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ELASTIC CONSTANTS AND THERMAL EXPANSION AVERAGES OF A NONTEXTURED POLYCRYSTAL

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This paper gives expressions for the overall average elastic constants and thermal expansion coefficients of a polycrystal in terms of its single crystal components. The polycrystal is assumed to be statistically homogeneous, isotropic, and perfectly disordered. Upper and lower bounds for the averages are easily found by assuming a uniform strain or stress. The upper bound follows from Voigt's assumption that the total strain is uniform within the polycrystal while the lower bound follows from Reuss' original assumption that the stress is uniform. A self-consistent estimate for the averages can be found if it is assumed that the overall response of the polycrystal is the same as the average response of each crystallite. The derivation method is based on Eshelby's theory of inclusions and inhomogeneities. We define an equivalent inclusion, which gives an expression for the strain disturbance of the inhomogeneity when external fields are applied. The equivalent inclusion is then used to represent the crystallites. For the self-consistent model the average response of the grains has to be the same as the overall response of the material, or the average strain disturbance must vanish. The result is an implicit equation for the average polycrystal elastic constants and an explicit equation for the average thermal expansion coefficients. For the particular case of cubic symmetry the results can be reduced to a cubic equation for the self-consistent shear modulus. For lower symmetry crystals it is best to calculate the self-consistent bulk and shear modulus numerically.

Introduction

A polycrystal, whose properties vary in a complicated fashion from point to point over a small microscopic length scale, may appear on average to be uniform or perhaps, more generally, its properties appear to vary smoothly. The determination of such overall properties from the properties and geometrical arrangement of the constituent monocrystal grains is our aim. In the simplest case the polycrystal is assumed to be statistically homogeneous, isotropic, and perfectly disordered. General expressions for averages can then be derived. Many different properties can be averaged, such as dielectric constants, diffusivity, elastic constants, electrical conductivity, magnetic permeability, magnetostriction, piezoelectric constants, thermal conductivity, or thermal expansion. In this paper we treat the elastic constants, which have already received more attention than most other physical properties, and the thermal expansion.

Elastic constants are fundamental physical data needed for the characterization of materials. In addition to their fundamental importance, elastic constants and properties derived from them are used as the starting point for the mechanical design of almost all products. Theoretical averaging methods for the calculation of the isotropic elastic constants of a polycrystal from the single crystal constants of

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its grains go back more than 100 years. Voigt [1887] assumed that the strain is constant throughout the polycrystal and he obtained a simple approximate solution. Many years later Reuss [1929] found a solution by assuming that the stress is constant. Hill [1952] showed that these two solutions provided upper and lower bounds of the possible average constants. In 1958 Kröner proposed a self-consistent theory and derived the self-consistent shear modulus of a cubic polycrystal, and Tomé [1998] showed how to incorporate the effect of thermal expansion into these models.

In this paper we develop a consistent intuitive notation to describe the concepts that have arisen in the field. The above developments are reviewed in this framework and additional results are presented. We try to keep the notation as clear as possible in the sometimes detailed calculations. Our major aim is to show how the relevant equations can be used to calculate explicit results; we give only selected results and refer to the literature for exhaustive listings. In this sense our paper has the character of a primer.

Relations for material properties are frequently expressed in terms of tensor equations, because tensors have clear rules for coordinate transformations and rotations. However, the relations are also frequently expressed in terms of matrices, because matrices allow straightforward mathematical calculations. The two methods can be used in parallel and are related to each other. We use both in this paper and represent them in symbolic form.

The analysis starts by defining the concept of an *effective medium*, which is a model that approximates the average state of the polycrystal and describes its average properties. In terms of this effective medium we can define *effective elastic constants*, which relate the average stress to the average strain in the effective medium. We can also define an *effective thermal expansion coefficient*. Various theories then derive effective properties as averages over crystallographic properties. The Voigt and Reuss models provide special cases of such an effective medium and the resulting effective properties give upper and lower bounds.

To get explicit scalar expressions for the effective properties from the symbolic equations we use the linear tensor invariants. The fundamental property of a tensor invariant is that it is independent of rotation in space and therefore isotropic. Hence the invariant is equal to its average. This method is used to derive explicit expressions for the effective elastic constants and thermal expansion coefficient in the simple theories.

Eshelby's theory of elastic inclusions and inhomogeneities is used to derive a self-consistent model. This is the method that was first used by Kröner [1958] to solve for the cubic polycrystal. There is, however, a more powerful and fundamental method to derive self-consistent estimates called *statistical continuum mechanics*, which we do not use in this paper. In an applied stress field, the inhomogeneity looks like an inclusion. We introduce the *equivalent inclusion* to determine the stress disturbance of the homogeneity by using the result of the inclusion. This allows us to solve for the strain disturbance of the inhomogeneity in an applied field.

The self-consistent model lets the equivalent inclusion represent a grain of the polycrystal. The strain disturbance then occurs because the local elastic and thermal properties of the grain differ from the average values for the polycrystal. The condition for self-consistency is that the average grain response is the same as the overall average of the polycrystal, or that the average disturbance vanishes. This leads to an implicit equation for the self-consistent effective elastic constants and an explicit equation for the self-consistent effective thermal expansion coefficient.

We next apply the results to crystals with cubic symmetry. For this case there are only three independent components of the single crystal elastic constants. The analysis can then be simplified considerably by using Walpole's notation for the decomposition of unity. This approach leads to the logical choice of the bulk modulus and shear modulus as the basic elastic constants to use in explicit calculations. When written out explicitly the equation for the self-consistent elastic constants is complicated but straightforward. The bulk modulus is isotropic. The equation for the self-consistent effective shear modulus can be reduced to a cubic equation, which was first obtained by Kröner [1958]. Finally, this equation can be solved explicitly in closed form. It is easy to calculate average numerical results for cubic crystals.

For lower crystal symmetries the solution of the implicit equation leads to high-order equations for the effective bulk and shear modulus. It is then best to continue the solution numerically. We present some results of these calculations.

