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Pressure derivatives of the elastic moduli of a polycrystalline aggregate of hexagonal metal: Calculations using monocrystal elastic-constant pressure derivatives

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The pressure deriviatives of the bulk, shear and Young's moduli, and of Poisson's ratio of a number of polycrystalline metals have been calculated using Hill's approximation. The pressure derivatives of the second-order elastic constants of the corresponding single-crystal hexagonal metals have been used for this purpose.

INTRODUCTION

The problem of calculating the elastic properties of a polycrystal from the elastic moduli and their pressure derivatives of the corresponding single crystal is complicated and has received repeated attention from various authors. Voigt[1] was the first to suggest how the fourth-rank elastic stiffness tensor C_{ijkl} could be averaged to obtain the two independent quasi-isotropic elastic constants: the bulk modulus B and the shear modulus G. A similar approach was used by Reuss[2] to average the compliance tensor S_{ijkl} under the basic assumption of uniform state of stress in the crystal. Hill[3] showed that the Voigt and the Reuss values are actually upper and lower bounds, respectively, for the elastic moduli of a polycrystal. If one accepts the concept of an effective elastic modulus of a polycrystal, according to which an aggregate of randomly oriented crystals may be replaced by an equivalent isotropic and homogeneous elastic body, then the Voigt and Reuss bounds are exact theoretical results. However, except for the case when the anisotropy of the crystal is small, these bounds are not close enough to provide a good estimate for the effective elastic moduli. In fact, Voigt and Reuss averages represent first-order bounds, and whether the Voigt average exceeds the Reuss average depends on whether some elastic anisotropy index such as $2C_{44}/(C_{11}-C_{12})$ exceeds, or is less than, unity. Hill[3] suggested that the arithmetic mean of the values calculated, using the Voigt and Reuss schemes, be used to express the most probable value for the polycrystalline solid. Later several attempts were made to find expressions for the effective elastic moduli of a polycrystal. Hashin and Shtrikman[4] used a variational approach and obtained the second-order bounds for cubic symmetry while Kröner and Köch[5] gave the third-order bounds. Recently, Gairola and Kröner[6] proposed a formulation for calculating all the bounds and the self-consistent value of the shear modulus for cubic symmetry. Ledbetter[7,8] cited eight methods for averaging cubic-symmetry elastic coefficients to calculate the elastic Debye θ and did extensive analysis on polycrystalline copper. Peresada[9] proposed a new method of estimation of elastic moduli of a polycrystal from single-crystal data of any symmetry which leads to results in good agreement with those obtained by Hill's approximation. A simple method, based on Hill's approximation, was suggested by Anderson[10] for calculating the Debye temperature. Further, it is possible to calculate the pressure derivatives of the elastic moduli and of the Poisson's ratio of the polycrystalline solid if the pressure derivatives of its single crystal are available either theoretically or experimentally. The pressure derivative of the shear modulus of a polycrystal is an experimentally measured quantity and hence it is of interest to compute the same theoretically.

The object of the present paper is to calculate the pressure derivatives of bulk, shear and Young's moduli, and of the Poisson's ratio of a number of polycrystalline metals using the pressure derivatives of the corresponding hexagonal single crystals.

FORMULAE FOR HEXAGONAL MATERIALS IN THE VOIGT AND REUSS SCHEMES

Voigt averages of C_{ij} for bulk B_v and shear G_v moduli of hexagonal materials are

$$9B_v = 2C_{11} + C_{33} + 2C_{12} + 4C_{13} \tag{1}$$

and

$$15G_v = 2C_{11} + C_{33} - C_{12} - 2C_{13} + 6C_{44} + 3C_{66}, \tag{2}$$

where

$$2C_{66} = C_{11} - C_{12}.$$

According to Reuss the bulk B_R and shear G_R moduli for materials with hexagonal symmetry are given by

$$B_R^{-1} = 2S_{11} + S_{33} + 2S_{12} + 4S_{13} \tag{3}$$

and

$$15G_R^{-1} = 8S_{11} + 4S_{33} - 4S_{12} - 8S_{13} + 6S_{44} + 3S_{66}, \tag{4}$$

where $S_{66} = 2(S_{11} - S_{12})$.

