Available online at www.sciencedirect.com
SCIENCE DIRECT®
ELSEVIER
C. R. Mecanique 331 (2003) 623–629
COMPTES RENDUS MECANIQUE

Characterization of a class of polycrystals whose effective elastic bulk moduli can be exactly determined

Qi-Chang He

Laboratoire de mécanique, Université de Marne-la-Vallée, 19, rue A. Nobel, 77420 Champs sur Marne, France

Received 3 June 2003; accepted after revision 9 July 2003

Presented by André Zaoui

Abstract

Necessary and sufficient conditions are established for the stress response of a linearly elastic material to an isotropic stain to be hydrostatic. In the 3D case, these conditions are satisfied not only by the isotropic and cubic materials but also by all other anisotropic materials provided appropriate restrictions are imposed. In the 2D case, only the isotropic and square materials have an isotropic stress response to an isotropic strain. Using a uniform field argument, the elastic bulk modulus of a polycrystal consisting of monocrystals compatible with the established conditions is shown to equal that of any constituent monocrystal. Thus, Hill's relevant result about a polycrystal composed of cubic monocrystals is generalized. ***To cite this article: Q.-C. He, C. R. Mecanique 331 (2003).***

Résumé

Caractérisation d'une classe de polycristaux dont les modules de compression isotrope effectifs peuvent exactement être déterminés. Les conditions nécessaires et suffisantes sont établies pour que la réponse en contrainte d'un matériau élastique linéaire à une déformation isotrope soit hydrostatique. Dans le cas 3D, ces conditions sont satisfaites non seulement par les matériaux isotropes et cubiques mais aussi par d'autres matériaux anisotropes si des restrictions appropriées sont imposées. Dans le cas 2D, les matériaux isotropes et à symétrie carrée sont les seuls pouvant avoir une réponse isotrope à une sollicitation isotrope. Utilisant un argument de champs uniformes, il est montré que le module de compression isotrope d'un polycristal composé de monocristaux compatibles avec les conditions établies est égal à celui d'un monocristal constituant quelconque. Ceci généralise le résultat de Hill établi pour un polycristal constitué de monocristaux cubiques. ***Pour citer cet article : Q.-C. He, C. R. Mecanique 331 (2003).***

Keywords: Computational solid mechanics; Anisotropic elasticity; Uniform hydrostatic stress; Bulk modulus; Polycrystals; Micromechanics

Mots-clés : Mécanique des solides numérique ; Elasticité anisotrope ; Contrainte hydrostatique uniforme ; Module de compression ; Polycristaux ; Micromécanique

E-mail address: he@univ-mlv.fr (Q.-C. He).

1631-0721/$ – see front matter
doi:10.1016/S1631-0721(03)00148-7

Version française abrégée

En 1952, Hill [1] a découvert que le module de compression isotrope effectif $\bar{\kappa}$ d'un polycristal constitué de monocristaux cubiques peut être exactement déterminé indépendamment des orientations de ces derniers et que, plus précisément, $\bar{\kappa}$ est égal au module de compression isotrope d'un monocristal constituant quelconque. L'objectif principal de ce travail est d'étendre le résultat de Hill à des polycristaux composés de monocristaux autres que les monocristaux cubiques. La clé pour atteindre cet objectif réside dans l'établissement des conditions nécessaires et suffisantes pour que la réponse d'un matériau élastique linéaire à une sollicitation isotrope soit isotrope et dans l'identification des symétries matérielles compatibles avec les conditions établies.

Le matériau considéré est élastique linéaire homogène. Le tenseur de contrainte S est lié au tenseur de déformation E par l'Éq. (1) dans laquelle $\mathbf{K}$ est le tenseur de rigidité élastique possédant les symétries indicielles habituelles (2). Ces dernières permettent d'écrire (1) sous la forme matricielle (3). Pour que la réponse en contrainte du matériau à une déformation isotrope soit hydrostatique, la satisfaction de l'Éq. (4) est à la fois nécessaire et suffisante et conduit aux conditions (5) recherchées. Autrement dit, la réponse du matériau à une sollicitation isotrope est isotrope si et seulement si les 5 conditions définies par (5) sont vérifiées.