Hooke's law

We start with a description of the elastic constants. For a single crystal, Hooke's law can be written as follows

$$\sigma_{ij} = c_{ijkl} e_{kl}, \qquad (i, j, k, l = 1, 2, 3), \tag{1}$$

where repeated indices are summed, σ and e are the stress and strain, both second rank tensors, and c is the elastic stiffness, a fourth rank tensor. Hooke's law can also be written in matrix form as

$$\sigma_i = c_{ij} e_j, \qquad (i, j = 1, \dots, 6), \tag{2}$$

where σ and e are the (6×1) stress and strain vectors and c is the (6×6) stiffness matrix. The two notations, tensors and matrices, are completely equivalent. The relation between them has been discussed in detail in [Nye 1960] and [Hearmon 1961]. The matrix form of the elastic stiffness or elastic moduli was introduced by Voigt [1887] and is frequently referred to as the Voigt notation or reduced notation. As in matrix theory, it is convenient to use the symbolic notation,

$$\sigma = ce, \tag{3}$$

to represent either of the foregoing equations. Equation (3) can be solved for the strain in terms of the stress:

$$e = \frac{\sigma}{c} = s\sigma,$$

where s, the elastic compliance, is the inverse of the stiffness c. We shall frequently use this divide notation, $1/c$, instead of the more common inverse notation, c^{-1}. The elastic properties of stiffness and compliance are usually referred to as the elastic constants of a material.

The effective medium

On a macroscopic scale a polycrystal may appear homogeneous or uniform, or perhaps, more generally, its properties appear to vary smoothly. Therefore we shall represent it by an effective medium, which is a model that approximately describes the overall average properties of the medium to some desired degree of accuracy. This then represents a gross description of the polycrystal. We also assume that in the effective medium the average stress $\langle\sigma\rangle$ and average strain $\langle e\rangle$ are related by the same simple form as Hooke's law for the single crystal

$$\langle\sigma\rangle = C\langle e\rangle, \tag{4}$$

where C is the effective stiffness. So the effective medium is homogeneous. We also assume that it is isotropic and perfectly disordered. The latter means that there is no texture, no characteristic grain shapes, no characteristic grain boundary geometry, no correlations between regions of the medium, such as periodicity. The effective stiffness thus represents the average stiffness of the polycrystal. The bracket notation stands for volume averages,

$$\langle\sigma\rangle = \frac{1}{V}\int\limits_V \sigma\, dV, \qquad \langle e\rangle = \frac{1}{V}\int\limits_V e\, dV,$$

and so the average stress or strain can almost be regarded as applied fields or boundary conditions. Equation (4) can now be solved for the average strain

$$\langle e\rangle = \frac{\langle\sigma\rangle}{C} = S\langle\sigma\rangle, \tag{5}$$

where S is the effective compliance. We have used the convention, suggested by Kröner [1958], that upper case letters are used for isotropic tensors or matrices that are material properties of the homogeneous effective medium. So upper case letters will represent the average properties of the polycrystal. Lower case letters are used for tensors or matrices that vary locally through the heterogeneous medium or the grains of the polycrystal and thus represent properties of the single crystal.

For an isotropic material there are only two independent elastic constants. Since the effective stiffness is isotropic, its tensor components can be expressed in terms of the two elastic constants as follows

$$C_{ijkl} = K\delta_{ij}\delta_{kl} + G\Big(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk} - \tfrac{2}{3}\,\delta_{ij}\delta_{kl}\Big), \tag{6}$$

where K is the effective bulk modulus, G the effective shear modulus, and δ the Kronecker delta defined as follows

$$\delta_{ij} \equiv \begin{cases} 1 & \text{if } i = j \\ 0 & \text{if } i \neq j \end{cases},$$
$$\delta_{kk} \equiv 3.$$

We can solve Equation (6) for K and G. If we calculate the two linear invariants of C we get

$$\begin{cases} C_{iijj} = 9K \\ C_{ijij} = 3K + 10G \end{cases} \quad \text{or} \quad \begin{cases} K = \tfrac{1}{9}\,C_{iijj} \\ G = \tfrac{1}{10}\Big(C_{ijij} - \tfrac{1}{3}\,C_{iijj}\Big). \end{cases} \tag{7}$$

Thus we have expressed the two scalar elastic constants K and G in terms of the two linear invariants of the stiffness tensor C. We can do the same manipulations with the effective compliance tensor

$$S_{ijkl} = \frac{1}{9K}\,\delta_{ij}\,\delta_{kl} + \frac{1}{4G}\Big(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk} - \tfrac{2}{3}\,\delta_{ij}\delta_{kl}\Big).$$

The linear invariants of S are

$$\begin{cases} S_{iijj} = \dfrac{1}{K} \\ S_{ijij} = \dfrac{1}{3K} + \dfrac{5}{2G} \end{cases} \qquad \text{or} \qquad \begin{cases} \dfrac{1}{K} = S_{iijj} \\ \dfrac{1}{G} = \dfrac{2}{5}\left(S_{ijij} - \dfrac{1}{3}\,S_{iijj}\right). \end{cases} \tag{8}$$

So now we have expressed the two elastic constants also in terms of the two linear invariants of the compliance tensor S.

The Voigt and Reuss models

To get actual expressions for the average elastic constants of a polycrystal in terms of the single crystal elastic constants, the [Voigt 1887] and [Reuss 1929] models are frequently invoked, because they provide an easy way to derive effective elastic constants. Furthermore, Hill [1952] showed that they provide bounds on those constants. Voigt assumed that there is a homogeneous or constant strain in the polycrystal, thus fulfilling compatibility, but not necessarily equilibrium. Reuss assumed a homogeneous or constant stress, thus fulfilling equilibrium, but not necessarily compatibility. For the Voigt model the actual strain is then equal to the average strain,

$$e = \langle e \rangle = \text{constant}, \tag{9}$$

and therefore we can decompose the average of the product of the stiffness and the strain into the product of the average stiffness and the average strain $\langle \sigma \rangle = \langle ce \rangle = \langle c \rangle \langle e \rangle$. Comparing with Equation (4) we find that for the Voigt model the effective stiffness is the average crystal stiffness,

$$C_V = \langle c \rangle, \tag{10}$$

which provides an upper bound on C. In the Reuss model we have

$$\sigma = \langle \sigma \rangle = \text{constant}, \tag{11}$$

and so $\langle e \rangle = \langle s\sigma \rangle = \langle s \rangle \langle \sigma \rangle$. Comparing with Equation (5) we find that for the Reuss model the effective compliance is the average crystal compliance,

$$S_R = \langle s \rangle \qquad \text{or} \qquad C_R = \langle c^{-1} \rangle^{-1}, \tag{12}$$

which provides an upper bound on S and a lower bound on C. To proceed further and get more explicit expressions for Equation (10) and Equation (12), we recall that fourth rank tensors have two linear invariants, and the fundamental property of invariants is that they are scalars and therefore do not depend on orientation in space. Therefore, each invariant is equal to its volume average. So we have

$$c_{iijj} = \langle c_{iijj} \rangle \qquad \text{and} \qquad c_{ijij} = \langle c_{ijij} \rangle. \tag{13}$$

