 & 0 & 0 & S_{1212} & 0 \\ 0 & 0 & 0 & 0 & 0 & S_{1212} \end{bmatrix}^c, \quad \alpha^c = \begin{bmatrix} \alpha_{11} \\ \alpha_{11} \\ \alpha_{11} \\ 0 \\ 0 \\ 0 \end{bmatrix}^c. \tag{22}$$

Consider now a polycrystal consisting of cubic crystals, and with the shear traction vanishing at some or all crystal interfaces. Subject the polycrystal to the loading

$$t_i(S) = \bar{\sigma} n_i, \quad \theta(S) = 0, \tag{23}$$

where $\bar{\sigma}$ is a hydrostatic stress. It is readily established that this loading induces in every crystal the following uniform hydrostatic stress and strain field:

$$\sigma^c_{ij}(\mathbf{x}) = \bar{\sigma}\,\delta_{ij}, \quad \varepsilon^c_{ij}(\mathbf{x}) = (S^c_{1111}+2S^c_{1122})\bar{\sigma}\,\delta_{ij} = (1/3\kappa_c)\bar{\sigma}\,\delta_{ij}, \tag{24}$$

where κ_c denotes the bulk modulus of the cubic crystals. These fields do not induce any slip at the frictionless boundaries, so that under (23) the average stress and strain in the polycrystal is also given by (24). Since by definition, however,

$$\bar{\varepsilon}^{pc}_{ij} = S^*_{ijkl}\bar{\sigma}^{pc}_{kl}, \tag{25}$$

it is seen that (24) and (25) imply

$$S^*_{ijkk} = \delta_{ij}/(3\kappa_c). \tag{26}$$

Equation (26) is a constraint condition on the effective compliance of a polycrystal which consists of cubic crystals and may have frictionless grain boundaries at several locations. It turns out that it is identical to that given by Walpole (1985) for the case of perfectly bonded cubic crystals. It is emphasized, however, that in spite of obeying the same form (26), the effective compliance is different in these two cases.

As far as the thermal expansion tensor of the polycrystal with cubic crystals and frictionless grain boundaries is concerned, it is easily observed, as in the case of perfectly bonded crystals, that it is equal to the thermal expansion tensor of the cubic crystals. To see this, we subject the polycrystal to:

$$t_i(S) = 0, \quad \theta(S) = \theta_0, \tag{27}$$

and notice that the stresses vanish throughout, whereas the strains are given by:

$$\varepsilon_{ij}^c(\mathbf{x}) = \alpha_{11}^c \theta_0 \, \delta_{ij}. \tag{28}$$

Thus, clearly,

$$\alpha_{ij}^* = \alpha_{11}^c \, \delta_{ij}. \tag{29}$$

It may be inquired whether the result in (29) can be obtained as a special case of (14) which was derived for the case of tetragonal, hexagonal or trigonal crystals. Obviously, a cubic crystal is a special case of the above classes so that eqn (14) should have a proper reduction in this instance. It is interesting to observe, however, that the apparent indeterminacy of this last equation in the special case of cubic crystals disappears only through the use of (26), after which (29) is readily recovered.

We finally mention that for a planar polycrystal with square symmetric crystals defined by

$$\begin{aligned} \varepsilon_{11}^c &= S_{1111}^c \sigma_{11}^c + S_{1122}^c \sigma_{22}^c + \alpha_{11}^c \theta_0, \\ \varepsilon_{22}^c &= S_{1122}^c \sigma_{11}^c + S_{1111}^c \sigma_{22}^c + \alpha_{11}^c \theta_0, \\ \varepsilon_{12}^c &= S_{1212}^c \sigma_{12}^c, \end{aligned} \tag{30}$$

the equations corresponding to (26) and (29), become

$$S_{\alpha\beta\gamma\gamma}^* = \delta_{\alpha\beta}(S_{1111}^c + S_{1122}^c), \quad \alpha_{\alpha\beta}^* = \alpha_{11}^c \, \delta_{\alpha\beta}. \tag{31}$$

3. POLYCRYSTALS WITH FRICTIONLESS GRAIN BOUNDARIES AND AN INCLUSION PHASE

In this section we consider a polycrystal which, in addition to having frictionless grain boundaries at some locations, contains an inclusion or impurity phase. The question is asked whether a microstructure independent relation for the effective thermal expansion tensor, of the type given in (14), exists for such a polycrystal. For three-dimensional polycrystals, it will be shown that the answer is positive, provided the crystals are cubic and the inclusion phase is cubic or isotropic. For two-dimensional polycrystals in plane stress (or plane strain) conditions, the answer is positive if the crystals are square symmetric, and the inclusion phase is square symmetric or isotropic.

