

# ELASTIC PROPERTIES OF POLYCRYSTALS†

## A Review

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The elastic properties of polycrystals depend on the single-crystal elastic constants of the crystallites which build up the polycrystal and on the manner in which the crystallites are connected. Because of the technical importance of polycrystalline materials a lot of papers deal with the problem to calculate effective elastic constants of polycrystals from single-crystal and structure properties. This paper gives a review concerning the most important theories and methods respecting this matter.

KEY WORDS Polycrystal, elasticity, inhomogeneity, ultrasound.

### 1. INTRODUCTION

A lot of technically important materials are polycrystalline. Their elastic properties depend on the single-crystal elastic constants of the crystallites which build up the polycrystal and on the manner in which the crystallites are connected. Effective elastic constants of polycrystalline materials can be calculated from single-crystal and structure properties. To solve this problem exactly, orientation and shape of each grain must be known. From these informations, the mean values of stress and strain in the whole polycrystal and thus its effective elastic constants are to be determined taking into account the boundary conditions of stress and strain at the grain boundaries. But this technique is not practicable because the calculations would become too complicated. Furthermore, in most cases the exact orientations and shapes of the grains are not known. This problem can be overcome while using orientation and grain shape distribution functions. The orientation distribution function indicates the statistical probability to find the different orientations within the polycrystal. It can be determined by texture measurements. In this case, orientation correlations of different grains are neglected. For the grain shape different assumptions more or less realistic are used. This paper gives a review concerning the most important theories and methods to calculate effective elastic constants of polycrystals from single-crystal and structure properties and points out its validity limitations.

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† Invited Review.

## 2. EFFECTIVE ELASTIC CONSTANTS OF MICROSCOPICALLY INHOMOGENEOUS ELASTIC MEDIA

In the linear approximation, the stress tensor  $\sigma_{ij}$  of an elastic material is connected with its strain tensor  $\varepsilon_{ij}$  by the Hooke's law

$$\sigma_{ij}(\mathbf{r}) = C_{ijkl}(\mathbf{r})\varepsilon_{kl}(\mathbf{r}), \quad (1a)$$

$$\varepsilon_{ij}(\mathbf{r}) = S_{ijkl}(\mathbf{r})\sigma_{kl}(\mathbf{r}). \quad (1b)$$

If the medium considered is inhomogeneous the elastic moduli tensor  $C_{ijkl}$  and the compliance tensor  $S_{ijkl} = (C^{-1})_{ijkl}$  and thus stress and strain are position dependent. In the case of macroscopical homogeneity effective elastic constants  $C_{ijkl}^{\text{eff}}$  and compliance moduli  $S_{ijkl}^{\text{eff}} = (C^{\text{eff}})^{-1}_{ijkl}$  can be defined which connect the mean (i.e. ensemble averaged) stress and strain tensors  $\langle \sigma_{ij} \rangle$  and  $\langle \varepsilon_{ij} \rangle$  by

$$\langle \sigma_{ij} \rangle = C_{ijkl}^{\text{eff}} \langle \varepsilon_{kl} \rangle, \quad (2a)$$

$$\langle \varepsilon_{ij} \rangle = S_{ijkl}^{\text{eff}} \langle \sigma_{kl} \rangle. \quad (2b)$$

The effective elastic constants depend on their local values  $C_{ijkl}(\mathbf{r})$  and  $S_{ijkl}(\mathbf{r})$  which are given by single-crystal and structure properties if the inhomogeneous medium considered is a polycrystal. In this paper, a review of several theories is given which allow to calculate the effective elastic constants from statistical information about the local values  $C_{ijkl}(\mathbf{r})$ . Each method needs simplifying assumptions which lead to validity limitations. In most cases, single-phase polycrystals are considered although the theories do not require this restriction.

## 3. CALCULATION OF EFFECTIVE ELASTIC CONSTANTS OF POLYCRYSTALS

### 3.1. *Approximate Relations between Ensemble-Averaged Stress and Strain Tensors*

3.1.1. *The Voigt approximation.* The ensemble average of Eq. (1a) is given by

$$\langle \sigma_{ij} \rangle = \langle C_{ijkl} \varepsilon_{kl} \rangle. \quad (3a)$$

Voigt (1887; 1928) assumed the strain to be the same and hence equal to its mean value in each grain. From this (3a) follows to be

$$\langle \sigma_{ij} \rangle = \langle C_{ijkl} \rangle \langle \varepsilon_{kl} \rangle, \quad (3b)$$

that is, the Voigt approximation of the effective elastic constants  $C_{ijkl}^V$  is equal to its ensemble averages,

$$C_{ijkl}^V = \langle C_{ijkl} \rangle. \quad (4a)$$

This approximation satisfies the boundary conditions for strain but generally not for stress.