Combining Equation (7), (10), and (13) we get for the Voigt model the result

$$\begin{aligned} K_V &= \tfrac{1}{9}\,c_{iijj}, \\ G_V &= \tfrac{1}{10}\left(c_{ijij} - \tfrac{1}{3}\,c_{iijj}\right). \end{aligned} \tag{14}$$

In detail, we have both in tensor and matrix notation

$$\begin{aligned} 9K_{\mathrm{V}} &= (c_{1111}+c_{2222}+c_{3333})+2(c_{1122}+c_{1133}+c_{2233}) = (c_{11}+c_{22}+c_{33})+2(c_{12}+c_{13}+c_{23}),\\ 15G_V &= (c_{1111}+c_{2222}+c_{3333})-(c_{1122}+c_{1133}+c_{2233})+3(c_{1212}+c_{1313}+c_{2323})\\ &= (c_{11}+c_{22}+c_{33})-(c_{12}+c_{13}+c_{23})+3(c_{44}+c_{55}+c_{66}). \end{aligned} \tag{15}$$

We also have for the compliance

$$s_{iijj} = \langle s_{iijj}\rangle \qquad \text{and} \qquad s_{ijij} = \langle s_{ijij}\rangle. \tag{16}$$

Combining Equation (8), (12), and (16) we get for the Reuss model the result

$$\frac{1}{K_R} = s_{iijj}, \qquad \frac{1}{G_R} = \frac{2}{5}\left(s_{ijij} - \frac{1}{3}s_{iijj}\right). \tag{17}$$

In detail, we have

$$\begin{aligned} \frac{1}{K_R} &= (s_{1111}+s_{2222}+s_{3333})+2(s_{1122}+s_{1133}+s_{2233}) = (s_{11}+s_{22}+s_{33})+2(s_{12}+s_{13}+s_{23}),\\ \frac{15}{G_R} &= 4(s_{1111}+s_{2222}+s_{3333})-4(s_{1122}+s_{1133}+s_{2233})+3(s_{1212}+s_{1313}+s_{2323})\\ &= 4(s_{11}+s_{22}+s_{33})-4(s_{12}+s_{13}+s_{23})+3(s_{44}+s_{55}+s_{66}). \end{aligned} \tag{18}$$

Hearmon [1961] has also derived these explicit equations, but by a different method. Hill [1952] showed that the Voigt and Reuss averages formed the least upper bound and the greatest lower bound, respectively, for the aggregate polycrystal.

Cubic polycrystal. For the special case of a cubic polycrystal, the Voigt relations (15) reduce to

$$3K_V = c_{11}+2c_{12}, \qquad 5G_V = c_{11}-c_{12}+3c_{44}. \tag{19}$$

and the Reuss relations, Equation (18), become

$$\frac{1}{3K_R} = s_{11}+2s_{12}, \qquad \frac{5}{G_R} = 4(s_{11}-s_{12})+3s_{44}. \tag{20}$$

The Voigt and Reuss bulk moduli are identical in this case, $K_V = K_R$, and also equal to the single crystal and effective polycrystal bulk modulus. This is only true for cubic symmetry; for other crystal symmetries, the various estimates of the effective bulk modulus differ from each other.

Thermal expansion

Tomé [1998] showed how thermal expansion can be incorporated into the elastic equations. The stress in Hooke's law is related to the elastic strain, so in this case the total strain must be adjusted for the effects of the thermal expansion in order to get the elastic strain. Equation (3) for the single crystal is therefore modified to

$$\sigma = c(e - \boldsymbol{\alpha}\delta T), \tag{21}$$

where $\boldsymbol{\alpha}$ is the single crystal thermal expansion coefficient, a second rank tensor or a (6×1) vector, and δT is a small temperature change that takes place uniformly throughout material. Equation (4) for the effective medium is modified to

$$\langle \sigma \rangle = C(\langle e \rangle - \boldsymbol{A}\delta T), \tag{22}$$

where $\boldsymbol{A}$ is the average thermal expansion coefficient of the effective medium. We emphasize the fact that $\boldsymbol{\alpha}$ and $\boldsymbol{A}$ are tensors or (6×1) vectors by writing them **boldface** to distinguish them from the scalars below. Equation (21) can be solved for the local strain in the single crystal,

$$e = s\sigma + \boldsymbol{\alpha}\delta T, \tag{23}$$

and Equation (22) for the average strain in the effective medium,

$$\langle e \rangle = S\langle \sigma \rangle + \boldsymbol{A}\delta T. \tag{24}$$

The stress or strain and the temperature change in these equations can be applied arbitrarily and therefore these quantities will be treated as independent variables.

The Voigt model. With Voigt's assumption of constant strain, Equation (9), Equations (21) and (22) lead to $C_V\langle e \rangle - C_V\boldsymbol{A}_V\delta T = \langle c \rangle\langle e \rangle - \langle c\boldsymbol{\alpha} \rangle\delta T$. Since this equation holds for an arbitrary average strain $\langle e \rangle$ and an arbitrary temperature change δT, we can equate their coefficients. The first equality gives the relation Equation (10), which we already found without taking the influence of a temperature change into account. The second equality is

$$C_V\boldsymbol{A}_V = \langle c\boldsymbol{\alpha} \rangle \qquad \text{or} \qquad \boldsymbol{A}_V = \frac{\langle c\boldsymbol{\alpha} \rangle}{C_V} = S_V\langle c\boldsymbol{\alpha} \rangle. \tag{25}$$