We first consider the three-dimensional polycrystal. The compliance and thermal expansion tensors of the cubic crystals are given by (22). The corresponding tensors of the inclusion phase will be denoted by $\mathbf{S}^p$ and α^p. The inclusion phase is cubic, but its principal directions may be arbitrarily oriented at different locations, so that it can be viewed as a different crystal. Naturally, this phase may be isotropic in which case

$$S_{1212}^p = 2(S_{1111}^p - S_{1122}^p). \tag{32}$$

As in the previous section, we assume that at some locations of the crystal–crystal and crystal–inclusion boundaries perfect bonding may prevail, whereas at others frictionless slip is present. Finally, a porous inclusion phase is obtained by letting $\mathbf{S}^p \to \infty$.

The first step is the search for a specific loading (σ'', θ_0):

$$t_i(S) = \sigma'' n_i, \quad \theta(S) = \theta_0, \tag{33}$$

which results in a hydrostatic stress and strain throughout. Let us assume that

$$\sigma^c_{ij}(\mathbf{x}) = \sigma^p_{ij}(\mathbf{x}) = \sigma''\,\delta_{ij}, \tag{34}$$

and obtain

$$\begin{aligned} \varepsilon^c_{ij}(\mathbf{x}) &= (S^c_{1111}+2S^c_{1122})\sigma''\,\delta_{ij}+\alpha^c_{11}\theta_0\,\delta_{ij}, \\ \varepsilon^p_{ij}(\mathbf{x}) &= (S^p_{1111}+2S^p_{1122})\sigma''\,\delta_{ij}+\alpha^p_{11}\theta_0\,\delta_{ij}. \end{aligned} \tag{35}$$

Demanding

$$\varepsilon^c_{ij}(\mathbf{x}) = \varepsilon^p_{ij}(\mathbf{x}), \tag{36}$$

provides:

$$\sigma'' = (\alpha^p_{11}-\alpha^c_{11})\theta_0/[(S^c_{1111}+2S^c_{1122})-(S^p_{1111}+2S^p_{1122})]. \tag{37}$$

Therefore, under (33), and with σ'' given by (35), the resulting stresses and strains in the polycrystal are hydrostatic and uniform, and summarized by:

$$\begin{aligned} \sigma^c_{ij}(\mathbf{x}) = \sigma^p_{ij}(\mathbf{x}) &= (\alpha^p_{11}-\alpha^c_{11})\theta_0\,\delta_{ij}/[(S^c_{1111}+2S^c_{1122})-(S^p_{1111}+2S^p_{1122})], \\ \varepsilon^c_{ij}(\mathbf{x}) = \varepsilon^p_{ij}(\mathbf{x}) &= \frac{[(S^c_{1111}+2S^c_{1122})\alpha^p_{11}-(S^p_{1111}+2S^p_{1122})\alpha^c_{11}]\theta_0}{(S^c_{1111}+2S^c_{1122})-(S^p_{1111}+2S^p_{1122})}\delta_{ij}. \end{aligned} \tag{38}$$

At this stage it is important to observe that if the crystals had an anisotropy which was higher than that of the cubic class, and the polycrystal contained an inclusion phase which was even isotropic, a hydrostatic uniform state of stress and strain could not have been generated under a loading of the type (33).

The effective thermal expansion tensor of the polycrystal is now obtained by subjecting the polycrystal to the loading in (10), and decomposing this loading in the form of (12), where σ'' replaces now $\hat{\sigma}$. Following the same superposition procedure of the previous section results in the following expression for the thermal expansion coefficient of the polycrystal:

$$\begin{aligned} \alpha^*_{ij} = {} & \frac{(S^c_{1111}+2S^c_{1122})\alpha^p_{11}-(S^p_{1111}+2S^p_{1122})\alpha^c_{11}}{[(S^c_{1111}+2S^c_{1122})-(S^p_{1111}+2S^p_{1122})]}\delta_{ij} \\ & -S^*_{ijkk}\frac{(\alpha^p_{11}-\alpha^c_{11})}{[(S^c_{1111}+2S^c_{1122})-(S^p_{1111}+2S^p_{1122})]}. \end{aligned} \tag{39}$$

The porous polycrystal is obtained by letting $\mathbf{S}^p \to \infty$, and results again in (29). Obviously, this result could also be directly derived by applying (10) to the polycrystal, and observing that a uniform field solution prevails with

$$\sigma^c_{ij}(\mathbf{x}) = 0, \quad \varepsilon^c_{ij}(\mathbf{x}) = \alpha^c_{11}\theta_0\,\delta_{ij}, \tag{40}$$

so that the result in (29) is immediate. Note, however, that this is a strict property of porous polycrystals with cubic crystals which may or may not have frictionless grain boundaries at some locations.

