Poisson's Ratio for Central-Force Polycrystals *

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The Poisson ratio ν of a polycrystalline aggregate was calculated for both the face-centered cubic and the body-centered cubic cases. A general two-body central-force interatomic potential was used. Deviations of ν from 0.25 were verified. A lower value of ν is predicted for the f.c.c. case than for the b.c.c. case. Observed values of ν for twenty-three cubic elements are discussed in terms of the predicted values. Effects of including volume-dependent electron-energy terms in the interatomic potential are discussed.

Introduction

The Poisson ratio ν of polycrystalline aggregates is of considerable interest both practically and theoretically. Poisson's ratio is used frequently in engineering design, and it relates directly to the nature of interatomic forces in solids.

Many authors (see Refs. [2-5] in Ref. [1]) have cited the deviation of ν from 1/4 as proof that the interatomic potential has a non-central component. Recently this view was disputed [1]. It was shown that 1/4 is the lower limit of ν for an aggregate of central-force crystals and that the upper limit is:

$$\nu_{\max} = \frac{1}{4}\,\frac{(2A^{-2}+A^{-1}+2)}{(A^{-2}+3A^{-1}+1)}, \qquad (1)$$

where

$$A = 2\,C_{44}/(C_{11}-C_{12}) \qquad (2)$$

is the Zener elastic anisotropy factor, where C_{11}, C_{12}, and C_{44} are the three independent Voigt elastic constants for the cubic-symmetry case. That a range of ν values is possible in a central-force model of polycrystals was pointed out also by Anderson and Demarest [2].

In this note, the problem of ν is reconsidered from the viewpoint of a general two-body central-force interatomic potential. For the two common cubic crystal structures, body-centered cubic and face-centered cubic, unique central-force values of ν are given. And it is suggested that these values relate to the problem of the occurrence of non-central interatomic forces in polycrystalline aggregates.

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Two-Body Central-Force Calculations

Most materials have non-central components in their interatomic forces. This is especially true in metals where the free electrons contribute some purely volume-dependent energy terms. However, because they are simple in both form and interpretation, two-body central-force interatomic potentials have been used to calculate a variety of properties of metals. Such calculations include: second-order elastic constants [3]; third-order elastic constants [4]; fourth-order elastic constants [5]; pressure dependence of the elastic constants [6]; composition dependence of the elastic constants [7]; Debye temperature [8]; mechanical stabilities [9]; theoretical strengths [10]; atomic vibrations and melting [11]; anharmonic properties [12]; equations of state [13]; diffusion [14]; properties of amorphous metals [15]; lattice parameters of intermetallic phases [16]; and properties of point defects such as vacancies and interstitials [17]. Thus, a basis for the general type of calculation described here is well established.

Theoretical Approach

If the interatomic potential is denoted $\Phi(\mathbf{r})$, then the Brugger elastic constants, which are fourth-rank tensors, are given at $T = 0$ K by:

$$C_{ijkl} = \frac{\partial^2 U}{\partial \eta_{ij}\,\partial \eta_{kl}} = \frac{1}{2V^0}\,[\sum D^2\,\Phi(\mathbf{r})\,r_i^0\,r_j^0\,r_k^0\,r_l^0]_{r=r^0}, \qquad (3)$$

where $D\,\Phi(\mathbf{r})$ denotes $(1/\mathbf{r})\,[\partial\Phi(\mathbf{r})/\partial r]$. The energy density U of the crystal is obtained by a sum over two-body atom-atom interaction energies:

$$U = (1/2\,V^0)\sum \Phi(\mathbf{r}), \qquad (4)$$

where V^0 is the undeformed atomic volume. The η_{ij} are components of the Lagrangean elastic strain matrix

$$\eta = \tfrac{1}{2}(\mathbf{J}^t \mathbf{J} - \mathbf{I}) , \qquad (5)$$

where $\mathbf{I}$ is the 3×3 identity matrix, t denotes transposition, and the deformation matrix $\mathbf{J}$ is defined by

$$\mathbf{r} = \mathbf{J}\,\mathbf{r}^0 , \qquad (6)$$

where $\mathbf{r}^0$ and $\mathbf{r}$ are the interatomic spacings in the initial state and in the deformed state, respectively. Details concerning this approach to elastic constants can be found elsewhere [18].

(a) Face-Centered Cubic Case

Face-centered cubic crystals have twelve nearest neighbors at $\langle \pm, 1 \pm 1, 0 \rangle a/2$, where a is the unit-cell dimension. In this case one obtains from Eq. (3):

$$C_{11}\,(=C_{1111}) = \frac{1}{2V^0}\left[8\left(\frac{a}{2}\right)^4 D^2\,\Phi\left(\frac{a}{\sqrt{2}}\right) + 2\,a^4 D^2\,\Phi(a) + \ldots\right] \qquad (7)$$

and

$$C_{12}\,(=C_{1122}) = C_{44}\,(=C_{2323}) = \frac{1}{2V^0}\left[4\left(\frac{a}{2}\right)^4 D^2\,\Phi\left(\frac{a}{\sqrt{2}}\right) + 0 + \ldots\right], \qquad (8)$$

where ... indicates contributions from pairs farther than second-nearest neighbors.