Tomé [1998] also found this result. Since the effective thermal expansion coefficient is isotropic, it can be expressed as $A_{ij} = A\delta_{ij}$, where A is the scalar effective thermal expansion coefficient. With the help of Equation (6), we can derive the relation

$$A = \frac{1}{9K} C_{iikl}A_{kl}. \tag{26}$$

We now take the linear invariant of Equation (25) and substitute it into Equation (26), remembering that the invariant is equal to its average, to get the effective thermal expansion coefficient for the Voigt model

$$A_V = \frac{1}{9K_V} c_{iikl}\alpha_{kl}. \tag{27}$$

In detail we have in both tensor and matrix notation

$$\begin{aligned}
9K_VA_V &= (c_{1111} + c_{1122} + c_{1133})\alpha_{11} + (c_{1122} + c_{2222} + c_{2233})\alpha_{22} \\
&\qquad + (c_{1133} + c_{2233} + c_{3333})\alpha_{33} + 2(c_{1112} + c_{1222} + c_{1233})\alpha_{12} \\
&\qquad\qquad + 2(c_{1113} + c_{1333} + c_{2213})\alpha_{13} + 2(c_{1123} + c_{2223} + c_{2333})\alpha_{23}, \\
&= (c_{11} + c_{12} + c_{13})\alpha_1 + (c_{12} + c_{22} + c_{23})\alpha_2 + (c_{13} + c_{23} + c_{33})\alpha_3 \\
&\qquad + 2(c_{14} + c_{24} + c_{34})\alpha_4 + 2(c_{15} + c_{25} + c_{35})\alpha_5 + 2(c_{16} + c_{26} + c_{36})\alpha_6.
\end{aligned} \tag{28}$$

Note that the effective thermal expansion coefficient of a polycrystal is coupled to the elastic constants in the Voigt model. For crystal structures where the off-diagonal terms of the elastic constant matrix vanish, such as cubic, hexagonal, tetragonal, and orthorhombic, the second line of Equation (28) vanishes and the equation simplifies considerably.

The Reuss model. With Reuss' assumption of constant stress, Equation (11), Equations (23) and (24) lead to $S_R\langle\sigma\rangle + \boldsymbol{A}_R\delta T = \langle s\rangle\langle\sigma\rangle + \langle\boldsymbol{\alpha}\rangle\delta T$. Since this equation holds for arbitrary average stress $\langle\sigma\rangle$ and arbitrary temperature change δT, we can equate their coefficients. The first equality gives the relation Equation (12), which we already found without the influence of temperature. The second equality is

$$\boldsymbol{A}_R = \langle\boldsymbol{\alpha}\rangle. \tag{29}$$

Tomé [1998] also found this result. The linear invariant of this equation is

$$A_R = \tfrac{1}{3}\,\alpha_{ii}. \tag{30}$$

In detail, we have the simple result

$$A_R = \tfrac{1}{3}\,(\alpha_{11}+\alpha_{22}+\alpha_{33}) = \tfrac{1}{3}(\alpha_1+\alpha_2+\alpha_3). \tag{31}$$

So in the Reuss model the overall thermal properties are independent of the elastic properties.

Eshelby's theory

To obtain a self-consistent estimate of the effective properties we use Eshelby's theory of elastic inclusions and inhomogeneities [Eshelby 1961]. That is the method Kröner [1958] first used to get a solution for the cubic polycrystal. Kröner [1972] later used statistical continuum mechanics to derive the same as well as additional results. The subject of inclusions, inhomogeneities, and the equivalent inclusion has been treated in detail by Mura [1982]. In the present treatment we also include Tomé's contribution for thermal expansion [Tomé 1998].

The inclusion. Consider an infinitely extended homogeneous material in domain D with elastic constants C everywhere, containing a domain Ω with a stress-free strain e^P, which is called the transformed inclusion. This inclusion causes a local stress σ' and strain e', which are related by Hooke's law

$$\begin{aligned} \sigma' &= C(e'-e^P), && \text{in } \Omega,\\ \sigma' &= Ce', && \text{in } D-\Omega. \end{aligned}$$

If e^P is uniform and Ω is an ellipsoid, then the stress σ' and strain e' are also uniform in Ω and related to e^P by

$$e' = Ee^P, \quad \text{in } \Omega, \tag{32}$$

where E is the Eshelby tensor, which is a constant. Let us apply a stress $\bar\sigma$ at infinity with a corresponding strain $\bar e$, and a temperature change δT. The bar is used to denote that these quantities will be overall average values. They are related by Hooke's law $\bar\sigma = C(\bar e - \boldsymbol{A}\delta T)$. The resulting total stress σ is then given by

$$\begin{aligned} \sigma &= \bar\sigma + \sigma' = C(\bar e + e' - e^P - \boldsymbol{A}\delta T), && \text{in } \Omega,\\ \sigma &= \bar\sigma + \sigma' = C(\bar e + e' - \boldsymbol{A}\delta T), && \text{in } D-\Omega. \end{aligned} \tag{33}$$

The prime represents deviations from the average value.

The inhomogeneity. Consider an infinitely extended material in domain D with the elastic constants C and thermal expansion A containing a domain Ω with the elastic constants c and thermal expansion α, which is called an inhomogeneity. We investigate the disturbance in an applied stress and temperature increment caused by the presence of this inhomogeneity. Let us again denote the applied stress at infinity by $\bar{\sigma}$ and the corresponding strain by $\bar{e}$, and the temperature increment by δT, while the stress disturbance and the strain disturbance are denoted by σ' and e', respectively. The total stress (actual stress) is σ, and the total strain is e. Hooke's law is written as

$$\begin{aligned} \sigma &= \bar{\sigma} + \sigma' = c(e - \boldsymbol{\alpha}\delta T) = c(\bar{e} + e' - \boldsymbol{\alpha}\delta T), && \text{in } \Omega, \\ \sigma &= \bar{\sigma} + \sigma' = C(e - \boldsymbol{A}\delta T) = C(\bar{e} + e' - \boldsymbol{A}\delta T), && \text{in } D - \Omega. \end{aligned} \tag{34}$$

The equivalent inclusion. The equivalent inclusion is a method to determine the stress disturbance of the inhomogeneity using the result of the inclusion. So the inclusion has been introduced arbitrarily in order to simulate the inhomogeneity problem. In an applied stress or strain field, the inhomogeneity looks like an inclusion. The necessary and sufficient condition for the equivalency of the stresses and strains in the above two problems of inhomogeneity and inclusion is

$$c(\bar{e} + e' - \boldsymbol{\alpha}\delta T) = C(\bar{e} + e' - e^P - \boldsymbol{A}\delta T), \qquad \text{in } \Omega. \tag{35}$$

This equation can solved for e' when the transformed inclusion problem, Equation (32), in the homogeneous material is solved for E. After obtaining e', the stress σ can be found from Equation (34) or Equation (33). If $\bar{\sigma}$ is a uniform stress and δT a uniform temperature change, e^P is also uniform in Ω and Eshelby's Equation (32) can be used. Substitution of Equation (32) into Equation (35) gives

$$c(\bar{e} + e' - \boldsymbol{\alpha}\delta T) = C\left(\bar{e} + e' - \frac{e'}{E} - \boldsymbol{A}\delta T\right), \qquad \text{in } \Omega.$$

The solution of this equation for the strain disturbance is

$$e' = E\,\frac{-\delta c\bar{e} + (c\boldsymbol{\alpha} - C\boldsymbol{A})\delta T}{\delta c E + C}, \tag{36}$$

where we have defined $\delta c \equiv c - C$. So Equation (36) represents the local strain disturbance at the inhomogeneity when a uniform strain $\bar{e}$ and temperature change δT is applied to the domain.