The Voigt approximation of the compliance tensor  $S_{ijkl}^V$  is the inverted elastic moduli tensor,

$$S_{ijkl}^V = (C^{V^{-1}})_{ijkl} = (\langle C \rangle^{-1})_{ijkl}. \quad (4b)$$

In single-phase polycrystals the position dependent variation of the elastic

constants is only caused by different orientations of the grains. The elastic constants of a grain with arbitrary orientation can be described by the single-crystal constants and a rotation. The averaged elastic constants follow from weighted integrations over all orientations. Weighting function is the orientation distribution function which describes the texture of the polycrystal considered. The Voigt approximation yields too large values for the effective elastic constants. Deviations from the actual values up to 20% or more occur depending on the elastic anisotropy (Chung and Buessem, 1967).

3.1.2. *The Reuss approximation.* Starting from the ensemble average of Eq. (1b)

$$\langle \varepsilon_{ij} \rangle = \langle S_{ijkl} \sigma_{kl} \rangle \quad (5a)$$

Reuss (1929) assumed the stress to be the same and hence equal to its mean value in each grain. The resulting elastic equation

$$\langle \varepsilon_{ij} \rangle = \langle S_{ijkl} \rangle \langle \sigma_{kl} \rangle \quad (5b)$$

yields the Reuss approximation of the compliance tensor to be equal to its ensemble average,

$$S_{ijkl}^R = \langle S_{ijkl} \rangle. \quad (6a)$$

The corresponding elastic constants are the elements of the inverted tensor,

$$C_{ijkl}^R = (S^{R^{-1}})_{ijkl} = (\langle S \rangle^{-1})_{ijkl}. \quad (6b)$$

The Reuss approximation satisfies the boundary conditions for stress but generally not for strain.

The averaged values of the elements of the compliance tensor can be calculated in the same way as the averaged elastic moduli which are needed for the Voigt approximation. The Reuss approximation yields too low values for the effective elastic constants.

3.1.3. *The Hill approximation.* Hill (1952) showed that the Voigt and the Reuss approximation are upper and lower bounds for the effective elastic constants of polycrystals and recommended to use the mean values of both approximations,

$$C_{ijkl}^H = \frac{1}{2}(C_{ijkl}^V + C_{ijkl}^R), \quad (7a)$$

$$S_{ijkl}^H = \frac{1}{2}(S_{ijkl}^V + S_{ijkl}^R). \quad (7b)$$

Hill's proposal cannot be justified by scientific arguments. It is only a phenomenological description of the elastic properties of polycrystalline materials which mostly yields good results but fails in the case of the large grain shape anisotropy.

The deviation of the Hill approximation from actual values is nearly independent of the orientation distribution of the grains (Kneer, 1965). Therefore, it is a good approximation to describe the texture dependence of the elastic properties of polycrystals. For example, Bunge (1968; 1974) used the Hill approximation to calculate the elastic moduli of cold rolled copper sheets and found a good agreement with experimental results.

3.1.4. *The Kröner approximation.* Kröner (1958) derived a relation for single-phase polycrystals connecting the ensemble average of the strain tensor  $\langle \varepsilon_{ij} \rangle$  and

the local stress  $\sigma_{ij}(\Omega)$  in a grain with an arbitrary orientation characterized by the solid angle  $\Omega$ , and vice versa, a relation connecting the ensemble average of the stress tensor  $\langle \sigma_{ij} \rangle$  and the local strain  $\varepsilon_{ij}(\Omega)$

$$\sigma_{ij}(\Omega) = p_{ijkl}(\Omega) \langle \varepsilon_{kl} \rangle, \quad (8a)$$

$$\varepsilon_{ij}(\Omega) = q_{ijkl}(\Omega) \langle \sigma_{kl} \rangle. \quad (8b)$$

From these equations the effective elastic moduli and the compliance tensor of the polycrystal considered follow to be equal to the ensemble averages of the tensor elements  $p_{ijkl}(\Omega)$  and  $q_{ijkl}(\Omega)$ , respectively,

$$C_{ijkl}^{\text{eff}} = \langle p_{ijkl} \rangle, \quad (9a)$$

$$S_{ijkl}^{\text{eff}} = \langle q_{ijkl} \rangle. \quad (9b)$$

In general, as well  $p_{ijkl}(\Omega)$  and  $q_{ijkl}(\Omega)$  as the local stress and strain components  $\sigma_{ij}(\Omega)$  and  $\varepsilon_{ij}(\Omega)$  are not only dependent on the orientation of the grain but also on its shape. Kröner assumed the stress-free grains to be spheres.

