

NAT'L INST. OF STAND & TECH

A11106 173453

NIST
PUBLICATIONS

REFERENCE

NISTIR 6944

Determination of the Single Crystal Elastic Constants by Diffraction from a Cubic Polycrystal

Roland DeWit
U. S. DEPARTMENT OF COMMERCE
Technology Administration
National Institute of Standards
and Technology
Metallurgy Division
Gaithersburg, MD 20899

QC
100
.456
#6944
2003

NIST
National Institute of Standards
and Technology
Technology Administration
U.S. Department of Commerce

***Determination of the Single Crystal
Elastic Constants by Diffraction from a
Cubic Polycrystal***

Roland DeWit

**U. S. DEPARTMENT OF COMMERCE
Technology Administration
National Institute of Standards
and Technology
Metallurgy Division
Gaithersburg, MD 20899**

January 2003



**U.S. DEPARTMENT OF COMMERCE
Donald L. Evans, Secretary**

**TECHNOLOGY ADMINISTRATION
Phillip J. Bond, Under Secretary for Technology**

**NATIONAL INSTITUTE OF STANDARDS
AND TECHNOLOGY
Arden L. Bement, Jr., Director**

Determination of the Single Crystal Elastic Constants by Diffraction from a Cubic Polycrystal

Roland deWit

Guest worker, National Institute of Standards and Technology, Materials Science and Engineering Laboratory, Metallurgy Division, Materials Performance Group, Gaithersburg MD 20899*

Abstract

Using the theory of statistical continuum mechanics, closed expressions are derived for the diffraction elastic constants of a cubic polycrystal that is statistically homogeneous, isotropic, and disordered. By measuring these constants for several diffracting planes of a single polycrystal, the single crystal elastic constants are determined.

Keywords

Continuum mechanics, cubic, diffraction, disordered, effective properties, elastic constants, homogeneous, isotropic, polycrystal

Introduction

The method of statistical continuum mechanics is used in this paper to derive the elastic constants or elastic moduli of a polycrystal. A polycrystal, whose properties vary in a complicated fashion from point to point over a small “microscopic” length scale, may appear “on average” to be uniform or perhaps, more generally, its properties appear to vary smoothly. The determination of these “overall” properties from the properties and geometrical arrangement of the constituent grains is the aim of statistical continuum mechanics. In the simplest case the polycrystal is assumed to be statistically homogeneous, isotropic, and disordered. General expressions for averages can then be derived. In this process Green’s functions and modifications thereof have proved to be of great value. The effects of diffraction from a cubic polycrystal are included in the present treatment.

The analysis starts by defining an “effective medium”, which is a model that approximates the average state of the polycrystal and describes its average properties. In terms of this effective medium we can define “effective elastic moduli”, which relate the average stress to the average strain in the effective medium. The Voigt and Reuss models provide special cases of such an effective medium and the resulting effective moduli give upper and lower bounds for other possible effective moduli.

This paper focuses attention on crystals with cubic symmetry. For this case there are only three independent components of the single crystal elastic moduli. The analysis can then be simplified

* Contribution of the National Institute of Standards and Technology. Not subject to copyright.

considerably by using Walpole's notation for the decomposition of "unity". This approach leads to a very convenient set of three fundamental components for the cubic elastic moduli.

Regarding the elastic moduli as a fourth rank tensor there exist two invariants, which are a combination of the tensor components that is independent of rotation in space. From this consideration we can derive a formula for the spatial average of the tensor. Furthermore by considering the directional form of Young's modulus for a cubic crystal we can derive a formula for the diffraction average.

For the application of statistical continuum mechanics we use the method of perturbation theory where a suitable effective medium is defined in terms of its deviation from a "comparison medium", which is known and chosen arbitrarily. From the classic equations of elasticity we then derive the basic integral equation, also known as the LSD equation, which relates the strain in the polycrystal to the strain in the comparison medium. It contains a term, called the modified Green's function that is derivable from the Green's function for the comparison medium. Solving this equation for the case of diffraction and averaging we get a formal expression for the "approximate effective diffraction elastic constants".