Ensuite, les conditions (5) sont exploitées pour chacune des 8 symétries élastiques tridimensionnelles (3D) possibles [7]. Quand le matériau est isotrope ou cubique, les conditions (5) sont automatiquement satisfaites. Si le matériau est orthotrope de révolution ou tétragonal ou trigonal, elles se réduisent à une seule condition (6). Dans le cas orthotrope, les conditions (5a) sont seulement nécessaires et suffisantes. Quand le matériau est monoclinique, il faut imposer (5a) et (7). Dans le cas triclinique général, nous retrouvons les conditions (5). La forme particulière (8) de $\mathbf{K}$ permet à $\mathbf{K}$ de rester triclinique et de vérifier (5), constituant ainsi une condition suffisante.

S'agissant de l'élasticité linéaire bidimensionnelle (2D) caractérisée par (9), notre problème consiste à exiger que la réponse en contrainte du matériau à une déformation équibiaxiale soit aussi équibiaxiale. Ce problème est formulé par (10) conduisant aux conditions nécessaires et suffisantes (11). En élasticité 2D, il y a seulement 4 symétries possibles [8]. En examinant ces symétries, nous arrivons à la conclusion que, contrairement aux résultats 3D trouvés, un matériau élastique linéaire 2D satisfaisant les conditions (11) est nécessairement isotrope ou de symétrie carrée.

Soit un polycristal constitué d'un nombre fini de monocristaux ayant les mêmes propriétés élastiques à des rotations près mais pouvant avoir des formes géométriques différentes. Soit $\mathbf{K}$ le tenseur de rigidité d'un monocristal constituant. Alors, le tenseur de rigidité $\mathbf{K}^{(p)}$ d'un monocristal p, est lié à $\mathbf{K}$ par (12). Le tenseur $R^{(p)}$ décrit la rotation du monocistal p par rapport au monocristal de référence et $\mathbf{R}^{(p)}$ correspond au tenseur de rotation d'ordre 4 induit par $R^{(p)}$. Quand $\mathbf{K}$ satisfait les conditions (5), le module de compression isotrope défini par (13) a l'expression (14) et l'Éq. (15) s'ensuit. Grâce à cette dernière, une déformation macroscopique isotrope engendre un champ de déformation locale isotrope uniforme et un champ de contrainte locale isotrope uniforme dans le polycristal. Par conséquent, le module de compression isotrope effectif $\bar{\kappa}$ de ce dernier est égal au module de compression isotrope κ d'un monocristal constituant quelconque, c'est-à-dire que nous avons la formule (16). Ainsi, le résultat de Hill susmentionné est généralisé à des polycristaux constitués de monocristaux qui ne sont pas nécessairement cubiques.

1. Introduction

As early as 1952, Hill [1] discovered that the effective (or macroscopic) elastic bulk modulus $\bar{\kappa}$ of a polycrystal consisting of cubic monocrystals can exactly be determined regardless of their orientations and, more precisely, is equal to the elastic bulk modulus κ of any constituent cubic monocrystal. The crucial observation leading to this remarkable microstructure-independent exact result is that the linearly elastic stress (strain) response of a cubic monocrystal to an isotropic strain (stress) loading is isotropic owing to the existence of three equivalent perpendicular material symmetry planes.

Recently, the aforementioned Hill's result has been rediscovered while being framed either within a general theory of uniform fields or in a general theory of exact relations (see [2–5] and the relevant references cited therein). Recently, He and Bary [6] have extended it to polycrystals made up of nonlinearly cubic monocrystals. However, even in the linearly elastic case, the problem remains open of whether it is possible to exactly determine the effective bulk modulus of a polycrystal consisting of monocrystals which do not present three equivalent perpendicular material symmetry planes. The main purpose of this work is to give an answer to this question.