To calculate the tensor elements  $p_{ijkl}(\Omega)$  and  $q_{ijkl}(\Omega)$ , an in the stress-free case spherical single crystal embedded in a homogeneous matrix characterized by the effective elastic constants of the polycrystal is considered. The differences between the elastic moduli of the grain and the matrix and a homogeneous external deformation  $\langle \varepsilon_{ij} \rangle$  cause the local stress  $\sigma_{ij}(\Omega)$  and local strain  $\varepsilon_{ij}(\Omega)$  which are connected by the elastic constants of the single crystal  $c_{ijkl}(\Omega)$ ,

$$\sigma_{ij}(\Omega) = c_{ijkl}(\Omega) \varepsilon_{kl}(\Omega). \quad (10)$$

The single crystal may be replaced by elastically deformed matrix material which in the stress-free case is not a sphere but its shape is determined by the condition that the local stress  $\sigma_{ij}(\Omega)$  and the stress in the matrix will not change. The elastic deformation of the inserted matrix material is related to the deviation of its shape from a sphere in the stress-free case (Eshelby, 1957) and connected with the local stress by the effective elastic constants of the polycrystal. With these relations a connection between the local strain  $\varepsilon_{ij}(\Omega)$  and the homogeneous external strain  $\langle \varepsilon_{ij} \rangle$  can be derived which inserted into Eq. (10) yields determination equations for the tensor components  $p_{ijkl}(\Omega)$ . The tensor elements  $q_{ijkl}(\Omega)$  can be determined analogously. The results are given in the following equations,

$$p_{ijkl}(\Omega) = c_{ijkl}(\Omega) + c_{ijmn}(\Omega) u_{mnkl}(\Omega), \quad (11a)$$

$$q_{ijkl}(\Omega) = S_{ijkl}^{\text{eff}} + u_{ijmn}(\Omega) S_{mnlk}^{\text{eff}}, \quad (11b)$$

$$u_{ijkl}(\Omega) = -(\nu(\Omega)^{-1})_{ijmn} (c_{mnlk}(\Omega) - C_{mnlk}^{\text{eff}}), \quad (11c)$$

$$v_{ijkl}(\Omega) = c_{ijkl}(\Omega) - C_{ijkl}^{\text{eff}} + C_{ijmn}^{\text{eff}} w_{mnlk}. \quad (11d)$$

The tensor elements  $w_{ijkl}$  only depend on the effective elastic constants of the polycrystal. In the case of macroscopic isotropy they are given by

$$w_{1111} + 2w_{1122} = \frac{3C_{11}^{\text{eff}}}{C_{11}^{\text{eff}} + 2C_{12}^{\text{eff}}}, \quad (12a)$$

$$w_{1212} = \frac{w_{1111} - w_{1122}}{2} = \frac{5}{4} \frac{3C_{11}^{\text{eff}}}{4C_{11}^{\text{eff}} - C_{12}^{\text{eff}}}, \quad (12b)$$

$$w_{1111} = w_{2222} = w_{3333}, \quad (12c)$$

$$w_{1122} = w_{1133} = w_{2233}, \quad (12d)$$

$$w_{1212} = w_{1313} = w_{2323}, \quad (12e)$$

$$w_{ijkl} = 0 \quad \text{else.} \quad (12f)$$

The  $C_{ij}^{\text{eff}}$  are the effective elastic constants  $C_{ijkl}^{\text{eff}}$  of the polycrystal in the matrix notation. Ensemble averaging of Eqs (11), that is if spherical grains are assumed, integration with respect to all orientations of the grains, yields determination equations for the effective elastic constants  $C_{ijkl}^{\text{eff}}$  and the elements of the compliance tensor  $S_{ijkl}^{\text{eff}}$ . If the approximation each grain to be a sphere is not used but a grain shape distribution is assumed which allow a gap-less assemblage of the polycrystal the resulting effective compliance tensor will turn out to be the inverse of the elastic moduli tensor. The separate calculation of  $C_{ijkl}^{\text{eff}}$  and  $S_{ijkl}^{\text{eff}}$  using the equations (11a) and (11b) and the assumption of spherical grains yields upper and lower bounds for the effective elastic constants and compliance tensor elements (Kröner, 1958). In general, the differences between these bounds are within measurement inaccuracy. The self-consistent theory of Kröner fulfills the boundary conditions for stress and strain statistically exact.

Analytical results are given for macroscopically isotropic polycrystals with crystallites of cubic (Hershey, 1954) and of any desired symmetry (Kröner, 1958). Analogous calculations were carried out for polycrystals with fibre (Kneer, 1965) and rolling texture (Morris, 1970). The complicated equations (11) and (12) yield rather simple results, namely a cubic equation for the effective shear modulus, in the case of cubic single-crystal symmetry and macroscopical isotropy.