The self-consistent model

We now take the equivalent inclusion to represent a grain in the polycrystal. The interpretation of Equation (36) is then as follows. The applied strain $\bar{e}$ and temperature change δT cause a strain disturbance e' in the grain because the local elastic and thermal properties of the grain differ from the average elastic and thermal properties of the polycrystal. The condition for self-consistency is that the average grain response is the same as the overall average for the polycrystal, or that the average disturbance vanishes:

$\langle e' \rangle = \mathbf{0}$. Since $\bar{e}$ and δT are independent and E is constant, we then get from Equation (36)

$$\left\langle \frac{\delta c}{\delta c E + C} \right\rangle = \mathbf{0}, \tag{37}$$

$$\left\langle \frac{c\boldsymbol{\alpha} - C\boldsymbol{A}}{\delta c E + C} \right\rangle = \mathbf{0}. \tag{38}$$

These equations are consistent with those of Tomé [1998]. Equation (37) is an implicit equation for the self-consistent effective elastic stiffness C. For cubic crystal symmetry it leads to a cubic equation for the self-consistent effective shear modulus, discussed below. It can also be solved for lower crystal symmetries, but then leads to a pair of high-order coupled equations for the effective bulk and shear modulus. For example, for hexagonal symmetry it leads to one equation that is quadratic in both K and G, and another equation that is quadratic in K and sixth order in G. In general, the simpler equation can be solved for K in terms of G and the result substituted into the other equation. It is then best to solve this latter equation numerically rather than symbolically. There are many solutions, but usually there is only one real positive one. The expression Equation (38) can be solved as

$$\boldsymbol{A} = \frac{\left\langle \frac{c\boldsymbol{\alpha}}{\delta c E + C} \right\rangle}{\left\langle \frac{C}{\delta c E + C} \right\rangle}, \tag{39}$$

once the stiffness C has been obtained. For numerical purposes, this equation is rather tedious and lengthy. The calculation can be simplified as follows. If we define the (6×1) vector

$$v = \frac{c\boldsymbol{\alpha}}{\delta c E + C},$$

and the (6×6) matrix

$$M = \left\langle \frac{C}{\delta c E + C} \right\rangle,$$

then the scalar effective thermal expansion coefficient is given by

$$A = \frac{v_1 + v_2 + v_3}{3(M_{11} + 2M_{12})}. \tag{40}$$

Upper limit. If we assume that the inhomogeneity is very soft, that is, $E = \mathbf{0}$, then Equations (37) and (39) reduce to

$$\langle c - C \rangle = \mathbf{0}, \quad \text{and} \quad \boldsymbol{A} = \left\langle \frac{c\boldsymbol{\alpha}}{C} \right\rangle,$$

which reduce to the Voigt solutions, Equation (10) and Equation (25).

Lower limit. If we assume the inhomogeneity is very hard, $E = \boldsymbol{I}$, then Equation (37) and Equation (39) reduce to

$$\left\langle \frac{c - C}{c} \right\rangle = \mathbf{0}, \qquad \boldsymbol{A} = \left\langle \frac{C}{c} \right\rangle^{-1} \langle \boldsymbol{\alpha} \rangle, \tag{41}$$

which reduce to the Reuss solutions, Equation (12) and Equation (29), when we note that from Equation (41) we have

$$\left\langle \frac{C}{c} \right\rangle^{-1} = \boldsymbol{I}. \tag{42}$$

The Walpole notation

Walpole [1981] introduced a notation that greatly simplifies symbolic manipulations for isotropic and cubic materials. A fourth-order tensor will generally have a structure that reflects some underlying geometric symmetry, like that of a crystal. An appropriate decomposition of the structure of a tensor can reflect valuable physical insight while offering to simplify greatly the calculation of various inverses and inner products. Isotropic tensors are the principal ones to be prepared for in detailed calculations and there is a smaller role for anisotropic tensors that reflect the symmetry of cubic crystals.

Isotropic case. Walpole decomposed unity as $\boldsymbol{I} = \boldsymbol{J} + \boldsymbol{K}$. In terms of fourth rank tensors these symbols are defined as

$$I_{ijkl} \equiv \tfrac{1}{2}(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}), \qquad J_{ijkl} \equiv \tfrac{1}{3}\,\delta_{ij}\delta_{kl},$$

$$K_{ijkl} \equiv \tfrac{1}{2}\left(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk} - \tfrac{2}{3}\,\delta_{ij}\delta_{kl}\right).$$

In terms of (6×6) matrices we have the definitions

$$\boldsymbol{I} \equiv \begin{pmatrix} 1&0&0&0&0&0\\ 0&1&0&0&0&0\\ 0&0&1&0&0&0\\ 0&0&0&1&0&0\\ 0&0&0&0&1&0\\ 0&0&0&0&0&1 \end{pmatrix}, \qquad \boldsymbol{J} \equiv \begin{pmatrix} \frac{1}{3}&\frac{1}{3}&\frac{1}{3}&0&0&0\\ \frac{1}{3}&\frac{1}{3}&\frac{1}{3}&0&0&0\\ \frac{1}{3}&\frac{1}{3}&\frac{1}{3}&0&0&0\\ 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ 0&0&0&0&0&0 \end{pmatrix}, \qquad \boldsymbol{K} \equiv \begin{pmatrix} \frac{2}{3}&-\frac{1}{3}&-\frac{1}{3}&0&0&0\\ -\frac{1}{3}&\frac{2}{3}&-\frac{1}{3}&0&0&0\\ -\frac{1}{3}&-\frac{1}{3}&\frac{2}{3}&0&0&0\\ 0&0&0&1&0&0\\ 0&0&0&0&1&0\\ 0&0&0&0&0&1 \end{pmatrix}.$$