The key to achieving our purpose resides in establishing necessary and sufficient conditions for a linearly elastic material to respond isotropically to an isotropic strain or stress, and in identifying what material symmetries are compatible with them. After finding three-dimensional (3D) necessary and sufficient conditions in Section 2, it is shown in Section 3 that, in addition to the isotropic and cubic materials, all other 3D anisotropic materials have the possibility of exhibiting an isotropic response to an isotropic loading. However, in the context of two-dimensional (2D) linear elasticity, it is shown in Section 4 that no materials other than the isotropic and square materials can have an isotropic response to an isotropic loading. Using a uniform field argument in Section 5, it is concluded that the effective elastic bulk modulus $\bar{\kappa}$ of any polycrystal made up of monocrystals consistent with the 3D necessary and sufficient conditions of Section 2 is equal to the elastic bulk modulus κ of any constituent monocrystal.

The notation adopted in this work is as follows. Scalars are denoted by Greek letters, and vectors by bold-face lower case Latin letters. Second- and fourth-order tensors are designated by light- and bold-face lower case Latin letters, respectively. The components of a vector, second- or fourth-order tensor are represented by the corresponding light-face letter with a suitable number of subscripts. In addition, use is made of the Kronecker tensor product $A\underline{\otimes}B$ of two second-order tensors A and B defined by $(A\underline{\otimes}B)_{ijkl} = (A_{ik}B_{jl} + A_{il}B_{jk})/2$.

2. Three-dimensional necessary and sufficient conditions

Consider a linearly elastic homogeneous material whose stress-strain relation is given by

$$S = \mathbf{K}E \tag{1}$$

where E is the (infinitesimal) strain tensor, S the (Cauchy) stress tensor and $\mathbf{K}$ the elastic stiffness tensor. Relative to a three-dimensional orthonomal basis $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$, the components K_{ijmn} of $\mathbf{K}$ have the usual minor and major symmetries

$$K_{ijmn} = K_{jimn} = K_{mnij} \tag{2}$$

The major symmetry $K_{ijmn} = K_{mnij}$ implies that hyperelasticity is concerned. In addition, $\mathbf{K}$ is assumed to be positive definite and bounded. Accounting for (2), it is convenient to express (1) in the following matrix form:

$$\begin{bmatrix} S_1 \\ S_2 \\ S_3 \\ \sqrt{2}S_4 \\ \sqrt{2}S_5 \\ \sqrt{2}S_6 \end{bmatrix} = \begin{bmatrix} K_{11} & K_{12} & K_{13} & \sqrt{2}K_{14} & \sqrt{2}K_{15} & \sqrt{2}K_{16} \\ K_{12} & K_{22} & K_{23} & \sqrt{2}K_{24} & \sqrt{2}K_{25} & \sqrt{2}K_{26} \\ K_{13} & K_{23} & K_{33} & \sqrt{2}K_{34} & \sqrt{2}K_{35} & \sqrt{2}K_{36} \\ \sqrt{2}K_{14} & \sqrt{2}K_{24} & \sqrt{2}K_{34} & 2K_{44} & 2K_{45} & 2K_{46} \\ \sqrt{2}K_{15} & \sqrt{2}K_{25} & \sqrt{2}K_{35} & 2K_{45} & 2K_{55} & 2K_{56} \\ \sqrt{2}K_{16} & \sqrt{2}K_{26} & \sqrt{2}K_{36} & 2K_{46} & 2K_{56} & 2K_{66} \end{bmatrix} \begin{bmatrix} E_1 \\ E_2 \\ E_3 \\ \sqrt{2}E_4 \\ \sqrt{2}E_5 \\ \sqrt{2}E_6 \end{bmatrix} \tag{3}$$

where the subscripts are identified as $1 \equiv 11,\ 2 \equiv 22,\ 3 \equiv 33,\ 4 \equiv 23,\ 5 \equiv 31$ and $6 \equiv 12$.