Relations between the stiffnesses C_{ij} and the compliances S_{ij} are given by Cline *et al.*[11] and by Nye.[12] Poisson's ratio σ and Young's modulus E, with the values of B and G determined by Voigt's or Reuss averaging procedures, can be computed from

$$2\sigma = \frac{3B - 2G}{3B + G} \tag{5}$$

and

$$9E^{-1} = 3G^{-1} + B^{-1}. \tag{6}$$

Based on energy arguments, Hill[3] proved that the arithmetic mean of Voigt and Reuss averages would yield a more accurate result than either individual average. This is expressed as

$$2M_H = M_V + M_R, \tag{7}$$

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TABLE I. Values of B', G', E', σ' in Hill's approximation. The first row against each metal gives our present calculated values while the second row gives the estimated values of Guinan and Steinberg. The references for SQEC and their pressure derivatives are given by the superscripts to the metals.

Sample No.	Metal	B'_H	G'_H	E'_H	σ'_H
1.	Sc[13,14]	2.91	0.95	2.63	0.035
		2.00	1.10	000	000
2.	Y[15,16]	3.30	0.99	2.91	0.085
		2.00	1.00	000	000
3.	Tb[17,18]	3.31	0.37	1.56	0.141
		2.68	0.46	000	000
4.	Ho[19,20]	3.29	0.74	2.43	0.115
		2.84	1.20	000	000
5.	Lu[21,22]	3.27	1.24	3.38	0.046
		3.00	0.88	000	000
6.	Tm[23]	4.15	1.49	4.15	0.079
		2.64	1.60	000	000
7.	Pr[24,25]	4.25	1.82	4.79	0.114
		2.20	000	000	000
8.	Nd[25,26]	4.18	1.78	4.69	0.043
		2.80	0.18	000	000
9.	Tl[27,28]	2.09	0.88	2.44	−0.072
		5.09	0.57	000	000
10.	Co[29,30]	3.47	1.98	5.04	−0.010
		4.26	1.80	000	000
11.	Mg[31,32]	4.05	1.62	4.30	0.040
		3.90	1.30	000	000
12.	Zn[33,34]	5.63	2.56	6.71	0.058
		6.40	2.30	000	000
13.	Be[35,36]	4.53	2.44	7.32	0.074
		4.60	2.10	000	000
14.	Zr[37]	4.11	0.04	0.55	0.062
		4.11	0.31	000	000
15.	Ti[38,39]	4.36	0.48	1.68	0.046
		4.37	0.63	000	000
16.	Re[40]	5.57	1.80	4.97	0.009
		5.41	2.0	000	000
17.	Er[41]	3.30	1.04	3.03	0.079
		3.31	0.83	000	000
18.	Dy[41]	3.26	0.43	1.73	0.132
		3.26	0.54	000	000
19.	Gd[41]	3.37	0.31	1.42	0.151
		3.37	0.21	000	000

TABLE II. Values of B', G', E', and σ' in Voigt and Reuss approximations. The first row against each metal gives the Voigt's bounds while the second row gives the Reuss bounds.

Sample No.	Metal	B'	G'	E'	σ'
1.	Sc	2.93	0.98	2.71	0.035
		2.89	0.92	2.56	0.035
2.	Y	3.30	1.01	2.95	0.082
		3.30	0.97	2.86	0.087
3.	Tb	3.32	0.37	1.57	0.142
		3.30	0.37	1.55	0.140
4.	Ho	3.29	0.75	2.45	0.114
		3.29	0.73	2.41	0.116
5.	Lu	3.27	1.24	3.37	0.046
		3.27	1.24	3.39	0.046
6.	Tm	4.0	1.31	3.74	0.085
		4.3	1.67	4.56	0.072
7.	Pr	4.25	1.78	4.71	0.134
		4.25	1.85	4.86	0.094
8.	Nd	4.35	1.91	5.02	0.040
		4.01	1.64	4.36	0.045
9.	Tl	2.06	0.70	1.94	−0.043
		2.12	1.06	2.94	−0.102
10.	Co	3.45	1.94	4.93	−0.008
		3.49	2.03	5.16	−0.011
11.	Mg	4.05	1.63	4.34	0.039
		4.05	1.60	4.26	0.041
12.	Zn	5.31	2.59	6.73	0.027
		5.93	2.53	6.70	0.089
13.	Be	4.62	2.63	7.69	0.073
		4.43	2.24	6.95	0.075
14.	Zr	4.13	0.06	0.61	0.062
		4.09	0.02	0.49	0.062
15.	Ti	4.37	0.48	1.68	0.048
		4.35	0.49	1.68	0.045
16.	Re	5.41	1.86	5.09	0.008
		5.73	1.74	4.86	0.011
17.	Er	3.31	1.06	3.07	0.078
		3.30	1.03	3.0	0.080
18.	Dy	3.26	0.43	1.74	0.132
		3.26	0.43	1.72	0.131
19.	Gd	3.38	0.31	1.44	0.151
		3.37	0.30	1.41	0.150

