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A calculation of the bulk modulus of polycrystalline materials

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It is shown that the bulk modulus of a polycrystalline material, composed of cubic single crystals, is the same as that of the constituent single crystal. The bulk modulus of the aggregate is independent of the distribution of the individual single crystals. The same results apply also to other polycrystalline systems, whose constituent single crystals undergo a pure uniform contraction when subjected to hydrostatic pressure.

1. Introduction

The elastic constants of polycrystalline materials depend in general on the elastic constants of the constituent single crystals and the orientation distribution of these over a given volume. Calculation of the exact elastic constants of a polycrystalline aggregate is in most cases not easy, even if the distribution of the individual single crystals is specified precisely. For isotropic polycrystals it might be thought at first sight that the elastic constants could be obtained from those of the individual single crystals by the method of simple averaging. This is, however, not so. If we regard the deformation of the polycrystal simply as the result of the deformation of the constituent single crystal, it would, in principle, be necessary to solve the equations of equilibrium for every single crystal, taking into account the appropriate boundary conditions at their surfaces of separation [1]. Thus, the relationship between the elastic properties of the whole polycrystal and those of its constituent single crystal depend on their actual form of the latter and the degree of correlation of their mutual orientations. A general relationship between the elastic constants of the polycrystal and the constituent single crystal of the same material is difficult to obtain. The problem becomes even more complicated when we consider polycrystals with texture, i.e. with anisotropic properties.

Calculations concerning the elastic constants of polycrystals have been based either on numerical simulations of the aggregate mass or have used some well known approximations such as those of Voigt [2] and Reuss [3]. These approximations in general give bounds for the values of the elastic constants of the polycrystal. Bishop and Hill [4] and Hill [5] considered an isotropic, statistically homogeneous polycrystal composed of cubic single crystals. For this case the upper and lower bounds for the bulk modulus of the polycrystal, obtained using the Voigt and Reuss approximations, were the same and equal to the bulk modulus of the cubic single crystal. While any aggregate theory should consider the conditions of both continuity and equilibrium, Bell [6] in his discussion of prediction of aggregate properties points out that the analysis of Bishop and Hill explicitly included only the continuity condition. By using a similar approach, Andrews [7] calculated the bulk modulus of a class of cubic polycrystals with texture; in this case too the approximations showed that the bulk modulus of the polycrystalline aggregate was the same as that of the component single crystal. This led him to speculate that for all polycrystals composed of cubic single crystals of the same material, the bulk modulus of the aggregate is the same as that of the individual single crystal. Lifshitz and Rozentsveig [8] have calculated with fair accuracy the moduli of an isotropic polycrystal when the elastic properties of the constituent single crystals are nearly isotropic. A first approximation to the elastic moduli of the polycrystal found it to be the same as the "isotropic" part of the single crystal modulus. A second approximation leads to additional terms which were quadratic in the "anisotropic" part of the modulus. However, these terms were found to be independent of the shape of the single crystals and the correlation of their orientations. More recently, Sowerby, Viana and Davies [9] have discussed a method, using a crystallite orientation distribution function (CODF), to correlate texture and mechanical properties of materials. The CODF expresses the probability that a crystallite has a certain orientation and this function can be obtained from a limited number of pole figure distributions. It is possible that such an approach can also be used to obtain the bulk modulus of polycrystalline materials from a knowledge of the single crystal's modulus.

In this paper, a purely analytical approach has been used to give an exact calculation of the bulk modulus of polycrystals, whose constituent single crystals have cubic symmetry. The results also hold for some classes of crystals besides those of cubic symmetry.

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2. Analysis

We assume familiarity with basic crystal elasticity theory and associated tensor notation. Details in this latter respect can be found in Nye [10] and Landau and Lifshitz [1].