### 3.2. Results from Equilibrium Conditions for the Displacement Vector

#### 3.2.1. Dynamic description of the elastic properties

3.2.1.1. Relations between ultrasonic propagation and effective elastic constants. In an elastic medium the equation of motion follows from the condition that the force components must be equal to the acceleration components (Hershey, 1954)

$$\frac{\partial}{\partial x_j} \sigma_{ij} = \rho \frac{\partial^2}{\partial t^2} s_i. \quad (13)$$

$\rho$  is the density of the medium. If the linearized relation between the displacement vector  $\mathbf{s}$  and the strain tensor  $\varepsilon_{ij}$

$$\varepsilon_{ij} = \frac{1}{2} \left( \frac{\partial s_i}{\partial x_j} + \frac{\partial s_j}{\partial x_i} \right) \quad (14)$$

and the Hooke's law given in Eq. (1) which connects stress and strain by the elastic constants  $C_{ijkl}$  is substituted into (13) one gets the equation of motion for the displacement vector,

$$\frac{\partial}{\partial x_j} \left( C_{ijkl} \frac{\partial s_k}{\partial x_l} \right) - \rho \frac{\partial^2}{\partial t^2} s_i = 0. \quad (15)$$

In an inhomogeneous medium the elastic constants  $C_{ijkl}$  and the density  $\rho$  are position dependent.

In the case of macroscopic homogeneity it is convenient to consider the ensemble average of the displacement vector  $\langle \mathbf{s} \rangle$ . Approximately, it is assumed that the averaging of solutions of the equation of motion yields plane waves. In this case,  $\langle \mathbf{s} \rangle$  obeys a similar equation of motion which contains the position independent effective elastic constants  $C_{ijkl}^{\text{eff}}$  and density  $\rho_{\text{eff}}$ ,

$$C_{ijkl}^{\text{eff}} \frac{\partial^2 \langle s_k \rangle}{\partial x_j \partial x_l} - \rho_{\text{eff}} \frac{\partial^2 \langle s_i \rangle}{\partial t^2} = 0. \quad (16)$$

In a single-phase polycrystal no density variations occur, and the effective density  $\rho_{\text{eff}}$  is identically equal to the in this case position independent density  $\rho$ .

If the ensemble average of the displacement vector is the plane wave

$$\begin{aligned} \langle \mathbf{s} \rangle &= \mathbf{e}_P e^{i\omega t - i\boldsymbol{\beta} \cdot \mathbf{r}}, & \boldsymbol{\beta} &= \beta \mathbf{e}_\beta, \\ \mathbf{e}_P &= (n_1, n_2, n_3), & \mathbf{e}_\beta &= (n_{\beta 1}, n_{\beta 2}, n_{\beta 3}) \end{aligned} \quad (17)$$

with the angular frequency  $\omega$ , the possibly complex propagation constant  $\beta$ , propagation into  $\mathbf{e}_{\beta^-}$ , and polarization in  $\mathbf{e}_P$ -direction the derivations in (16) can be carried out and one gets

$$C_{ijkl}^{\text{eff}} n_{\beta j} n_{\beta l} n_k \beta^2 - \rho_{\text{eff}} \omega^2 n_i = 0. \quad (18)$$

From this equation the effective elastic constants can be determined if the propagation constants of plane ultrasonic waves in the inhomogeneous medium considered are known. For example, if  $\langle \mathbf{s} \rangle$  is the plane compressional wave propagating into  $\mathbf{e}_i$ -direction (its propagation constant is denoted by  $\beta_{Li}$ ) one has

$$C_{iii}^{\text{eff}} = \frac{\rho_{\text{eff}} \omega^2}{\beta_{Li}^2}. \quad (19a)$$

The plane shear wave with propagation into  $\mathbf{e}_i$ - and polarization in  $\mathbf{e}_j$ -direction (its propagation constant is denoted by  $\beta_{Tij}$ ) yields

$$C_{jji}^{\text{eff}} = \frac{\rho_{\text{eff}} \omega^2}{\beta_{Tij}^2}. \quad (19b)$$

In the macroscopically isotropic case these two propagation constants and therefore the effective elastic constants, too, are independent on direction and the remaining effective elastic constants are given by

$$C_{ijj}^{\text{eff}} = C_{iii}^{\text{eff}} - 2C_{ijj}^{\text{eff}}, \quad (19c)$$

$$C_{ijk}^{\text{eff}} = 0 \quad \text{else.} \quad (19d)$$

If texture is present, one gets directional dependent ultrasonic propagation constants, and, as a consequence, directional dependent effective elastic constants and effective anisotropy factors

$$A_k^{\text{eff}} = C_{kkk}^{\text{eff}} - C_{ijj}^{\text{eff}} - 2C_{ijj}^{\text{eff}}, \quad i \neq j \neq k, \quad i, j, k = 1, 2, 3 \quad (20)$$

not equal to zero. In this case, pure compressional and shear waves only occur if

propagation and polarization are parallel to symmetry axes of texture which complicates the calculation of the whole effective elastic moduli tensor.

