

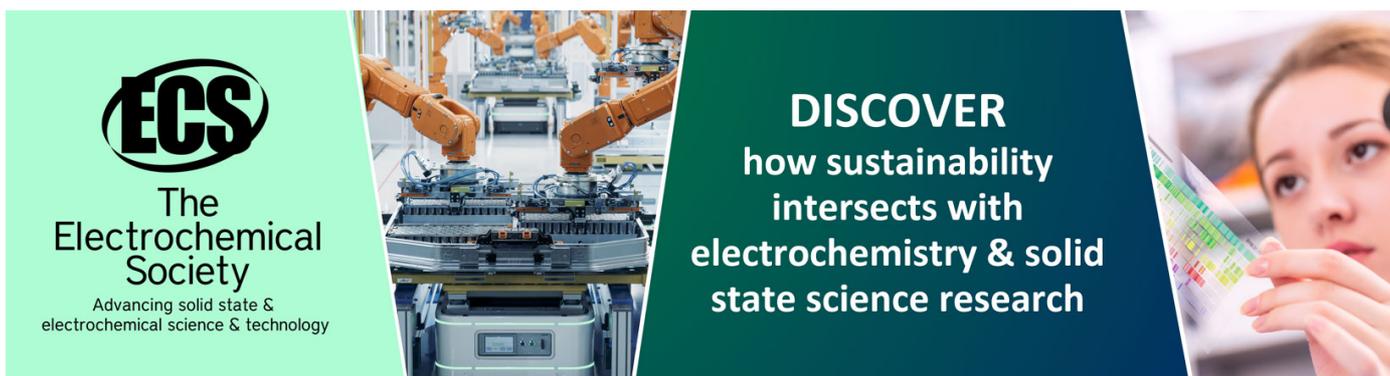
## Elastic moduli of polycrystalline cubic metals

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## Elastic moduli of polycrystalline cubic metals

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**Abstract.** It was noted previously (Date and Andrews 1969) that the expression  $2/E+1/G=\text{constant}$  applied to some polycrystalline cubic metals, as it would to bar specimens cut from single crystals. The value of the constant would be somewhat different. Reynolds (1970) showed that the relationship was one of a number connected with the rotated average moduli for bar specimens. It was thought that these relationships would be sufficient to enable the elastic constants to be determined from measurements on polycrystalline specimens. These would be true or modified single-crystal constants.

The present paper represents a further stage and aims to clarify and extend the previous work. It is shown that the orientation-independent relationships referred to are not in fact independent of each other and are insufficient to enable the constants to be found. Some useful results do, however, follow. Thus, the methods of Reuss, Voigt and Hill lead to the same calculation of bulk modulus for polycrystalline materials and show that it should be identical with the single-crystal value.

It is also shown why polycrystalline cubic metals behave in an isotropic manner when the grains are completely randomly oriented. Departures from randomness (development of an orientation texture) render increasingly invalid the widely accepted relationship between  $E$ ,  $G$  and  $\nu$  (Poisson's ratio), viz.  $E=2G(1+\nu)$ . The effect is more pronounced, the greater the anisotropy of the single crystals. As a consequence values of  $\nu$  obtained by the engineering formula may be spurious and unreliable. If, however, practical values of  $E$  and  $G$  are used to reveal such values of  $\nu$ , a knowledge of the average value of the ratio can be used to provide values of  $E$  and  $G$  for untextured materials.

### 1. Introduction

The problem of relating the fundamental elastic properties of anisotropic single crystals to those of polycrystalline bulk materials has been the subject of a considerable research effort but there are still a number of unresolved problems. In general it is accepted that the properties of the polycrystalline material will be represented by the single-crystal values averaged over all orientations and secondly that some accommodation is needed due to the change in properties from grain to grain across grain boundaries where there is a change in orientation. The approximation of Voigt (1928) assumed uniform strain throughout the material and this gives relationships in terms of elastic stiffness ( $c_{ij}$ ). The alternative 'uniform stress' approach of Reuss (1929) leads to expressions in terms of elastic compliances ( $s_{ij}$ ). Practical measurements appear to lie in between and Hill (1952) suggested that the average should be taken of the two approximations. Further contributions have been made, for example, by Markham (1962) and Schreiber *et al* (1973). Experimental work has generally relied on a comparison between measured and

calculated properties, requiring a knowledge of the single-crystal constants (see for example Davies *et al* 1972).