Next we consider a polycrystalline thin film under plane stress conditions and square symmetric crystals, described in (30). The polycrystal contains an inclusion phase which is also square symmetric, and free slip is allowed to occur at arbitrary locations. We subject first the planar polycrystal to a loading in the form

$$t_\alpha(S) = \sigma''' n_\alpha, \quad t_3(S) = 0, \quad \theta(S) = \theta_0, \tag{41}$$

and look for a stress σ''' which results in a uniform dilatational plane fields. Assuming

$$\sigma^c_{\alpha\beta}(\mathbf{x}) = \sigma^p_{\alpha\beta}(\mathbf{x}) = \sigma''' \delta_{\alpha\beta}, \tag{42}$$

and demanding

$$\varepsilon^c_{\alpha\beta}(\mathbf{x}) = (S^c_{1111} + S^c_{1122})\sigma''' \delta_{\alpha\beta} + \alpha^c_{11}\theta_0 \delta_{\alpha\beta} = \varepsilon^p_{\alpha\beta}(\mathbf{x}) = (S^p_{1111} + S^p_{1122})\sigma''' \delta_{\alpha\beta} + \alpha^p_{11}\theta_0 \delta_{\alpha\beta}, \tag{43}$$

readily provides the sought value of σ'''. With this value of σ''', and the superposition scheme in (12), we obtain the following effective planar thermal expansion tensor of the polycrystal

$$\alpha^*_{\alpha\beta} = \frac{\alpha^p_{11}(S^c_{1111} + S^c_{1122}) - \alpha^c_{11}(S^p_{1111} + S^p_{1122})}{(S^c_{1111} + S^c_{1122}) - (S^p_{1111} + S^p_{1122})} \delta_{\alpha\beta} - S^*_{\alpha\beta\gamma\gamma} \frac{\alpha^p_{11} - \alpha^c_{11}}{(S^c_{1111} + S^c_{1122}) - (S^p_{1111} + S^p_{1122})}. \tag{44}$$

4. CONCLUDING REMARKS

As a first remark, it is pointed out that the results in this paper would also continue to be valid if, at some locations of the crystal boundaries, the tangential component of the displacement vector suffers a discontinuity which is proportional to the shear traction there in the form of

$$[\mathbf{u}_t]_\Gamma = \mathbf{k}\mathbf{t}_t \tag{45}$$

where $[\mathbf{u}_t]_\Gamma$ denotes the jump in the tangential displacement vector $\mathbf{u}_t$ at certain locations of the grain boundary denoted by Γ, $\mathbf{t}_t$ is the shear traction, and $\mathbf{k}$ is a second order tensor representing a certain flexibility of that interface. The validity of the claim becomes transparent when it is observed that the hydrostatic state of stress and strain created by a loading of the type (2) and (3) for example, with $\hat{\sigma}$ given by (7), continues to prevail throughout, even if, at some locations of the grain boundaries, conditions of the type (45) are present; eqn (14) is therefore valid in this instance as well. The same conclusion holds for (18), (26), (29), (31), (39), and (44). Making use of the representation of the type in (45) brings in however the important question of a more realistic description of the conditions at the grain boundaries, an issue which we have preferred to avoid in this paper by adhering to the limiting situation of completely relaxed shear stresses at possible locations and putting thus the emphasis on the simplicity, exactness, and microstructure independent property of the derived relations.