The decomposition is idempotent and orthogonal:

$$\boldsymbol{J}\boldsymbol{J} = \boldsymbol{J}, \qquad \boldsymbol{K}\boldsymbol{K} = \boldsymbol{K}, \qquad \boldsymbol{J}\boldsymbol{K} = \boldsymbol{K}\boldsymbol{J} = \boldsymbol{0}.$$

The linear invariants are

$$\begin{aligned} I_{iijj} &= 3, & J_{iijj} &= 3, & K_{iijj} &= 0,\\ I_{ijij} &= 6, & J_{ijij} &= 1, & K_{ijij} &= 5. \end{aligned} \tag{43}$$

In the matrix notation the first invariant is the sum of all elements in the upper left quadrant, and the second invariant is the sum of all the diagonal elements. With this notation the effective stiffness, Equation (6), can now be written in symbolic notation

$$C = 3K\boldsymbol{J} + 2G\boldsymbol{K}. \tag{44}$$

We see that decomposition reflects a split into an isotropic or dilatational part and a deviatoric or shear part. The Eshelby tensor for a spherical inclusion can be found in many texts [Kröner 1958; Eshelby 1961; Kröner 1972; Walpole 1981; Mura 1982; Tomé 1998] and in this notation it can be written

$$E = \frac{3K}{4G + 3K}\boldsymbol{J} + \frac{6}{5}\frac{2G + K}{4G + 3K}\boldsymbol{K}.$$

Cubic symmetry. For a cubic crystal, Walpole further decomposed $\boldsymbol{K}$ as $\boldsymbol{K} = \boldsymbol{K}' + \boldsymbol{K}''$. For the tensor definitions of these symbols see Walpole. In terms of (6×6) matrices,

$$\boldsymbol{K}' \equiv \begin{pmatrix} \frac{2}{3} & -\frac{1}{3} & -\frac{1}{3} & 0 & 0 & 0 \\ -\frac{1}{3} & \frac{2}{3} & -\frac{1}{3} & 0 & 0 & 0 \\ -\frac{1}{3} & -\frac{1}{3} & \frac{2}{3} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}, \qquad \boldsymbol{K}'' \equiv \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}.$$

This decomposition is also idempotent and orthogonal:

$$\begin{aligned} \boldsymbol{K}'\boldsymbol{K}' &= \boldsymbol{K}', \\ \boldsymbol{K}''\boldsymbol{K}'' &= \boldsymbol{K}'', \\ \boldsymbol{K}'\boldsymbol{K}'' = \boldsymbol{K}''\boldsymbol{K}' &= \boldsymbol{0}, \\ \boldsymbol{J}\boldsymbol{K}' = \boldsymbol{K}'\boldsymbol{J} &= \boldsymbol{0}, \\ \boldsymbol{J}\boldsymbol{K}'' = \boldsymbol{K}''\boldsymbol{J} &= \boldsymbol{0}. \end{aligned} \tag{45}$$

The linear invariants are

$$\begin{aligned} K'_{iijj} &= 0, \qquad & K''_{iijj} &= 0, \\ K'_{ijij} &= 2, \qquad & K''_{ijij} &= 3. \end{aligned} \tag{46}$$

With this notation the cubic crystal elastic stiffness can be written in a form that resembles the isotropic case

$$c = 3\kappa \boldsymbol{J} + 2\mu' \boldsymbol{K}' + 2\mu'' \boldsymbol{K}'', \tag{47}$$

where κ is the bulk modulus. Here μ' and μ'' are the $\{001\}\langle 110\rangle$ and $\{001\}\langle 100\rangle$ shear resistance of the crystal, respectively. For cubic crystals these moduli can be regarded as more fundamental elastic constants than the stiffness and compliance. They are related as follows

$$\begin{aligned} \kappa &= \frac{1}{3}(c_{11} + 2c_{12}) = \frac{1}{3(s_{11} + 2s_{12})}, \\ \mu' &= \frac{1}{2}(c_{11} - c_{12}) = \frac{1}{2(s_{11} - s_{12})}, \\ \mu'' &= c_{44} = \frac{1}{s_{44}}. \end{aligned} \tag{48}$$

The relations Equation (45) make it simple to calculate inverses, such as the elastic compliance

$$s = \frac{1}{c} = \frac{\boldsymbol{J}}{3\kappa} + \frac{\boldsymbol{K}'}{2\mu'} + \frac{\boldsymbol{K}''}{2\mu''}. \tag{49}$$

To prove this relation, take the matrix product of Equations (47) and (49) and show that it is unity.

Cubic crystal symmetry

We next apply some of the foregoing equations to the special case of cubic symmetry. For cubic symmetry, the results are much simpler than for all the lower crystal structures.

Voigt model. We illustrate the application of the concepts first to the Voigt model. From Equations (14), (47), (43), and (46) we have $K_V = \kappa$, and

$$G_V = \frac{2}{5}\mu' + \frac{3}{5}\mu''. \tag{50}$$

These results are the same as Equation (19). Furthermore, Equation (50) illustrates a general rule for averaging the cubic shear components, that is, take two fifths the coefficient of $\boldsymbol{K}'$ plus three fifths the coefficient of $\boldsymbol{K}''$.

Reuss model. For the Reuss model, we have from Equations (49), (43), and (46) $K_R = \kappa$ and

$$\frac{5}{G_R} = \frac{2}{\mu'} + \frac{3}{\mu''}. \tag{51}$$

These results are the same as Equation (20). Equation (51) illustrates the general rule mentioned above.