The present paper extends the conclusions of earlier work by Date and Andrews (1969) and Reynolds (1970). It is intended to facilitate the interpretation of the properties of polycrystalline materials, particularly where the single-crystal constants are not necessarily known or are conceivably *modified* by the incorporation into polycrystals and by alloying. Such for example is the case with many steels whether based on the body-centred cubic  $\alpha$ -iron structure or the face-centred  $\gamma$ -iron structure. Alloy elements in solid solution have systematic effects on increasing or decreasing the moduli  $E$  and  $G$ , which are generally not large but can, as in the case of Ni or C, alter the moduli by amounts up to 7% of the value for pure Fe. The subject was investigated in detail by Speich *et al* (1972). It is recognised that the presence of second-phase particles may also have an effect depending on their type, quantity and distribution of the particles.

The present approach is that, if the elastic properties of polycrystalline bars are deduced on the basis of either the Voigt or the Reuss assumptions, then certain combinations of these properties lead to an elimination of the orientation dependence. Some of these properties and the combinations correspond to, and may in certain cases be equal to, measured values expressed in terms of  $E$ ,  $G$  or  $\nu$  (Poisson's ratio). Where the equality does not apply directly the implication is that the measured values should lie between those indicated by the two approximations (in the manner noted in the first paragraph). Alternatively the true values of the elastic constants  $c_{ij}$ , or compliances  $s_{ij}$ , may not be known, as in the case of many practical alloys such as steels. The experimentally measured values, and the derived relations might therefore be used to determine 'quasi-single-crystal constants' for the polycrystalline material.

A related problem arises from the use of formulae strictly only applicable to isotropic materials, to polycrystalline materials in which the individual grains are markedly anisotropic. A notable example is the use of a common relationship between  $E$ ,  $G$  and  $\nu$  which becomes increasingly invalid if the polycrystalline metal develops a texture. This problem was noted previously (Date and Andrews 1969) but is further considered here and some practical applications are indicated.

## 2. Basic and derived relationships

The basic average moduli for cubic materials based on the two assumptions referred to were given by Reynolds (1970) and are summarised here for convenience of reference in table 1. The practically determined moduli which have been indicated are not necessarily exact equalities and cannot be simultaneously so for both approximations (unless  $c=s=0$ ). They refer to bar axes along OZ (subscript 33). In this table and table 2, the orientation factor  $\Delta$  is the sum  $(l^2m^2 + m^2n^2 + n^2l^2)$  when  $l$ ,  $m$ ,  $n$  are the direction cosines for the axis of the specimen with reference to the crystal axes.

Equations (1)–(6) in table 1 may then be used to give the derived relationships (13)–(18) on the left-hand side of table 2. The equivalent derivations for expressions in terms of  $C_{ij}$  or  $c_{ij}$  are on the right-hand side, viz. equations (19)–(24) derived from (7) to (12).

In table 2, equation (13) is the expression noted by Date and Andrews (1969) and confirmed by Armstrong and Mordike (1970). The expression was found to apply to single crystals and also to polycrystalline steels. It was used to relate elastic moduli for different directions in a material with a partially developed orientation texture. It also enabled the variation of moduli with composition to be established when the results were

Table 1. Basic average moduli for cubic materials.