Let the material undergo an isotropic strain $E = \varepsilon I$ with I being the second-order identity tensor and ε a scalar. Except if the material is isotropic or cubic, the resulting stress response is generally not hydrostatic, i.e., $S \neq \sigma I$ with σ a scalar. In the present work, we look for particular anisotropic materials, in addition to the cubic one, such that their stress response to an isotropic strain is indeed hydrostatic. This implies that the stiffness tensor $\mathbf{K}$ must have the property that $\mathbf{K}(\varepsilon I) = \sigma I$, i.e.,

$$\mathbf{K}I = 3\kappa I \tag{4}$$

where $\kappa = \sigma/(3\varepsilon)$ represents the bulk modulus. This is an eigenvalue problem requiring that the second-order identity tensor I be an eigentensor of $\mathbf{K}$. Using the matrix components of $\mathbf{K}$ as in (3), it is immediate that (4) holds if and only if

$$K_{11} + K_{12} + K_{13} = K_{12} + K_{22} + K_{23} = K_{13} + K_{23} + K_{33} \tag{5a}$$

$$K_{14} + K_{24} + K_{34} = 0, \qquad K_{15} + K_{25} + K_{35} = 0, \qquad K_{16} + K_{26} + K_{36} = 0 \tag{5b}$$

These 5 conditions characterize all linearly elastic materials such that their stress response to an isotropic strain is also isotropic. As a direct consequence, any material satisfying (5) cannot have more than 16 independent elastic moduli. Recall that its stiffness tensor $\mathbf{K}$ must additionally be positive definite and bounded.

3. Specification of 3D necessary and sufficient conditions for each elastic symmetry

In [7], it was proved that there are only 8 possible symmetry classes for all 3D elastic tensors: isotropic, transversely isotropic, cubic, tetragonal, orthotropic, trigonal, monoclinic and triclinic. For each of these 8 symmetry classes, the non-zero matrix components of $\mathbf{K}$ relative to a privileged axis system and the relations between them can also be found in [7]. Now we proceed to examine the necessary and sufficient conditions (5) for every symmetry class.

In the *isotropic* case, the conditions (5) are trivially satisfied for the non-zero components of $\mathbf{K}$ which are $K_{11} = K_{22} = K_{33},\ K_{12} = K_{13} = K_{23}$ and $K_{44} = K_{55} = K_{66} = (K_{11} - K_{12})/2$. In the *cubic* case, the non-zero components of $\mathbf{K}$ relative its symmetry axe system are $K_{11} = K_{22} = K_{33},\ K_{12} = K_{13} = K_{23}$ and $K_{44} = K_{55} = K_{66}$, so that the conditions (5) are also directly verified. It is a basic result of linear elasticity that the stress response of an isotropic or a cubic material to an isotropic strain is hydrostatic.

Given a *transversely isotropic* material, the basis unit vector $\mathbf{e}_3$ can be chosen to characterize the rotational symmetry axe without loss of generality. Correspondingly, the non-zero components of $\mathbf{K}$ are $K_{11} = K_{22},\ K_{33},\ K_{12},\ K_{13} = K_{23},\ K_{44} = K_{55}$ and $K_{66} = (K_{11} - K_{12})/2$. The conditions (5) are simplified into

$$K_{11} + K_{12} = K_{13} + K_{33} \tag{6}$$

This condition reduces the number of independent material parameters from 5 to 4 but does not change the transversely isotropic character of the material.

When a material is *tetragonal*, the non-zero components of $\mathbf{K}$ relative to an appropriate system of axes are $K_{11} = K_{22},\ K_{33},\ K_{12},\ K_{13} = K_{23},\ K_{44} = K_{55}$ and K_{66}, the conditions (5) reduce also to Eq. (6). Thus, we see that the necessary and sufficient condition is the same for the transversely isotropic and tetragonal materials. However, note that the number of independent material parameters is reduced from 6 to 5 in the tetragonal situation.

If a material is *orthotropic* with respect to the planes normal to the basis vectors $\mathbf{e}_1,\ \mathbf{e}_2$ and $\mathbf{e}_3$, the non-zero components of $\mathbf{K}$ are $K_{ij}\ (i, j = 1, 2, 3)$ and $K_{\alpha\alpha}\ (\alpha = 4, 5, 6)$. In this case, the two conditions in (5a) constitute the searched necessary and sufficient conditions while preserving the orthotropic character of the material. The number of independent material parameters becomes 7.