Self-consistent model. In terms of the Walpole notation we have from Equation (44) and Equation (47)

$$\delta c \equiv c - C = 3(\kappa - K)\boldsymbol{J} + 2(\mu' - G)\boldsymbol{K}' + 2(\mu'' - G)\boldsymbol{K}''.$$

Using this we can also write

$$\frac{C}{\delta c} = \frac{K}{\kappa - K}\boldsymbol{J} + \frac{G}{\mu' - G}\boldsymbol{K}' + \frac{G}{\mu'' - G}\boldsymbol{K}''.$$

Therefore

$$\frac{\delta c}{\delta c E + C} = \frac{\boldsymbol{I}}{E + \frac{C}{\delta c}} = \frac{\boldsymbol{J}}{\frac{3K}{4G+3K} + \frac{K}{\kappa - K}} + \frac{\boldsymbol{K}'}{\frac{6}{5}\frac{2G+K}{4G+3K} + \frac{G}{\mu' - G}} + \frac{\boldsymbol{K}''}{\frac{6}{5}\frac{2G+K}{4G+3K} + \frac{G}{\mu'' - G}}. \tag{52}$$

Setting the average equal to zero, Equation (37), we have

$$\frac{\boldsymbol{J}}{\frac{3K}{4G+3K} + \frac{K}{\kappa - K}} + \frac{2}{5}\frac{\boldsymbol{K}}{\frac{6}{5}\frac{2G+K}{4G+3K} + \frac{G}{\mu' - G}} + \frac{3}{5}\frac{\boldsymbol{K}}{\frac{6}{5}\frac{2G+K}{4G+3K} + \frac{G}{\mu'' - G}} = \boldsymbol{0}.$$

Since $\boldsymbol{J}$ and $\boldsymbol{K}$ are independent, their coefficients must vanish separately

$$\frac{1}{\frac{3K}{4G+3K} + \frac{K}{\kappa - K}} = 0, \qquad \frac{2}{\frac{6}{5}\frac{2G+K}{4G+3K} + \frac{G}{\mu' - G}} + \frac{3}{\frac{6}{5}\frac{2G+K}{4G+3K} + \frac{G}{\mu'' - G}} = 0.$$

The first equation can also be obtained by setting the first invariant of Equation (52) equal to zero, and has the solution

$$K = \kappa. \tag{53}$$

The second equation can also be found by setting the second invariant of Equation (52) equal to zero, and can be reduced to the form

$$8G^3+(9\kappa+4\mu')G^2-3(\kappa+4\mu')\mu''G-6\kappa\mu'\mu''=0. \tag{54}$$

This is a cubic equation for the self-consistent effective shear modulus G of a cubic polycrystal that is statistically homogeneous, isotropic, and perfectly disordered. It was first obtained by Kröner [1958]. Hershey [1954] previously obtained a quartic equation that included Equation (54) as a factor.

The solution. There are general closed form solutions for cubic equations. If we write Equation (54) as follows

$$\gamma_3G^3+\gamma_2G^2+\gamma_1G+\gamma_0=0, \tag{55}$$

with the coefficients

$$\begin{aligned} \gamma_3 &\equiv 8, & \gamma_2 &\equiv 9\kappa+4\mu', \\ \gamma_1 &\equiv -3(\kappa+4\mu')\mu'', & \gamma_0 &\equiv -6\kappa\mu'\mu'', \end{aligned} \tag{56}$$

and define

$$p\equiv\sqrt{\left(\frac{\gamma_2}{3}\right)^2-\frac{\gamma_1\gamma_3}{3}}, \qquad q\equiv-2\left(\frac{\gamma_2}{3}\right)^3+\frac{\gamma_1\gamma_2\gamma_3}{3}-\gamma_0\gamma_3^2, \tag{57}$$

then the only nonnegative solution of Equation (55) for the effective self-consistent shear modulus of a cubic polycrystal is

$$G=2\frac{p}{\gamma_3}\cos\left[\frac{1}{3}\arccos\left(\frac{q}{2p^3}\right)\right]-\frac{\gamma_2}{3\gamma_3}. \tag{58}$$

It is now straightforward to calculate the average cubic polycrystal shear modulus from the single crystal elastic constants. Ledbetter calls this approach the Hershey–Kröner–Eshelby model. He measured elastic constants for copper [Ledbetter 1981] and stainless steel [Ledbetter 1984] and found that among nine different averaging models this model works best.

Thermal expansion. For a cubic crystal the thermal expansion coefficient is isotropic: $\alpha_{ij}=\alpha\delta_{ij}$. Therefore all cases, that is the Voigt model Equation (27), the Reuss model Equation (30), and the self-consistent model Equation (38), reduce to $A=\alpha$. Since the thermal expansion is isotropic in cubic crystals there is no difference between the polycrystal and the single crystal.

Some numerical results for cubic crystals. Table 1 shows the single crystal elastic constants of several cubic crystals at room temperature. The values are obtained from the handbook by Simmons and Wang [1971] except that those for calcium are from [Ledbetter and Kim 2001].

We have chosen a set of materials covering a wide range of anisotropy, where the Zener anisotropy factor is given from the formula [Zener 1948]

$$A=\frac{\mu''}{\mu'}=\frac{2c_{44}}{c_{11}-c_{12}}=\frac{2(s_{11}-s_{12})}{s_{44}}.$$

Table 2 shows values of the average bulk and shear modulus for cubic polycrystals calculated from the data in Table 1, using Equations (48), (53), (50), (51), (56), (57), and (58). The Voigt and Reuss values

Material	c_{11}	c_{12}	c_{44}	Anisotropy
Aluminum	1.073	0.609	0.283	1.22
Calcium	1.076	0.125	0.5758	1.21
Calcium Fluoride	1.628	0.433	0.334	0.56
Copper	1.684	1.214	0.754	3.21
Diamond	9.5	3.9	4.3	1.54
Gold	1.7893	1.4863	0.4367	2.88
Lead	0.466	0.392	0.1441	3.89
Lithium	0.135	0.1144	0.0878	8.52
Silver	1.24	0.934	0.461	3.01
Silver Chloride	0.601	0.362	0.0625	0.52
Sodium	0.0526	0.0404	0.0426	6.98
Sodium Chloride	0.487	0.124	0.126	0.69

Table 1. Single crystal elastic constants for several cubic crystals in units of Mbar.

Material	K	G_V	G_R	G_{VRH}	G_S
Aluminum	0.764	0.263	0.260	0.261	0.261
Calcium	0.442	0.536	0.531	0.533	0.533
Calcium Fluoride	0.831	0.439	0.406	0.423	0.422
Copper	1.371	0.546	0.400	0.473	0.482
Diamond	5.767	3.700	3.541	3.621	3.625
Gold	1.587	0.323	0.249	0.286	0.292
Lead	0.416	0.101	0.067	0.084	0.087
Lithium	0.121	0.057	0.022	0.039	0.040
Silver	1.036	0.338	0.255	0.297	0.302
Silver Chloride	0.442	0.085	0.077	0.081	0.081
Sodium	0.045	0.028	0.013	0.020	0.021
Sodium Chloride	0.245	0.148	0.144	0.146	0.146

Table 2. Average elastic constants for several cubic polycrystals in units of Mbar. The bulk modulus is denoted by K and the shear modulus by G. The subscripts denote Voigt (V), Reuss (R), Hill (VRH), and self-consistent (S).

always bracket the self-consistent value. The Hill average is defined as the arithmetic mean of the Voigt and Reuss average [Hill 1952]:

$$G_{\mathrm{VRH}} = \tfrac{1}{2}\,(G_V + G_R).$$

It is often close to the self-consistent value, G_S. More exhaustive listings are given in [Kröner 1972] and [Ledbetter and Kim 2001].