(a) Uniform stress averages of block compliances (Reuss)		(b) Uniform strain approximation (Voigt)	
$S_{11} = s_{11} - (\frac{3}{4}\Delta + \frac{1}{4})s$	(1)	$C_{11} = c_{11} - (\frac{3}{4}\Delta + \frac{1}{4})c$	(7)
$S_{33} = s_{11} - 2\Delta s \simeq \frac{1}{E}$	(2)	$C_{33} = c_{11} - 2\Delta c \simeq \frac{E(1-\nu)}{(1+\nu)(1-2\nu)}$	(8)
$S_{13} = s_{12} + \Delta s \simeq -\frac{\nu}{E}$	(3)	$C_{13} = c_{12} + \Delta c \simeq \frac{E\nu}{(1+\nu)(1-2\nu)}$	(9)
$S_{12} = s_{12} + \frac{1}{4}(1-\Delta)s$	(4)	$C_{12} = c_{12} + \frac{1}{4}(1-\Delta)c$	(10)
$S_{44} = s_{44} + 4\Delta s \simeq \frac{1}{G}$	(5)	$C_{44} = c_{44} + \Delta c \simeq G$	(11)
$s = (s_{11} - s_{12}) - \frac{1}{2}s_{44}$	(6)	$c = (c_{11} - c_{12}) - 2c_{44}$	(12)

$S_{ij}$ ,  $C_{ij}$  refer to the polycrystalline material and  $s_{ij}$ ,  $c_{ij}$  to the single crystals.

likely to be affected by varying degrees of texture. In the paper by Reynolds (1970), it was pointed out that equation (13) was one of a number of expressions eliminating the orientation factor  $\Delta$ . It was thought that it would be possible to determine the constants  $s_{ij}$  or  $c_{ij}$  from practical measurements by using these relations.

It is found however that they are not independent, and so insufficient to give a complete solution for all the constants. At the same time it is noted that the constant for equation (13) (i.e.  $(2s_{11} + s_{44})$  in the single crystal) was not the same for the steels for which the expression was established as for pure iron. The difference could be due to the error between results calculated on the uniform stress average (Reuss) and the polycrystalline properties. In this case, therefore,  $2/E + 1/G$  (polycrystalline) constant represents a value modified from  $(2s_{11} + s_{44})$  for the single crystal of pure iron. The difference could be due to the inherent limitation of the Reuss assumption, plus any modifications due to the alloying effects.

In connecting the two equations (13) and (19) in table 2 it is seen that the latter must also contain Poisson's ratio  $\nu$  and so is not so readily applicable unless independent measurements of  $\nu$  can be made as well as of  $E$  and  $G$ .

The equations in the second row of table 2, viz. (14) and (20), are more directly related. The conversions from compliances to constants or vice versa are achieved by formulae given in a number of textbooks, e.g. those by Nye (1957), Hearmon (1961), and Schreiber *et al* (1973). From these conversions it is easily seen that *inter alia*

$$(c_{11} + 2c_{12})^{-1} = (s_{11} + 2s_{12}).$$

It follows that equations (14) and (20) are directly related and interchangeable. The two approximations (and also Hill's mean) therefore lead to the same results. It is thus reasonable to make these expressions as equal to (rather than equivalent to) the practical quantities given on the right-hand side in terms of  $K$ ,  $E$  and  $\nu$ . If  $K$  could be determined experimentally (on bar material) this would give a correct value of  $\nu$  and of the sums equated above.

It also follows that if the single-crystal constants are known,  $3K$  can be calculated for these and thus is also a true value for the polycrystalline material. The implication of equation (20) is that the bulk modulus is unaltered by assembling single crystals into a polycrystalline mass. This is a significant conclusion and may have some useful

**Table 2.** Derived relationships. The expressions in the first four rows depend on the elimination of  $\Delta$ , but are not independent. The expressions in the last two rows contain  $\Delta$ .