Specializing to cubic crystal symmetry we derive the Gairola-Kröner formula, which gives the "approximate effective diffraction shear modulus" of the effective medium that represents the polycrystal and is given explicitly in terms of the three single crystal elastic moduli and the diffraction parameter. This formula gives various effective medium approximations for the polycrystal depending on the choice of the comparison medium.

When the comparison medium is set equal to the effective medium there is no more deviation between the two and the result gives the "self-consistent" moduli. For the cubic case this leads to a third order polynomial equation for the self-consistent shear modulus.

The two "diffraction elastic constants" of a polycrystal, which are conventionally used to express the results of diffraction experiments, can be defined in terms of two of the isotropic elastic moduli, like the bulk and shear modulus. For the cubic case these can then be expressed explicitly in terms of the three cubic single crystal elastic moduli and the diffraction parameter.

Values of the diffraction elastic constants have been measured for several reflection planes in some cubic polycrystals. These results can be used to determine the single crystal elastic constants by a regression analysis. In chi-square we take the two diffraction elastic constants as the dependent variables and the diffraction parameter as the independent variable. Then chi-square is minimized with respect to the three cubic elastic constants, which are the unknown parameters. In this way the three cubic elastic constants are determined. The results for steel, copper, and aluminum are presented.

Hooke's Law

For a single crystal Hooke's law can be written as

$$\sigma_{ij} = c_{ijkl} e_{kl} \quad (i, j, k, l = 1, 2, 3) \quad (1)$$

where repeated indices are summed, σ and e are the stress and strain, second rank tensors, and c is the elastic stiffness, a fourth rank tensor. Hooke's law can also be written in matrix form as

$$\sigma_i = c_{ij} e_j \quad (i, j = 1, \dots, 9) \quad \text{or} \quad (i, j = 1, \dots, 6) \quad (2)$$

where σ and e are the stress and strain vectors and c is the stiffness matrix. The matrix form of the elastic constants or elastic moduli is frequently referred to as the Voigt¹ notation. The three notations are completely equivalent and in this paper we shall use the symbolic notation

$$\sigma = ce \quad (3)$$

to represent any of the foregoing equations. Equation (3) can be solved for the strain in terms of the stress as follows

$$e = \frac{\sigma}{c} = s\sigma \quad (4)$$

where s , the elastic compliance, is the “inverse” of the stiffness c .

The Effective Medium

On a macroscopic scale a polycrystal may be approximated as a homogeneous medium. It can therefore be represented by an *effective medium*, which is a model that approximately describes the average properties of the medium to some desired degree of accuracy. In the effective medium the average stress $\langle \sigma \rangle$ and average strain $\langle e \rangle$ are related as follows

$$\langle \sigma \rangle = C \langle e \rangle \quad (5)$$

where C is the *effective stiffness*. So the effective medium is homogeneous. In this paper we shall assume that it is also isotropic and disordered. Equation (5) can be solved for the average strain

$$\langle e \rangle = \frac{\langle \sigma \rangle}{C} = S \langle \sigma \rangle \quad (6)$$

where S is the *effective compliance*. We use the convention that capital letters are used for a fourth rank tensor if the tensor is constant and thus represents the property of a homogeneous medium or the average property of a polycrystal. We use lower case letters for a fourth rank tensor if the tensor varies through the heterogeneous medium or polycrystal and thus represents the property of a single crystal.

The Voigt and Reuss Models

Frequently the Voigt¹ and Reuss² models are invoked to find bounds on the effective elastic moduli. Voigt assumed there is a constant strain and Reuss a constant stress in the polycrystal. For the Voigt model the actual strain then equals the average strain

$$e = \langle e \rangle \quad (7)$$

and so we have the following decomposition between the stiffness and the strain

$$\langle \sigma \rangle = \langle ce \rangle = \langle c \rangle \langle e \rangle \quad (8)$$

Comparing with (5) we find that for the Voigt model the effective stiffness is the average stiffness

$$C_V = \langle c \rangle \quad (9)$$

In the Reuss case we have

$$\sigma = \langle \sigma \rangle \quad (10)$$

and so

$$\langle e \rangle = \langle s\sigma \rangle = \langle s \rangle \langle \sigma \rangle \quad (11)$$