Consider a cubic single crystal subjected to a uniform hydrostatic pressure p. If K is the bulk modulus of this crystal then

$$p = -K\Delta \tag{1}$$

where Δ is the uniform dilatation or fractional change in volume of the single crystal. For the case of crystals with cubic symmetry such a relation holds because the linear compressibility is isotropic [10]; a sphere of a cubic crystal when subjected to a hydrostatic pressure remains a sphere. Under these conditions the stress (σ_{ij}) and strain (ε_{ij}) in the solid are

$$\sigma_{ij} = -p\delta_{ij} \tag{2a}$$

and

$$\varepsilon_{ij} = \tfrac{1}{3}\Delta\delta_{ij} \tag{2b}$$

where δ_{ij} is the Kronecker delta function; $\delta_{ij} = 0$, for $i \neq j$, and is unity otherwise. Now, $\varepsilon_{ii} = \Delta$ and therefore the fractional linear change in length, i.e. the strain ε_{ij}, is one third of the dilatation. The stress–strain relationship for the cubic single crystal can be assumed to be

$$\sigma_{ij} = c'_{ijkl}\varepsilon_{kl} \tag{3}$$

where c'_{ijkl} is the stiffness constant tensor for the cubic crystal in the four suffix notation [10]. By substituting Equations 1 and 2 in Equation 3 and simplifying we obtain

$$c'_{ijkl}\delta_{kl} = 3K\delta_{ij} \tag{4}$$

Now, the polycrystal is made up of a number of single crystals in various orientations and hence the stiffness constant tensor $c_{ijkl}(\boldsymbol{r})$ in the polycrystal is a function of position $\boldsymbol{r}$, thus

$$c_{ijkl}(\boldsymbol{r}) = M_{mi}(\boldsymbol{r})\,M_{nj}(\boldsymbol{r})\,c'_{mnop}M_{ok}(\boldsymbol{r})\,M_{pl}(\boldsymbol{r}) \tag{5}$$

where c'_{mnop} is the stiffness constant tensor of the single crystal in its principal axis system and the $M_{rs}(\boldsymbol{r})$ is a rotation matrix that rotates the coordinate system from the principal axes of the single crystal at position $\boldsymbol{r}$ to the global axis system of the polycrystalline material. Equation 5 defines the stiffness constant tensor of the polycrystal at position $\boldsymbol{r}$ in its global axis system.

If this polycrystal is subjected to external traction and is in equilibrium then the stress and strain in the polycrystal satisfy the equilibrium equations

$$\sum_{j=1}^{3}\frac{\partial\sigma_{ij}}{\partial x_j} = 0 \quad i = 1, 2, 3 \tag{6}$$

and the equation of compatibility.

Let the polycrystalline material be subjected to external forces or displacements, which give rise to stresses and strains in the individual single crystals. We shall assume that the stress and strain in a single crystal is uniform. Then the effective stiffness constant tensor of the polycrystal $\bar{c}_{ijkl}$ is defined as [10]

$$\bar{c}_{ijkl}\langle\varepsilon_{kl}\rangle = \langle c_{ijkl}\varepsilon_{kl}\rangle \tag{7}$$

where the angular brackets denote an average of the respective quantities over a whole aggregate. With every single crystal of the polycrystalline aggregate is associated a rotation matrix $M_{rs}(\boldsymbol{r})$. The rotation matrices are orthogonal and satisfy the equations,

$$M_{ik}M_{jk} = M_{ki}M_{kj} = \delta_{ij} \tag{8}$$

In view of the orthogonality relation Equation 8 and the fact that c'_{mnop} satisfies Equation 4, it is easily verified by substitution that the tensor $c_{ijkl}(\boldsymbol{r})$ also satisfies Equation 4. Now Equations 1 to 3 are satisfied simultaneously if and only if Equation 4 holds under identical conditions. Therefore the state of stress and strain everywhere in the polycrystal corresponds to a pure hydrostatic pressure and to uniform dilatation respectively. Moreover, if these are assumed to be independent of position the corresponding stress and strain clearly satisfy the equilibrium and compatibility equations and the boundary conditions as well as being the same in every constituent single crystal of the aggregate. By the uniqueness theorems of elasticity the above solutions, therefore, completely represent the state of stress and strain everywhere in the polycrystal. Substituting these values of stress and strain in Equation 7 gives,