where M_H, M_V, and M_R represent the Hill, Voigt, and Reuss averages, respectively, of any elastic quantity. The pressure derivatives B'_V, G'_V, B'_R, G'_R, σ', and E' are obtained from formulae (1)–(6) and from the relations between S_{ij} and C_{ij} for hexagonal symmetry:

$$9B'_V = (2C'_{11} + C'_{33} + 2C'_{12} + 4C'_{13}), \tag{8}$$

$$15G'_V = (2C'_{11} + C'_{33} - C'_{12} - 2C'_{13} + 6C'_{44} + 3C'_{66}), \tag{9}$$

$$\frac{-B'_R}{B_R^2} = (2S'_{11} + S'_{33} + 2S'_{12} + 4S'_{13}), \tag{10}$$

$$\frac{-15G'_R}{G_R^2} = (8S'_{11} + 4S'_{33} - 4S'_{12} - 8S'_{13} + 6S'_{44} + 3S'_{66}), \tag{11}$$

$$\sigma' = \frac{1}{2(3B+G)^2}[(3B+G)(3B'-2G') - (3B-2G)(3B'+G')], \tag{12}$$

$$E' = \frac{E^2}{9}\left(\frac{3G'}{G^2} + \frac{B'}{B^2}\right). \tag{13}$$

DISCUSSION

The pressure derivatives of the bulk, shear, and Young's moduli, and of the Poisson's ratio of a number of polycrystalline metals have been calculated using the pressure derivatives of the single-crystal second-order elastic constants (SOEC). These data are extremely useful from the engineering point of view and the pressure derivatives of E and σ are reported for the first time for these polycrystalline

metals. Guinan and Steinberg[42] have clearly demonstrated by their calculations of the Grüneisen parameters of the alkali metals and of some hexagonal metals that the direct pressure derivative approach is to be preferred to Barsch's[43] scheme. These authors derived an equation [Eq. (31) in Ref. 42] for the pressure derivative of the shear modulus G'_H under the assumption that the average of the individual Grüneisen parameters (GPs) over all the modes γ_0^1 is equal to the average over only the low-frequency acoustic modes $\overline{\gamma}_A$. This assumption is valid for a crystal of low anisotropy while hexagonal elements show a wide variation in the degree of anisotropy. Besides, the hexagonal elements exhibit large departures from the ideal c/a ratio. As a matter of fact, these authors used $(\gamma_0^1 - \frac{1}{3})$ instead of γ_0^1 while calculating G'_H for hexagonal metals, to take into account the effect of the departure of the c/a ratio from the ideal value. In spite of this, their estimated G'_H value agrees with experiment within 30% for 10 of the 12 hexagonal metals. For Zr, the estimated value differs by a factor of 8. These authors conclude that their formula for G'_H derived under acoustic approximation does not hold for the crystal class of hexagonal symmetry. The formula for B'_H [Eq. (32) in Ref. 42] obtained from shock wave data suffers from the same defect that it does not give reliable results for structures of high anisotropy and is derived under the assumption that material strength effects are very small. Our calculated values of the pressure derivatives of the elastic moduli of the polycrystals are presented in Table I. The calculations for polycrystal zinc have been performed using theoretical pressure derivatives of its SOEC since the experimental pressure derivative of C_{13} was not reported by Swartz and Elbaum.[44] In Table II the Voigt and the Reuss bounds for the 19 crystals are given.

One interesting point of our calculations is the negative value for the pressure derivative of the Poisson's ratio of the quasi-isotropic metals Tl and Co. This implies that at high pressures the values of the lattice parameters change and affect the value of the c/a ratio. This leads to lattice instability and to a possible hcp→bcc transformation in these elements under high pressures.

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