In general, the frequency dependent description of ultrasonic propagation leads to complex propagation constants containing the sound velocities and the attenuation of the waves by scattering at the grain boundaries so that the effective elastic constants resulting from Eq. (18) are complex, too. The limiting case frequency equal zero yields the common real values.

3.2.1.2. *Calculation of ultrasonic propagation constants in polycrystals.* A series of papers deal with the problem to calculate the complex propagation constants of ultrasonic waves in polycrystals (Ranganathan, Dattagupta, 1979; Lifshits, Parkhomovskii, 1948 and 1950; Usov, Fokin, Shermergor, 1972 and 1976; Grigorev, Shermergor, 1981; Stanke, Kino, 1984; Hireskorn, 1982, 1983, 1985, 1986, 1988). Only the most general theories (Stanke, Kino, 1984; Hireskorn, 1982, 1983, 1985, 1986, 1988) which more or less include the others shall be considered in this paper.

Starting point is the equation of motion (15) of the displacement vector  $\mathbf{s}$ . If the inhomogeneity of the polycrystal considered is small it can be solved using perturbation theory. The zeroth order of the equation of motion is chosen to describe a homogeneous isotropic medium with wave numbers  $k$  and  $\kappa$  for the compressional and shear waves, respectively,

$$\hat{L}_0 \mathbf{s}^0 = \mathbf{C}_{jkl}^0 \frac{\partial^2 s_k^0}{\partial x_j \partial x_l} + \rho_0 \omega^2 \mathbf{s}^0 = 0, \quad (21a)$$

$$\mathbf{C}_{jkl}^0 = (C_{1jkl}^0, C_{2jkl}^0, C_{3jkl}^0),$$

$$C_{iii}^0 = \frac{\rho_0 \omega^2}{k^2}; \quad i = 1, 2, 3;$$

$$C_{ijij}^0 = \frac{\rho_0 \omega^2}{\kappa^2}; \quad i, j = 1, 2, 3; \quad i \neq j;$$

$$C_{ijij}^0 = \rho_0 \omega^2 \left( \frac{1}{k^2} - \frac{2}{\kappa^2} \right); \quad i, j = 1, 2, 3; \quad i \neq j; \quad (21b)$$

$$C_{ijkl}^0 = 0 \quad \text{else.}$$

It is convenient to choose the density  $\rho_0$  and in the case of macroscopic isotropy even the elastic constants  $C_{ijkl}^0$  of the homogeneous isotropic approximation to be equal to the corresponding averaged values of the polycrystal. The deviation of the exact equation of motion from this homogeneous isotropic approximation

$$\varepsilon \hat{L}_1 \mathbf{s} = (\hat{L}_0 - \hat{L}) \mathbf{s} = -\rho' \omega^2 \mathbf{s} - \frac{\partial}{\partial x_j} \left( \mathbf{C}'_{jkl} \frac{\partial s_k}{\partial x_l} \right),$$

$$\rho' = \rho - \rho_0, \quad \mathbf{C}'_{jkl} = \mathbf{C}_{jkl} - \mathbf{C}_{jkl}^0 = (C'_{1jkl}, C'_{2jkl}, C'_{3jkl}) \quad (22)$$

is assumed to be small. That is, the relative mean quadratic differences  $\varepsilon_{\text{long}}^2$  and  $\varepsilon_{\text{trans}}^2$  of the wave numbers  $k_p$  and  $\kappa_p$  in the inhomogeneous material considered

and its values in the zeroth order approximation have to be much less than 1,

$$\varepsilon_{\text{long}}^2 = \frac{\langle (k_p - k)^2 \rangle}{k^2} \ll 1, \quad (23a)$$

$$\varepsilon_{\text{trans}}^2 = \frac{\langle (\kappa_p - \kappa)^2 \rangle}{\kappa^2} \ll 1. \quad (23b)$$

In a single-phase polycrystal  $\varepsilon_{\text{long}}$  and  $\varepsilon_{\text{trans}}$  are mainly determined by the ratio of the anisotropy factor and the single-crystal elastic constants. With this assumption the equation of motion can be expanded with respect to the inhomogeneity. The expansion yields the ensemble average of the displacement vector to be equal to an infinite series of operators acting on the solution of the homogeneous isotropic approximation of the equation

$$\langle \mathbf{s} \rangle = \left\{ 1 + \varepsilon \hat{L}_0^{-1} \sum_{\nu=0}^{\infty} \varepsilon^{\nu} \langle \hat{L}_1 (\hat{L}_0^{-1} \hat{L}_1)^{\nu} \rangle \right\} \mathbf{s}^0. \quad (24a)$$

The inverse operator  $\hat{L}_0^{-1}$  follows from the Green's function of the operator  $\hat{L}_0$  which is given in the literature (Lifshits, Parkhomovskii, 1950; Hirsekorn, 1988).