Consider a general *trigonal* material whose non-zero components of $\mathbf{K}$ are $K_{11} = K_{22},\ K_{33}, K_{12},\ K_{13} = K_{23},\ K_{44} = K_{55},\ K_{66} = (K_{11} - K_{12})/2$ and $K_{15} = -K_{25} = -K_{46}$. Then, the conditions (5b) are automatically satisfied while the conditions (5a) reduce to (6). When the latter holds, the number of independent material parameters becomes 5 and the trigonal character is conserved.

Let be given a general *monoclinic* material for which the zero component of $\mathbf{K}$ are $K_{14} = K_{15} = K_{24} = K_{25} = K_{34} = K_{35} = K_{46} = K_{56} = 0$. In this case, the conditions (5) are simplified into (5a) and

$$K_{16} + K_{26} + K_{36} = 0 \tag{7}$$

So, three conditions are to be verified and reduce the number of independent material parameters from 13 to 10. A particularly simple monoclinic material fulfilling the three conditions is the one such that the non-zero components of $\mathbf{K}$ are $K_{11} = K_{22} = K_{33},\ K_{12} = K_{13} = K_{23},\ K_{44},\ K_{55},\ K_{66}$ and K_{45}.

The conditions (5) are necessary and sufficient conditions for a general *triclinic* (or *totally anisotropic*) material. We observe that the lower right corner 3×3 matrix of $\mathbf{K}$ in (3) is not involved in the conditions (5). Then, simple sufficient conditions for (5a) and (5b) to hold trivially consist in prescribing the matrix of $\mathbf{K}$ as follows:

$$[\mathbf{K}] = \begin{bmatrix} K_{11} & K_{12} & K_{12} & 0 & 0 & 0 \\ K_{12} & K_{11} & K_{12} & 0 & 0 & 0 \\ K_{12} & K_{12} & K_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & 2K_{44} & 2K_{45} & 2K_{46} \\ 0 & 0 & 0 & 2K_{45} & 2K_{55} & 2K_{56} \\ 0 & 0 & 0 & 2K_{46} & 2K_{56} & 2K_{66} \end{bmatrix} \tag{8}$$

In this expression, the upper left corner 3×3 matrix of $\mathbf{K}$ is identical to the corresponding one for a cubic material. However, if $K_{11},\ K_{12},\ K_{44},\ K_{55},\ K_{66},\ K_{45},\ K_{46}$ and K_{56} are 8 independent material parameters, the symmetry group of $\mathbf{K}$ can be shown to be $\{I,\ -I\}$ so that the triclinic character of $\mathbf{K}$ is not destroyed by a reduction of the number of independent material parameters.

It is clear from the foregoing discussion that, in addition to the isotropic and cubic materials, all other linearly elastic materials can exhibit an isotropic stress response to an isotropic strain provided appropriate conditions are imposed to some elastic moduli. This conclusion, which seems not to have been reported in the literature, is the key to the extension of Hill's result about the effective elastic bulk modulus of polycrystals made up of cubic monocrystals.

4. Two-dimensional necessary and sufficient conditions

All the foregoing results are relevant to three-dimensional linear elasticity. It is useful to obtain the corresponding results for two-dimensional linear elasticity. In the latter case, the general stress-strain relation takes the following matrix form:

$$\begin{bmatrix} S_1 \\ S_2 \\ \sqrt{2}S_6 \end{bmatrix} = \begin{bmatrix} K_{11} & K_{12} & \sqrt{2}K_{16} \\ K_{12} & K_{22} & \sqrt{2}K_{26} \\ \sqrt{2}K_{16} & \sqrt{2}K_{26} & 2K_{66} \end{bmatrix} \begin{bmatrix} E_1 \\ E_2 \\ \sqrt{2}E_6 \end{bmatrix} \tag{9}$$