As a second remark, it is observed that the key to the derivation of the microstructure independent relations in the present paper has been the possibility of finding a very specific external loading which generates in the polycrystal a hydrostatic uniform state of stress and strain throughout in the three-dimensional case, and a planar dilatational one in the two-dimensional case. The necessity of this requirement has limited the existence of (14), for instance, to the case of tetragonal, hexagonal or trigonal crystals; similar limitations on the admissible symmetry classes of the constituent crystals and inclusion phase are present for the other connections. In this regard, it is noted that given a polycrystal with crystals having a higher anisotropy than that of the tetragonal class, one can devise certain artificial restrictions among the crystal properties which would allow to derive microstructure independent relations for the effective properties of polycrystals. As pointed out by Avellaneda *et al.* (1996), the value of the exact formulae in these cases would only lie in the fact that they would provide a stringent test for several possible approximate methods. Consider, for example, a three-dimensional anisotropic polycrystal with orthorhombic crystals defined by

$$\mathbf{S}^c = \begin{bmatrix} S_{1111} & S_{1122} & S_{1133} & 0 & 0 & 0 \\ S_{1122} & S_{2222} & S_{2233} & 0 & 0 & 0 \\ S_{1133} & S_{2233} & S_{3333} & 0 & 0 & 0 \\ 0 & 0 & 0 & S_{3232} & 0 & 0 \\ 0 & 0 & 0 & 0 & S_{3131} & 0 \\ 0 & 0 & 0 & 0 & 0 & S_{1212} \end{bmatrix}^c, \quad \alpha^c = \begin{bmatrix} \alpha_{11} \\ \alpha_{22} \\ \alpha_{33} \\ 0 \\ 0 \\ 0 \end{bmatrix}^c. \tag{46}$$

Let us, however, artificially demand that

$$S^c_{1111} + S^c_{1133} = S^c_{2222} + S^c_{2233}, \quad \alpha^c_{11} = \alpha^c_{22}. \tag{47}$$

Frictionless grain boundaries are again assumed to be present at possible locations. It is readily observed that application of (2) and (3) to this polycrystal results in a uniform hydrastatic stress and strain field if $\hat{\sigma}$ is given by (7) with S^c_1 still being defined by $(8)_1$, but S^c_3 being replaced by:

$$S^c_3 = S^c_{1133} + S^c_{2233} + S^c_{3333}. \tag{48}$$

With the restriction in (47), the microstructure independent relation (14) continues now to be valid for the case in which the crystal properties are given in (46).

Similarly, if in (46) one has

$$S^c_{1111} + S^c_{1122} + S^c_{1133} = S^c_{1122} + S^c_{2222} + S^c_{2233} = S^c_{1133} + S^c_{2233} + S^c_{3333}, \tag{49}$$

then a constrain condition of the type (26) for the components of the compliance tensor can be derived for this polycrystal. Such results, based on suitable restrictions on the constituent properties, can also be obtained for polycrystals containing an inclusion phase but will not be pursued further here.

It should finally be noted that the thermoelastic behaviour of a solid can be expressed in terms of the stiffness and thermal stress tensors $(\mathbf{L}, \beta)$ instead of the $(\mathbf{S}, \alpha)$ tensors adopted in the present paper. Although a passage from one set of variables to the other is always possible, since this involves an inversion operation of tensors it is not clear whether simple expressions of the type derived here in the $(\mathbf{S}, \alpha)$ setting will result in similarly simple expressions in $(\mathbf{L}, \beta)$. It can be shown however that independent derivation in this latter set of variables, which turns out to be fully dual to that in the present paper, can be given by applying, in the three-dimensional case for example, boundary conditions of the type

$$u_i(S) = \hat{\varepsilon} x_i, \quad \theta(S) = \theta_0, \tag{50}$$

instead of (2) and (3), and looking for a strain $\hat{\varepsilon}$ which would result in uniform hydrostatic stress and strain fields throughout. For the sake of brevity we have not given the details of this derivation, but simply indicate here that there is a one to one correspondence between the derived relations and their counterparts in the $(\mathbf{L}, \beta)$ variables; the components of $\mathbf{S}$ and α in the derived relations have to be replaced by the same components of $\mathbf{L}$ and β.

Some care is needed, however, in handling the relations concerning the plane polycrystal; specifically, if eqns (16) and (17), for example, are meant to refer to the plane stress conditions, then the corresponding equations arrived at by the replacement procedure will refer to the plane strain case. It is important to emphasize here that a one to one correspondence between any kind of relations in the $(\mathbf{S}, \alpha)$ and $(\mathbf{L}, \beta)$ variables *should not be taken for granted*, and is not present, as a matter of fact, in the connections derived by the author (Benveniste (1996)) for the case of a polycrystal which consists of elongated crystals and cylindrical inclusions and is in a state of generalized plane strain. The reason behind the existence of a one to one correspondence in the case of the relations derived in this paper lies in the fact that the fields which have led to the derivation of these connections are uniform *both* in the strains and stresses, as in (9) for instance.

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