Other crystal symmetries

For symmetries lower than cubic, Equation (37) is better solved numerically. Tables 3 and 4 give the single crystal elastic constants and thermal expansion coefficients of several different crystal structures at room temperature [Simmons and Wang 1971; Krishnan et al. 1979].

The anisotropy factor for these crystal structures is a generalization of the Zener factor and is given by

$$AI = \frac{2(c_{44}+c_{55}+c_{66})}{c_{11}+c_{22}+c_{33}-c_{12}-c_{13}-c_{23}}.$$

To obtain the self-consistent values, Equation (37) is solved simultaneously for the bulk modulus, K, and the shear modulus, G, which are then denoted by K_S and G_S. The results are given in Table 5. The Voigt and Reuss values are given by Equations (15) and (18). As before, the Hill values are the arithmetic mean of the Voigt and Reuss averages, and lie close to the self-consistent values.

Material	Crystal	c_{11}	c_{12}	c_{13}	c_{23}	c_{14}	c_{22}
Titanium	hexagonal	1.624	0.92	0.69	0.69	0.0	1.624
Zirconium	hexagonal	1.434	0.728	0.653	0.653	0.0	1.434
Indium	tetragonal	0.445	0.395	0.405	0.405	0.0	0.445
Tin	tetragonal	0.86	0.35	0.3	0.3	0.0	0.86
Calcite	trigonal	1.4626	0.597	0.5076	0.5076	−0.2076	1.4626
Quartz	trigonal	0.8501	0.0696	0.1412	0.1412	0.1678	0.8501
Aragonite	orthorhombic	1.5958	0.3663	0.0197	0.1591	0.0	0.8697
Uranium	orthorhombic	2.148	0.465	0.218	1.076	0.0	1.986

Table 3. Single crystal elastic constants for several crystals in units of Mbar.

Material	c_{33}	c_{44}	c_{55}	c_{66}	Anisotropy	α_1	α_2	α_3
Titanium	1.807	0.467	0.467	0.352	0.93	9.55	9.55	10.65
Zirconium	1.648	0.32	0.32	0.353	0.80	5.7	5.7	11.4
Indium	0.444	0.0655	0.0655	0.122	3.92	1.2	1.3	−0.81
Tin	1.33	0.49	0.49	0.53	1.44	14.64	14.64	28.14
Calcite	0.8531	0.3405	0.3405	0.4328	1.03	−5.6	−5.6	25
Quartz	1.0535	0.5722	0.5722	0.39025	1.28	13	13	8
Aragonite	0.8503	0.4132	0.2564	0.4274	0.79	35	17	10
Uranium	2.671	1.244	0.734	0.743	1.08	25.41	0.65	20.65

Table 4. Single crystal elastic constants in units of Mbar and thermal expansion coefficients in units of $10^{-6}K^{-1}$ for several crystals.

Material	K_V	K_R	K_{VRH}	K_S	G_V	G_R	G_{VRH}	G_S
Titanium	1.073	1.073	1.073	1.073	0.441	0.426	0.434	0.434
Zirconium	0.954	0.952	0.953	0.953	0.364	0.356	0.360	0.360
Indium	0.416	0.416	0.416	0.416	0.0592	0.0372	0.0482	0.0491
Tin	0.550	0.535	0.543	0.542	0.442	0.410	0.426	0.428
Calcite	0.778	0.716	0.747	0.750	0.367	0.269	0.318	0.315
Quartz	0.384	0.377	0.381	0.381	0.467	0.405	0.436	0.433
Aragonite	0.490	0.447	0.468	0.464	0.404	0.367	0.385	0.383
Uranium	1.147	1.114	1.131	1.128	0.881	0.807	0.844	0.842

Table 5. Average elastic constants for several polycrystals in units of Mbar. The bulk modulus is denoted by K and the shear modulus by G. The subscripts denote Voigt (V), Reuss (R), Hill (VRH), and self-consistent (S).

Table 6 shows the effective thermal expansion coefficients calculated from Equations (28), (31), and (40).

Summary

The concept of effective medium and effective material properties has been described, in particular for elastic constants and thermal expansion. The effective properties are used to represent the overall average properties of a polycrystal. The concept is then applied to the particular cases of the Voigt, Reuss, and self-consistent models to obtain expressions for the overall average properties of a polycrystal in terms of the single crystal components. The self-consistent model is derived by invoking Eshelby's theory of inclusion and inhomogeneities. It gives an implicit equation for the self-consistent elastic constants and an explicit equation for the self-consistent thermal expansion coefficient. A brief description is given of the Walpole notation for isotropic and cubic materials. For the particular case of cubic symmetry the

Material	A_V	A_R	A_{VRH}	A_S	Crystal
Titanium	9.913	9.917	9.915	9.915	hexagonal
Zirconium	7.662	7.600	7.631	7.629	hexagonal
Indium	0.527	0.530	0.528	0.527	tetragonal
Tin	19.90	19.14	19.52	19.52	tetragonal
Calcite	2.564	4.60	3.582	3.440	trigonal
Quartz	11.07	11.33	11.20	11.20	trigonal
Aragonite	23.46	20.67	22.06	21.79	orthorhombic
Uranium	15.12	15.57	15.34	15.39	orthorhombic

Table 6. Average thermal expansion coefficients in units of $10^{-6}K^{-1}$ for several polycrystals of different crystal symmetries.

bulk modulus and thermal expansion are isotropic and the self-consistent shear modulus satisfies a cubic equation, which can be solved explicitly. Some numerical results calculated from the solution are listed. For lower crystal symmetries, the equations are solved numerically. Results are given for the average bulk modulus, shear modulus, and thermal expansion coefficients of various hexagonal, tetragonal, trigonal, and orthorhombic polycrystals. In general, it is found that the Hill average is close to the self-consistent value.

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