The 2D counterpart of the eigenvalue problem (4) is given by

$$\mathbf{K1} = 2\kappa \mathbf{1} \tag{10}$$

where $\mathbf{1}$ denotes the 2D second-order identity tensor and κ is to be interpreted as the area modulus. In fact, Eq. (10) requires the response of a material to an equibiaxial strain to be an equibiaxial stress in the plane under consideration. For (10) to hold, it is necessary and sufficient that

$$K_{11} = K_{22} \tag{11a}$$

$$K_{16} + K_{26} = 0 \tag{11b}$$

These conditions are much simpler than the 3D necessary and sufficient conditions (5).

As in Section 3, let us examine the conditions (11) relative to every 2D elastic symmetry. In [8], He and Zheng proved that there are only 4 possible 2D elastic symmetries, which are isotropic, square, orthotropic and biclinic. In the *isotropic* and *square* cases, the conditions (11) are automatically fulfilled because $K_{11} = K_{22}$ and $K_{16} = K_{26} = 0$ by choosing an appropriate axis system for the square case. In the *orthotropic* case, (11b) is satisfied since $K_{16} = K_{26} = 0$, while (11a) needs being imposed. However, when $K_{11} = K_{22}$ and $K_{16} = K_{26} = 0,\ \mathbf{K}$ becomes square. So, a 2D orthotropic material verifying the conditions (11) is necessarily square. In the biclinic case, both (11a) and (11b) have to be imposed. Nevertheless, if (11a) and (11b) are effectively satisfied, it has been shown in [8] that there exits a rotation about the basis vector $\mathbf{e}_3$ by which the matrix components $K'_{\alpha\beta}$ of $\mathbf{K}$ relative to the rotated basis vectors $\{\mathbf{e}'_1, \mathbf{e}'_2\}$ are such that $K'_{11} = K'_{22}$ and $K'_{16} = K'_{26} = 0$, and $\mathbf{K}$ becomes also square.

Hence, we arrive at the conclusion that, in 2D linear elasticity, apart from the isotropic and square materials, there are no other materials such that their response to an equibiaxial loading is equibiaxial. This 2D conclusion contrasts sharply with the 3D results obtained in Section 3.

5. Effective elastic bulk moduli of a class of polycrystals

Now we consider a polycrystal consisting of a finite number n of monocrystals which have the same elastic properties to within some rotations, but which can take different geometrical forms. The interfaces between the monocrystals are assumed to be perfect. Let $\mathbf{K}$ denote the elastic stiffness tensor of a monocrystal whose orientation is taken to be the reference one. Then, the elastic stiffness tensor $\mathbf{K}^{(p)}$ of any constituent monocrystal, say monocrystal p with $1 \leqslant p \leqslant n$, is related to $\mathbf{K}$ by

$$\mathbf{K}^{(p)} = \mathbf{R}^{(p)}\mathbf{K}\mathbf{R}^{(p)\mathrm{T}} \quad \text{with } \mathbf{R}^{(p)} = R^{(p)}\underline{\overline{\otimes}}R^{(p)}, \mathbf{R}^{(p)\mathrm{T}} = R^{(p)\mathrm{T}}\underline{\overline{\otimes}}R^{(p)\mathrm{T}} \tag{12}$$

Above $R^{(p)}$ is the second-order tensor defining the rotation of monocrystal p relative to the reference monocrystal, and $R^{(p)\mathrm{T}}$ is the transposition of $R^{(p)}$.

We are interested in the case when the elastic stiffness tensor $\mathbf{K}$ satisfies the conditions (5). Then, Eq. (4) holds with κ being given by

$$\kappa = \frac{1}{9}\,\mathrm{tr}(\mathbf{K}I) = \frac{1}{9}(I : \mathbf{K}I) \tag{13}$$

This is an invariant (and the only linear invariant) of $\mathbf{K}$ under every all rotations. Accounting for the hypothesis that the conditions (5a) are verified, it follows from (13) that

$$\kappa = \frac{1}{3}(K_{11} + K_{12} + K_{13}) = \frac{1}{3}(K_{12} + K_{22} + K_{23}) = \frac{1}{3}(K_{13} + K_{23} + K_{33}) \tag{14}$$

More importantly, using Eqs. (4) and (12) and the formula $(A\underline{\overline{\otimes}}B)E = AEB^{\mathrm{T}}$ for any second-order symmetric tensor E, we obtain

$$\mathbf{K}^{(p)}I = 3\kappa I \tag{15}$$

for any constituent monocrystal p.