(a) Based on uniform stress average (Reuss)			(b) Based on uniform strain averages (Voigt)		
Equation no.	Expression in terms of $s_{ij}$ and $s_{kl}$	Practical equivalent or identity	Equation no.	Expression in terms of $C_{ij}$ and $c_{kl}$	Practical equivalent or identity
(13)	$2S_{33} + S_{44} = 2s_{11} + s_{44}$	$\frac{2}{E} + \frac{1}{G}$	(19)	$C_{33} + 2C_{44} = c_{11} + 2c_{44}$	$\frac{E(1-\nu)}{(1+\nu)(1-2\nu)} + 2G$
(14)	$S_{33} + 2S_{13} = s_{11} + 2s_{12}$ $= (c_{11} + 2c_{12})^{-1}$	$\frac{1}{3K} = \frac{1-2\nu}{E}$	(20)	$C_{33} + 2C_{13} = c_{11} + 2c_{12}$ $= (s_{11} + 2s_{12})^{-1}$	$\frac{E}{3K} = \frac{E}{(1-2\nu)}$
(15)	$S_{44} - 4S_{13} = s_{44} - 4s_{12}$	$\frac{1}{G} + \frac{4\nu}{E}$	(21)	$C_{44} - C_{13} = c_{44} - c_{12}$	$G - \frac{E\nu}{(1+\nu)(1-2\nu)}$
(16)	$3S_{12} - S_{11} = 3s_{12} - s_{11} + s$ $= 2s_{12} - \frac{1}{2}s_{44}$	$-\frac{1}{2} \left( \frac{1}{G} + \frac{4\nu}{E} \right)$	(22)	$3C_{12} - C_{11} = 3c_{12} - c_{11} + c$ $= 2(c_{12} - c_{44})$	$\frac{2E\nu}{(1+\nu)(1-2\nu)} - 2G$
(17)	$S_{33} - S_{13} - \frac{1}{2}S_{44} = s(1 - 5\Delta)$	$\frac{(1+\nu)}{E} - \frac{1}{2G} = s(1 - 5\Delta)$	(23)	$C_{33} - C_{13} - 2C_{44} = c(1 - 5\Delta)$	$\frac{E}{(1+\nu)} - 2G = c(1 - 5\Delta)$
(18)	$-\frac{S_{13}}{S_{33}} = -\frac{(s_{12} + s\Delta)}{(s_{11} - 2s\Delta)}$	$\nu$	(24)	$\frac{C_{13}}{C_{33} + C_{13}} = \frac{c_{12} + c\Delta}{(c_{11} + c_{12}) - c\Delta}$	$\nu$

consequences except that the direct experimental measurement of  $K$  for a polycrystalline metal would be very difficult.

In table 2, it is also readily seen that equations (13), (14) and (15) are not independent. An expression eliminating  $\Delta$  from equations involving  $s_{11}$ , and depending on strains normal to  $0Z$ , leads to equation (16) which is not independent of (15). There are thus only two independent relationships. Parallel results are obtained in terms of the Voigt approximation on the right-hand side of the table. Reynolds' expectation of being able to use orientation-independent relations to determine separate values of  $c_{ij}$  and  $s_{ij}$  is therefore not fulfilled.

Another relationship involving three (rather than two) of the rotated averages in table 1 is, however, derived and appears in equation (17) and in equation (23) for the two conditions respectively. These equations show why a polycrystalline material will show isotropic properties even when the single crystals are anisotropic. The expressions equate to zero if either:

- (a)  $s = c = 0$  (isotropic single crystals); or
- (b)  $\Delta = 0.2$ , as it does for random orientation.