For further calculations the truncated series which contains all terms up to quadratic order in  $\varepsilon$ , that is the second order Born approximation, is used (Hirsekorn, 1982, 1983, 1985, 1986),

$$\langle \mathbf{s} \rangle = \{ 1 + \varepsilon \hat{L}_0^{-1} \langle \hat{L}_1 \rangle + \varepsilon^2 \hat{L}_0^{-1} \langle \hat{L}_1 \hat{L}_0^{-1} \hat{L}_1 \rangle \} \mathbf{s}^0. \quad (24b)$$

Equations (17) and (24b) allow calculation of the complex propagation constants  $\beta$  of plane ultrasonic waves in dependence on its propagation and polarization direction. The Born approximation causes a validity limitation for large frequencies by the relations

$$ka \ll \frac{1}{\varepsilon_{\text{long}}} = \frac{k}{\{ \langle (k_p - k)^2 \rangle \}^{1/2}}, \quad \kappa a \ll \frac{1}{\varepsilon_{\text{trans}}} = \frac{\kappa}{\{ \langle (\kappa_p - \kappa)^2 \rangle \}^{1/2}}. \quad (25)$$

$a$  is the mean grain radius.

Analytical calculations were carried out for single-phase polycrystals of cubic crystal symmetry with randomly oriented grains (Hirsekorn, 1982 and 1983) and for those with texture of orthorhombic symmetry (Hirsekorn, 1985 and 1986), e.g. rolling or fibre texture. In the case of single-phase polycrystals no density variations occur. The calculations are based upon two additional assumptions:

a) All grains have the same size and shape, and integrals over a grain volume are approximately equal to the corresponding integrals over a sphere of the same volume.

b) The probability to have a special set of material constants is the same for each grain, and there is no correlation between them from grain to grain.

The assumption of same size and shape for all grains causes periodic oscillations of the sound velocities and scattering coefficients as function of frequency.

Using the fact that the operator  $\hat{L}_0$  acting on  $\mathbf{s}^0$  yields zero from the infinite series (24a) determining the ensemble average of the displacement vector of the homogeneous isotropic solution  $\mathbf{s}^0$  can be eliminated. With the assumption of

small inhomogeneity the resulting infinite series

$$\hat{L}_0 \langle \mathbf{s} \rangle = \varepsilon \sum_{\nu=0}^{\infty} \varepsilon^{\nu} \langle \hat{L}_1 (\hat{L}_0^{-1} \hat{L}_1)^{\nu} \rangle \sum_{\mu=0}^{\infty} \left\{ -\varepsilon \hat{L}_0^{-1} \sum_{\nu=0}^{\infty} \varepsilon^{\nu} \langle \hat{L}_1 (\hat{L}_0^{-1} \hat{L}_1)^{\nu} \rangle \right\}^{\mu} \langle \mathbf{s} \rangle \quad (26a)$$

approximately can be truncated (Keller approximation). If only terms up to second order in  $\varepsilon$  are taken into account (Stanke, Kino, 1984; Hirsekorn, 1988) the ensemble average of the displacement vector obeys the equation

$$\langle \hat{L}_0 - \varepsilon \langle \hat{L}_1 \rangle - \varepsilon^2 (\langle \hat{L}_1 \hat{L}_0^{-1} \hat{L}_1 \rangle - \langle \hat{L}_1 \rangle \hat{L}_0^{-1} \langle \hat{L}_1 \rangle) \rangle \langle \mathbf{s} \rangle = 0. \quad (26b)$$

The Keller approximation causes no validity limitation for large frequencies but yields only numerically solvable determination equations for the complex propagation constants of plane ultrasonic waves. This method was first applied to macroscopically isotropic single-phase polycrystals of cubic crystal symmetry (Stanke, Kino, 1984), and later generalized to macroscopically isotropic multi-phase polycrystals with phases of cubic, hexagonal, or orthorhombic crystal symmetry (Hirsekorn, 1988). These calculations do not contain the assumption of same size and shape for all grains but use a directional independent size and shape distribution. As a consequence, the oscillations of the sound velocities and scattering coefficients as function of frequency disappear. The assumptions, that the probability to have a special set of material constants is the same for each grain, and that there is no correlation between them from grain to grain are maintained.

As to be expected, in the Rayleigh and resonance region the numerical results calculated from the Born and the Keller approximation only differ insignificantly, but there are to be found essential differences within the region of geometric reflection (Stanke, Kino, 1984).

For accuracy improvement as well the Born as the Keller approximation can be used in higher than second order. The zeroth order of both approximations are identically equal to the Voigt approximation of the effective elastic constants if a macroscopically isotropic polycrystal is considered. The equation of motion can be solved analogously using the Reuss approximation as zeroth order of the expansion.