Next, consider the domain Ω occupied by a polycrystalline aggregate and impose on its boundary $\partial\Omega$ a uniform displacement boundary condition $\mathbf{u}(\mathbf{x}) = \overline{E}\mathbf{x}$ with $\overline{E} = \bar{\varepsilon}I$ being an isotropic macroscopic strain. Owing to (15), the linear displacement field $u(\mathbf{x}) = \bar{\varepsilon}\mathbf{x}$ and the uniform strain and stress fields $E(\mathbf{x}) = \bar{\varepsilon}I$ and $S(\mathbf{x}) = 3\kappa\bar{\varepsilon}I$ constitute a solution to the corresponding simple boundary value problem, and this solution is known to be unique. So, the macroscopic stress $\overline{S}$ is isotropic and given by $\overline{S} = 3\kappa\bar{\varepsilon}I$. Thus, we conclude that the effective elastic bulk modulus $\bar{\kappa}$ of the polycrystalline aggregate equals the bulk modulus of any constituent monocrystal:

$$\bar{\kappa} = \kappa \tag{16}$$

From the discussion of Section 3, it is clear that this result is valid not only for the polycrystals composed of cubic monocrystals but also for the polycrystals consisting of either transversely isotropic or tetragonal or orthotropic or trigonal or monoclinic or even triclinic monocrystals consistent with the conditions (5). Thus, the well-known result of Hill [1] is generalized to a large class of polycrystals.

6. Closing comments

Although motivated by the wish to characterize polycrystals such that their effective elastic bulk moduli can be exactly determined, the results presented in Sections 2 and 3 have wider usefulness. For example, in the well-known two-phase coated sphere assemblage model of Hashin [9], the materials constituting the core and the spherical shell are both assumed to be isotropic. Using the results of Sections 2 and 3, we see that, with no effect on Hashin's formula for the effective elastic bulk modulus, the core material can in fact be any material compatible with the conditions (5) and may in particular be totally anisotropic. Nevertheless, from a practical standpoint, it remains to clarify how closely some real anisotropic materials, different from the cubic materials, can verify the conditions (5).

References

[1] R. Hill, The elastic behavior of a crystalline aggregate, Proc. Phys. Soc. London Ser. A 65 (1952) 349–354.
[2] Y. Grabovsky, Exact relations for effective tensors of polycrystals. I. Necessary conditions, Arch. Rational Mech. Anal. 143 (1998) 309–330.
[3] Y. Grabovsky, D.S. Sage, Exact relations for effective tensors of polycrystals. II. Applications to elasticity and piezoelectricity, Arch. Rational Mech. Anal. 143 (1998) 331–356.
[4] Y. Grabovsky, G.W. Milton, D.S. Sage, Exact relations for effective tensors of composites: necessary and sufficient conditions, Comm. Pure Appl. Math. 53 (2000) 300–353.
[5] G.W. Milton, The Theory of Composites, Cambridge University Press, Cambridge, 2002.
[6] Q.-C. He, B. Bary, Exact relations for the effective properties of nonlinear elastic inhomogeneous materials, J. Multiscale Comput. Eng. (2003), in press.
[7] S. Forte, M. Vialleno, Symmetry classes for elasticity tensors, J. Elasticity 43 (1996) 81–108.
[8] Q.-C. He, Q.-S. Zheng, On the symmetries of 2D elastic and hyperelastic tensors, J. Elasticity 43 (1996) 203–225.
[9] Z. Hashin, The elastic moduli of heterogeneous materials, J. Appl. Mech. 29 (1962) 143–150.