(b) Body-Centered Cubic Case

Body-centered cubic crystals have eight nearest neighbors at $\langle \pm 1, \pm 1, \pm 1 \rangle a/2$ and six second-nearest neighbors at $\langle \pm 1, 0, 0 \rangle a$. In this case one obtains from Eq. (3):

$$C_{11} = \frac{1}{2V^0}\left[8\left(\frac{a}{2}\right)^4 D^2\,\Phi\left(\frac{\sqrt{3}}{2}a\right) + 2\,a^4 D^2\,\Phi(a) + 8\,a^4 D^2\,\Phi(\sqrt{2}\,a) + \ldots\right] \qquad (9)$$

and

$$C_{12} = C_{44} = \frac{1}{2V^0}\left[8\left(\frac{a}{2}\right)^4 D^2\,\Phi\left(\frac{\sqrt{3}}{2}a\right) + O + 4\,a^4 D^2\,\Phi(\sqrt{2}\,a) + \ldots\right]. \qquad (10)$$

Thus, the elastic constants C_{ij} can be determined simply through 2 nn interactions for a general central-force interatomic potential for both f.c.c. and b.c.c. crystal structures. The quantities $D^2\,\Phi(r_i)$ are unspecified here since they vary with the interatomic potential. In considering ν, which is a ratio of elastic constants, the $D^2\,\Phi(r_i)$ are unnecessary, as shown below.

From the C_{ij}, ν is calculated by first averaging the C_{ij} to obtain the macroscopic polycrystalline shear modulus G and then using the standard relationship:

$$\nu = \frac{1}{2}\,\frac{3B - 2G}{3B + G} , \qquad (11)$$

where the bulk modulus B, which is a rotational invariant of the C_{ij} matrix, is given by

$$B = \tfrac{1}{3}(C_{11} + 2\,C_{12}) . \qquad (12)$$

If the strain tensor is uniform in the polycrystal, then from Voigt [19]:

$$G_V = \tfrac{1}{5}(C_{11} - C_{12} + 3\,C_{44}) . \qquad (13)$$

However, if stress is uniform throughout the polycrystal, then from Reuss [20]:

$$G_R = \frac{5\,C'\,C_{44}}{3\,C' + 2\,C_{44}} . \qquad (14)$$

Since, in reality, neither strain nor stress are uniform in an aggregate, Hill [21] suggested that G should be determined from an arithmetic average of G_V and G_R. Thus,

$$G_H = \tfrac{1}{2}(G_V + G_R) . \qquad (15)$$

While many more sophisticated elastic-constant averaging methods have been proposed [22], Hill's average corresponds reasonably well with observation; and, for simplicity, it will be used here.

Results

Results of these calculations for ν, together with intermediate results for B and G are shown in Table 1. In the Table, f_1 is a short-hand notation for $D^2\,\Phi(1\,nn)$ for the f.c.c. case; b_1 and b_2 denote $D^2\,\Phi(1\,nn)$ and $D^2\,\Phi(2\,nn)$ for the b.c.c. case. The value of $G_R(1\,nn + 2\,nn)$ for the b.c.c. case is not exactly zero. However, for any reasonable values of b_2 and b_1 it follows that $G_R/B \cong 0.02$ for the b.c.c. $(1\,nn + 2\,nn)$ case. Results are given through $1\,nn$ for the f.c.c. case and through $2\,nn$ for the b.c.c. since these sets of nearest-neighbor interactions usually account reasonably well for most properties of these two types of crystals.

Table 1. Elastic constants of a polycrystalline aggregate calculated from a general central-force two-body interatomic potential using a Voigt-Reuss-Hill arithmetic average of the C_{ij} (subscripts V = Voigt, R = Reuss, H = V-R-H).

Elastic constant	Face-centered cubic 1 *nn*	Body-centered cubic 1 *nn*	1 *nn*+2 *nn*
B	$\frac{2}{3} f_1$	b_1	$\frac{1}{3}(3\,b_1+b_2)$
G_V	$\frac{2}{5} f_1$	$\frac{3}{5} b_1$	$\frac{1}{5}(3\,b_1+b_2)$
G_R	$\frac{5}{14} f_1$	0	0 (see text)
G_H	$\frac{53}{140} f_1$	$\frac{3}{10} b_1$	$\frac{1}{10}(3\,b_1+b_2)$
ν_V	0.250	0.250	0.250
ν_R	0.273	0.500	0.500
ν_H	0.261	0.364	0.364
ν (obs.)	0.353 (avg. of 10)	0.328 (avg. of 12)	

Discussion

Single-crystal elastic data (C_{11}, C_{12}, and C_{44}) are available for eleven f.c.c. elements and for twelve b.c.c. elements. The deviation of the ratio C_{12}/C_{44} from unity can be taken as an index (necessary but not sufficient) for the existence of non-central forces. The ratio of the observed value of ν to the central-force value of ν calculated here is plotted versus C_{12}/C_{44} in Figure 1. Both C_{ij} and