In both cases the expression is then identical with the formulation

$$E = 2G(1 + \nu)$$

or

$$\nu = \frac{E}{2G} - 1. \quad (25)$$

Attention may also be drawn to the practical equivalent moduli given in relation to equations (8) and (9) in table 1. These expressions depend on the stress-strain relationships:

$$\sigma_3 = C_{13}\epsilon_1 + C_{23}\epsilon_2 + C_{33}\epsilon_3 = C_{33}\epsilon_3 + 2C_{13}\epsilon_1 \quad (C_{13} = C_{23}, \epsilon_1 = \epsilon_2).$$

But  $\sigma_3 = E\epsilon_3$  and  $\epsilon_1 = -\nu\epsilon_3$ . Therefore

$$E = C_{33} - 2\nu C_{13}. \quad (26)$$

By treating (20) and (26) as simultaneous equations for  $C_{33}$  and  $C_{13}$ , one obtains the expressions in (8), (9), containing  $E$  and  $\nu$ . One may also write

$$\begin{aligned} \sigma_3 &= C_{13}(\epsilon_1 + \epsilon_2 + \epsilon_3) + (C_{33} - C_{13})\epsilon_3 \\ &= \frac{\nu E}{(1 + \nu)(1 - 2\nu)}\epsilon + \frac{E}{(1 + \nu)}\epsilon_3. \end{aligned} \quad (27)$$

Equation (27) is a more general form of the equation for isotropic materials containing Lamé constants. The constants no longer refer to isotropic materials and so  $E/(1 + \nu)$  is not to be equated to  $2\mu$  or  $2G$ .

Also from equations (2) and (3) and from (8) and (9), the final equations in table 2 follow. These give two different values of Poisson's ratio derived from the otherwise fundamentally correct use of strain ratios.

### 3. The problem of Poisson's ratio

The two values of the ratio given by equations (18) and (24) in table 2 may be regarded as correct values. If, however, equation (25) is used in conjunction with separate calculation of  $E$  and  $G$  from the basic constants, two further values of  $\nu$  result. The equations

for these are indicated in a footnote to table 3. There are thus *four* different calculations of Poisson's ratio.

The numerical values in table 3 illustrate how the calculations would apply in a concrete case for which the single-crystal constants are known—viz.  $\alpha$ -iron. This table illustrates the amount of variation possible between the extreme limits of the orientation function  $\Delta$ . This is zero for the directions  $\langle 100 \rangle$  and has a maximum value of  $\frac{1}{2}$  for  $\langle 111 \rangle$ . The random value of 0.2 gives an identical value of  $\nu$  for the Reuss approximation whether the strain ratio or isotropic formula (25) is used. The Voigt approximation gives a corresponding identity at a somewhat different value.

Table 3. Derivations of Poisson's ratio illustrated by numerical values for pure  $\alpha$ -iron.

(a) Equations in terms of $s_{ij}$				(b) Equations in terms of $c_{ij}$			
Equation and derivation	Values of $\nu$ for $\Delta$			Equation and derivation	Values of $\nu$ for $\Delta$		
	0	0.2	0.333		0	0.2	0.333
(18): see table 1; ratio in terms of true strains	0.366	0.303	0.212	(24): see table 1; ratio in terms of true strains.	0.366	0.269	0.212
(28): see below†; ratio from equation (25) assuming $E$ and $G$ in terms of compliances.	-0.437	0.303	1.364	(29): see below†; ratio from equation (25) assuming $E$ and $G$ in terms of constants.	-0.437	0.269	0.993

† Equation (28) requires  $\nu = (E/2G) - 1$  or

$$\nu = \frac{S_{44} - 2S_{33}}{2S_{33}} = \frac{(s_{44} - 2s_{11}) + 8s\Delta}{2s_{11} - 4s\Delta} = \frac{E}{2} [(s_{44} - 2s_{11}) + 8s\Delta]. \quad (28)$$

Correspondingly, for the right-hand columns, equation (29) depends on the use of (3) and elimination of  $E$  and  $G$  in terms of the  $C$ 's. Thus:

$$\begin{aligned} \frac{E}{2G} - 1 = \nu &= \frac{(C_{33} + 2C_{13})(C_{33} - C_{13})}{2(C_{33} + C_{13})C_{44}} - 1 \\ &= \frac{(c_{11} + 2c_{12})(c_{11} - c_{12} - 3c\Delta)}{2(c_{11} + c_{12} - c\Delta)(c_{44} + c\Delta)} - 1. \end{aligned} \quad (29)$$

Also from the table, it is seen that at the extreme limits of  $\Delta$ , the two approximations give the same values of  $\nu$  for the strain-ratio derivation. On the other hand, the applications of the isotropic formula to the anisotropic condition clearly leads to absurd values of  $\nu$  at these extremes.