$$\bar{c}_{ijkl}\langle\varepsilon_{kl}\rangle = \bar{c}_{ijkk}\frac{\Delta}{3} \tag{9}$$

and $\langle c_{ijkl}\varepsilon_{kl}\rangle = \langle c_{ijkk}\rangle(\Delta/3) = 3K\delta_{ij}(\Delta/3) = K\Delta\delta_{ij}$. We have used the identity that $c_{ijkk} = c_{ijkl}\delta_{kl} = 3K\delta_{ij}$ from Equation 4.

It remains to be shown that K is also the bulk modulus of the polycrystal. Since $\bar{c}_{ijkl}\langle\varepsilon_{kl}\rangle = \langle c_{ijkl}\varepsilon_{kl}\rangle$ from Equation 5, then using Equation 9 we see that $\bar{c}_{ijkk}(\Delta/3) = K\Delta\delta_{ij}$ or $\bar{c}_{ijkk} = 3K\delta_{ij}$. This shows that the effective stiffness constant tensor of the polycrystal also satisfies Equation 4.

From Equation 3 we obtain the following equation for the average stress ($\bar{\sigma}_{ij}$) in the polycrystal

$$\bar{\sigma}_{ij} = \langle c_{ijkl}\varepsilon_{kl}\rangle = K\Delta\delta_{ij} \tag{10}$$

However, since the state of stress everywhere in the polycrystal is a uniform hydrostatic pressure p, we find using Equation 2a in Equation 10, the following relationship between hydrostatic pressure and dilatation for the polycrystal

$$p = -K\Delta$$

K is the same as that of the single crystal. Hence we have shown that the bulk modulus of the polycrystal and of the constituent single cubic crystal are the same.

3. Remarks

Our analysis has been carried out for the case of polycrystals composed of constituent cubic single crystals. In proceeding through the analysis it is seen that our derivation holds, in general, as long as Equation 4 holds for the individual single crystal system. This is certainly true for cubic single crystal systems but it may also be valid in crystals having other types of symmetries. In particular it is true for polycrystals composed of single crystals, whose response to a hydrostatic pressure is a pure contraction.

In our derivation we have made no assumptions as to the nature of the distribution of the single crystals in the polycrystalline aggregate. Hence the results derived hold for any distribution of single crystals in the aggregate. In practical terms, this implies for instance that the bulk modulus of a rolled polycrystalline copper sheet will be the same as that of an isotropic sheet of the same metal. Furthermore, that bulk modulus is equal to that of a single crystal of copper.

The experimentally determined bulk modulus of single crystal cubic boron nitride and single crystal cubic diamond are 3×10^3 and $4.4 \times 10^3 \mathrm{N\,m^{-2}}$ respectively [11]. These values are within 10% of the corresponding values for polycrystalline CBN and diamond (which are directly bonded without a binder) [11, 12]. Experimental values of the bulk modulus of some cubic metal crystals tabulated in Gilman [13] also show good agreement with the bulk modulus of the corresponding polycrystals obtained from the CRC handbook. A survey of the literature however has not yielded systematic experimental results of the bulk modulus of single and polycrystals.

It may be possible to extend this analysis to other types of crystal systems as well as to polycrystals composed of more than one kind of single crystal material.

4. Conclusions

An analysis has been presented to calculate the bulk modulus of polycrystalline materials composed of cubic single crystals of a single material. The bulk modulus of the aggregate is shown to be independent of the distribution of the constituent single crystals and is equal to the bulk modulus of the constituent cubic single crystal. The same analysis also applies to systems possessing some symmetries of the cubic crystal, in particular those single crystals whose response to a hydrostatic pressure is a uniform contraction.

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