**3.2.2. The static equilibrium condition.** The dynamic description of the elastic properties of a polycrystal includes static results which are the limiting case frequency equal to zero. The asymptotic behaviour at low frequencies of the complex propagation constants of ultrasonic waves can be seen by expansion with respect to small values of  $ka$  and  $ka$ , respectively (Stanke, Kino, 1984; Hirsekorn, 1982, 1983, 1985, 1986, 1988). The sound velocities retain a constant part and a term quadratic in frequency while the scattering coefficients are proportional to the fourth power of frequency in the Rayleigh region. Therefore, at frequency equal to zero the imaginary parts of the complex propagation constants (scattering coefficients) vanish and only the real parts (wave numbers) remain which, substituted into Eq. (18), yield real values for the effective elastic constants of the polycrystal considered.

The same results can be maintained if instead of the equation of motion the

static equilibrium condition for the displacement vector

$$\frac{\partial}{\partial x_j} \left( C_{ijkl} \frac{\partial s_k}{\partial x_l} \right) = 0 \quad (27)$$

is solved. Lifshits and Rosentsweig (1946) calculated the effective elastic constants of macroscopically isotropic single-phase polycrystals of cubic or hexagonal crystal symmetry up to terms of quadratic order in the inhomogeneity which is characterized by the anisotropy factor in the case of single-phase polycrystals.

By Hashin and Shtrikman (1962) additionally the effective compliance tensor elements are determined in the same order of accuracy, and there is shown that the results valid up to quadratic order, analogously to the Voigt and Reuss approximation which contain only the linear terms with respect to the anisotropy factor, represent upper and lower bounds for the real effective elastic constants of polycrystals.

The dynamic description of the elastic properties of polycrystals outlined in the preceding chapter is correct up to second order in the inhomogeneity, too. Its results at frequency equal to zero are identical with those given by Lifshits and Rosentsweig (1946) and by Hashin and Shtrikman (1962).

As has been done in the case of the equation of motion, the static equilibrium Eq. (27) is solved with the Green's function technique. A fictitious homogeneous reference material with the static equilibrium condition

$$C_{ijkl}^0 \frac{\partial^2 s_k^0}{\partial x_j \partial x_l} = 0 \quad (28a)$$

and the position independent elastic moduli  $C_{ijkl}^0$  is defined. The Green's function  $g_{ik}(\mathbf{r} - \mathbf{r}')$  of Eq. (28a) which obeys the relation

$$C_{ijkl}^0 \frac{\partial^2}{\partial x_j \partial x_l} g_{mk}(\mathbf{r} - \mathbf{r}') = \delta_{im} \delta(\mathbf{r} - \mathbf{r}') \quad (28b)$$

yields the integral representation of the static equilibrium condition of the polycrystal (27) as follows:

$$s_i(\mathbf{r}) = s_i^0(\mathbf{r}) - \int d^3 r' g_{ik}(\mathbf{r} - \mathbf{r}') \frac{\partial}{\partial x'_l} \left( C'_{klmn}(\mathbf{r}') \frac{\partial s_m(\mathbf{r}')}{\partial x'_n} \right), \quad (29)$$

$$C'_{ijkl} = C_{ijkl} - C_{ijkl}^0.$$

The displacement vector  $\mathbf{s}^0(\mathbf{r})$  represents a solution of equation (28a). If the fictitious homogeneous reference material is a good zeroth order approximation of the polycrystal considered so that the deviations  $C'_{ijkl}$  of the actual elastic constants from those of the reference material can be looked at as a small perturbation, Eq. (29) can be solved approximately by expanding with respect to the inhomogeneity and taking into account only a finite number of terms.

By partial integration and subsequent differentiation Eq. (29) can be converted into an integral equation for the strain tensor (Lippmann-Schwinger type

equation):

$$\varepsilon_{ij}(\mathbf{r}) = \varepsilon_{ij}^0(\mathbf{r}) + \int d^3r' G_{ijkl}(\mathbf{r}, \mathbf{r}') C'_{klmn}(\mathbf{r}') \varepsilon_{mn}(\mathbf{r}'), \quad (30)$$

$$G_{ijkl}(\mathbf{r}, \mathbf{r}') = \frac{1}{2} \frac{\partial}{\partial x'_i} \left( \frac{\partial}{\partial x_j} g_{ik}(\mathbf{r} - \mathbf{r}') + \frac{\partial}{\partial x_i} g_{jk}(\mathbf{r} - \mathbf{r}') \right).$$

From this equation a formally exact solution for the effective elasticity tensor of a polycrystal can be derived (Zeller, Dederichs, 1973; Dederichs, Zeller, 1972; Fokin, Shermergor, 1969; Fokin, 1972; Gubernatis, Krumhansl, 1975). Corresponding results can be found for the effective compliance tensor (Dederichs, Zeller, 1972) if the integral equation for the stress tensor is posed. It is shown that the formal solution for the effective elasticity tensor is identically equal to the Kröner approximation if the elastic moduli of the used homogeneous reference body are chosen to be equal to the effective elastic constants of the polycrystal considered (Shermergor, Patlazhan, 1976).