The results in table 3 are thus seen to confirm and justify further the view previously expressed that the engineering (isotropic) formula, expressing  $\nu$  in terms of measured values of  $E$  and  $G$ , should be used with very much caution. This is particularly the case when the polycrystalline material may not be completely isotropic, as when an orientation texture has developed. An evident case where unusual values of the ratio have been obtained in this way is to be found in recent work of Wawra (1973, 1974a,b).

#### 4. Practical applications

Apart from the fact that the appearance of dubious values of Poisson's ratio may be used as a direct indication of the presence of some degree of anisotropy in the polycrystalline

metal, other practical procedures may follow. Extensive determinations have been made of elastic moduli for many types of steel and it is expected that these results will be published (K W Andrews, M Atkins and E H F Date unpublished results).

The use of an equation based on (13) in table 2, in the form

$$\frac{2}{E} + \frac{1}{G} = S_0 \quad (30)$$

for these steels and other polycrystalline materials, implies that the moduli are more strongly affected by the conditions required for the Reuss approximation. The fact that the constant  $S_0$  differs from a single-crystal value may be partly due to an effective change in  $s_{11}$  and  $s_{44}$  which would close the gap between the Reuss and Hill approximations. There could also be a contribution from the presence of alloy elements or second phases. More than one of these factors may influence the final results.

In cases where considerable numbers of steels of the same or similar types have been studied and there is very little variation in the values of Poisson's ratio which are consistent with random orientation although determined from  $E$  and  $G$ , then an average value is recognised as the ratio for random orientation. Subsequently any unusual values of the ratio differing significantly from this value may be used to modify the values of  $E$  and  $G$ . As determined, these are appropriate to the material with some degree of orientation texture and can go on record for this condition. The modified or adjusted values, then, correspond to completely random orientation for the same material—the adjusted values are obtained by the formulae

$$G_r = \frac{(2 + \nu_r)}{S_0(1 + \nu_r)} \quad E_r = \frac{2(2 + \nu_r)}{S_0} \quad (31)$$

In these expressions  $\nu_r$  is the value established or assumed for random orientation.

Alternatively, when the value of Poisson's ratio derived from  $E$  and  $G$  directly differs considerably from the random value, a true or corrected value can be obtained from a formula of the type

$$\nu_2 = a - b \cdot \nu_1 \quad (32)$$

where the subscript 1 refers to the original value and 2 to the corrected value. Some values of the constants  $a$  and  $b$  which have been obtained are listed in table 4. In these cases the constants for the pure metals were used to arrive at approximate constants for the steels, which corresponded to observed values of  $\nu_r$  and  $S_0$ . Analytical expressions for the constants  $a$  and  $b$  can be derived from single-crystal or other values of the  $s_{ij}$  from the formulae (28) and (29) at the foot of table 3.

Table 4. Constants in the equation  $\nu_2 = a - b\nu_1$  for correcting Poisson's ratio.

Material	$a$	$b$	Value of $\nu$ when $\nu_1 = \nu_2 = \nu_r^\dagger$
Pure $\alpha$ -iron	0.329	0.0856	0.303
Average of ferritic steels	0.306	0.0972	0.279
Average of austenitic steels	0.307 <sub>5</sub>	0.0962	0.280
Pure nickel	0.336	0.0819	0.311

$\dagger$  The subscript 1 refers to the value calculated from equation (25), the subscript 2 to the corrected value and r to the value for random orientation with  $\Delta = 0.2$ .

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