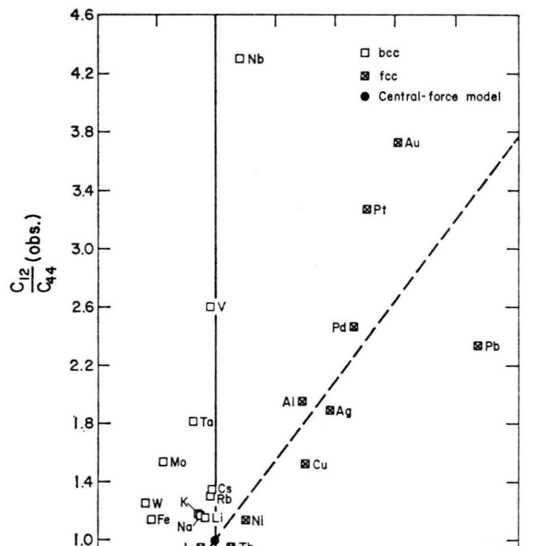

Fig. 1. Reduced elastic constant C_{12}/C_{44} versus ratio of observed and calculated Poisson ratios for cubic metals. For central interatomic forces, $C_{12}=C_{44}$ is a necessary condition called the Cauchy relationship.

ν (obs.) data were taken mainly from Simmons and Wang [23]. Very rough correspondences exist between these two parameters; there is a suggestion (indicated by the straight lines) that the f.c.c. and b.c.c. cases may behave differently. It is interesting that with one exception ν (obs.)/ν (calc.) exceeds unity for the f.c.c. elements; the exception is iridium, the only element considered for which low-temperature elastic constants were unavailable; normally ν decreases with lower temperatures and this would make iridium even more exceptional. Similarly, with one exception (niobium) all the ratios of ν(obs.)/ν(calc.) for the b.c.c. case are smaller than unity. In other words, it is suggested that 0.261 and 0.364 may be effective lower and upper bounds for the f.c.c. and the b.c.c. cases, respectively. The observed fluctuations from these bounds are much larger in the f.c.c. case. Anderson [24] showed that ν (obs.)/ν (calc.) is smaller than unity for alkali halides.

Some speculative remarks are appropriate concerning why the present calculations are reasonably successful in predicting Poisson's ratio for metals, which are known to have strong non-central forces due to their free electrons. (The upper and lower theoretical limits on Poisson's ratio are 0.5 and −1.0.) First, a large part of the contributions to the C_{ij}'s comes from nearest-neighbor interactions alone. Second, ν is a ratio of polycrystalline-averaged C_{ij}'s; thus, scaling errors are canceled and small incremental errors tend to be canceled.

An attempt was made to improve the present calculations by introducing volume-dependent terms into the interatomic potential. Thus:

$$\Phi(\mathbf{r}, v) = \frac{1}{2\,V^0} \sum \Phi(\mathbf{r}) + \sum_{\alpha} A_\alpha \, v_\alpha^{\,n_\alpha} \quad (16)$$

where A_α and n_α are constants for various types of contributions denoted by α, and v is the reduced volume V/V^0. Three such structure-independent energies were considered: kinetic, exchange, and correlation energies of the electron gas. General expressions for the contributions of these energies to the C_{ij}'s were given by Cousins [25]. In most cases, agreement between observed and calculated values of ν was unaffected or worsened by including the effects of these electron-electron interactions. It was concluded that the model described by Eq. (16), although used frequently, is incorrect, at least for some of the elastic constants.

In both the f.c.c. and b.c.c. cases, the effect of a real (non-central-force) interatomic potential is to shift ν closer to a value of 1/3, a value often assumed to be typical for metals. Reasons for these shifts are unclear, and further study on this problem may be appropriate. It is also unclear why C_{12}/C_{44} tends to be increased by non-central forces. Finally, it is pointed out that the present results are contrary to MacDonald's [26] contention that "general properties of a crystal may not necessarily be realized on a nearest-neighbor model".

Conclusions

Conclusions of the present study are:

(1) It is confirmed that the lower limit of ν for central-force polycrystals is 0.25. This value corresponds to uniform strain, the case where the Voigt average of the C_{ij}'s is appropriate.

(2) If non-central forces are absent, then ν(f.c.c.) = 0.261 and ν(b.c.c.) = 0.364.

(3) The choice of method (Voigt, Reuss, Hill, etc.) for averaging the C_{ij}'s to obtain G and ν is much more important in the b.c.c. case than in the f.c.c. case.

(4) Including volume-dependent energy terms of the form Av^n in the interatomic potential does not improve agreement between calculated and observed ν values.

(5) A nearest-neighbor model can predict the Poisson's ratio of cubic solids reasonably well.

(6) For the elements considered, agreement with a central-force value of ν is much better in the b.c.c. case than the f.c.c. case. (While not considered here, second-neighbor interactions in the f.c.c. case tend to increase ν and reduce the disagreement.)

(7) In the b.c.c. case, calculated values of ν are lower than observed values; this is reversed in the f.c.c. case.

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