The formal results can be expanded with respect to the inhomogeneity up to any order desired. Analytical results are given up to third order for macroscopically isotropic polycrystals of cubic crystal symmetry (Zeller, Dederichs, 1973). It is shown that in general all approximations of odd order in the inhomogeneity of the elasticity tensor give upper bounds for the effective elastic constants. Lower bounds are given by the analogous approximation of odd order for the compliance tensor (Dederichs, Zeller, 1972). Kröner (1977) extended the theory to include the bounds of even order in the inhomogeneity and indicated how these bounds can be made optimum taking into account the given statistical informations. The numerical evaluation for polycrystalline copper (Kröner, 1974) shows clearly the moving together of the upper and lower bounds with ascending order in the inhomogeneity.

The calculation of terms of higher order in the inhomogeneity needs more and more information about the polycrystal. For example, the linear and the quadratic term only depend on the orientation distribution of the grains but not on their shapes and sizes. Contrary to this, the calculation of the third order term presumes the knowledge of grain shape. Analytical solutions can be found only for spherical or ellipsoidal grains (Zeller, Dederichs, 1973). The complete mathematical formalism (Kröner, 1978) shows how the formal solutions of Lippmann-Schwinger type equations depend on correlation functions of any order and how a material in a statistical sense perfectly homogeneous, isotropic, and disordered can be defined. It is obvious that generally the effective elasticity and compliance tensors approximately calculated by expansion with respect to the inhomogeneity represent upper and lower bounds for the real effective elastic constants only if the polycrystal considered fulfills the used suppositions.

Several papers deal with the analytic and numeric evaluation of the formal solutions for the effective elastic constants of polycrystals for special cases. Self-consistent results following from the formally exact solutions are given for polycrystalline copper with axial texture (Kuzmenko, Korneev, Shermergor, 1983). General expressions which yield the effective elastic constants up to second-order terms of macroscopically isotropic polycrystals with any single-crystal symmetry are derived (Middya, Paul, Basu, 1985) and evaluated for

hexagonal, tetragonal, trigonal, orthorhombic, and monoclinic symmetry (Middya, Basu, 1986; Paul, Middya, Basu, 1986). The results for cubic single-crystal symmetry are already given by Zeller and Dederichs (1973).

#### 4. CONCLUDING REMARKS

There are to distinguish three essentially different methods to calculate the effective moduli and compliance tensors of polycrystals from single-crystal and structure properties:

1. Single-crystal properties are averaged; e.g. the effective elastic constants are set to be equal to the corresponding averaged single-crystal elastic moduli while the effective compliance tensor follows from the effective elastic moduli tensor by inversion (Voigt approximation), or vice versa, the elements of the effective compliance tensor are determined by averaging the corresponding single-crystal quantities, and the inversion of this tensor yields the effective elastic moduli (Reuss approximation), or the mean values of both approximations are taken (Hill approximation).
2. The self-consistency method from Kröner derives an effective stress-strain relation taking into account the boundary conditions of stress and strain at the grain boundaries statistically exact.
3. The equation of motion (dynamic description) or the static equilibrium condition (limiting case frequency equal to zero) of the displacement vector are solved approximately using the assumption of small inhomogeneity in the polycrystal considered or formally exact with subsequent self-consistent evaluation.

If a frequency dependent description of the elastic properties of a polycrystal is required only the third method is applicable. The most accurate and theoretically well-founded static method is the self-consistency method. But its evaluation is rather lengthy, needs exact suppositions concerning the statistical properties of the polycrystal, and the yielded numerical results are in many cases nearly the same as follows from the Hill approximation.

The formal solution of the static equilibrium condition of the displacement vector is identical with the self-consistency method of Kröner if the elastic constants of the used reference body are set equal to the effective elastic constants of the polycrystal considered (Gubernatis, Krumhansl, 1975). Expansion with respect to small inhomogeneity of the formal solutions yields upper and lower bounds for the effective elastic constants.

Most of the calculations are carried out for single-phase polycrystals although the theories do not require this restriction. Analytical results are given as well for macroscopically isotropic polycrystals as for those with texture of orthorhombic symmetry with cubic, hexagonal, or orthorhombic single-crystal symmetry. In order to describe the elastic properties of multi-phase polycrystals the analytical evaluations should be generalized.

This paper deals with elastic properties of inhomogeneous media, especially polycrystals. Another important field adjacent to this matter is the elastic-plastic behaviour of microinhomogeneous materials. A promising method to handle this

problem is the extension of the self-consistent approach to plasticity (Berveiller, Hihhi, Zaoui, 1981; Zaoui, 1985). The theory of plasticity is not as firmly based and developed as the linear elastic one, but in spite of many approximations and simplifications it can be used to describe several aspects of metal forming.

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