Comparing with (6) we find that for the Reuss model the effective compliance is the average compliance

$$S_R = \langle s \rangle \quad (12)$$

The Voigt and Reuss effective moduli form upper and lower bounds on the effective stiffness of the medium. There are two invariants for fourth rank tensors and the fundamental property of invariants is that they do not depend on orientation in space. If the average moduli are assumed to be independent of orientation, that is, if we assume the effective medium is isotropic, then each invariant is equal to its average. Then we have from (9) for the Voigt model

$$C_{ijj}^V = c_{ijj} \quad \text{and} \quad C_{ijj}^V = c_{ijj} \quad (13)$$

Similarly we have from (12) for the Reuss model

$$S_{ijj}^R = s_{ijj} \quad \text{and} \quad S_{ijj}^R = s_{ijj} \quad (14)$$

For an isotropic material there are only two independent elastic moduli. Equations (13) and (14) are therefore easily solved for the isotropic effective elastic moduli of the Voigt and Reuss models.

Cubic Crystal Symmetry

We shall further confine ourselves to the specific results of cubic crystal symmetry. There are then only three independent components of the single crystal elastic moduli. The analysis is simplified if we use the Walpole³ notation for the decomposition of “unity”

$$I = J + K = J + K' + K'' \quad (15)$$

The first equality gives the isotropic and the second the cubic decomposition. The isotropic and cubic bases are isotropic, idempotent and orthogonal to each other. See Walpole’s paper for details. The terms in (15) can be either tensors or matrices. The isotropic Voigt and Reuss effective moduli can then be written in terms of the following spectral decomposition

$$C_V = 3K_V J + 2G_V K \quad (16)$$

$$S_R = \frac{J}{3K_R} + \frac{K}{2G_R} \quad (17)$$

where K and G are the effective bulk and shear modulus, respectively. Similarly, the cubic stiffness and compliance have the decompositions

$$c = 3\kappa J + 2\mu' K' + 2\mu'' K'' \quad (18)$$

$$s = \frac{J}{3\kappa} + \frac{K'}{2\mu'} + \frac{K''}{2\mu''} \quad (19)$$

in terms of the single crystal bulk modulus κ and the two shear moduli μ' and μ'' , which represent the shear moduli in the [100] and [111] crystal directions, respectively. These fundamental components of the cubic elastic moduli, as discussed by Walpole, are very convenient to use in the calculations and are related to the standard elastic moduli in the Voigt notation by

$$\begin{cases} \kappa = \frac{1}{3}(c_{11} + 2c_{12}) = \frac{1}{3(s_{11} + 2s_{12})} \\ \mu' = \frac{1}{2}(c_{11} - c_{12}) = \frac{1}{2(s_{11} - s_{12})} \\ \mu'' = c_{44} = \frac{1}{s_{44}} \end{cases} \quad (20)$$

From the first equation of (13) we find the Voigt bulk modulus $K_V = \kappa$ and from the second we find the effective Voigt shear modulus,

$$G_V = \frac{2}{3}\mu' + \frac{3}{5}\mu'' \quad (21)$$

Similarly, from the first equation of (14) we find $K_R = \kappa$ and from the second we find the effective Reuss shear modulus, G_R ,

$$\frac{1}{G_R} = \frac{2}{5\mu'} + \frac{3}{5\mu''} \quad (22)$$

By examining (9), (16), (18), and (21) we conclude that we have found a rule for the orientation averaging of a cubic, homogeneous, isotropic, disordered fourth rank tensor. If the tensor is given by

$$t = aJ + b'K' + b''K'' \quad (23)$$

then the effective average is

$$\langle t \rangle = aJ + \left(\frac{2}{5}b' + \frac{3}{5}b''\right)K \quad (24)$$

This rule can be used alternatively to derive equations (21) and (22).

Young's Modulus and Diffraction

For a cubic single crystal Nye⁴ derived the reciprocal of Young's modulus in the direction $[hkl]$ as follows

$$E_{hkl}^{-1} = s_{11}^{hkl} = s_{11} - (2s_{11} - 2s_{12} - s_{44})\Gamma \quad (25)$$

where

$$\Gamma = \frac{h^2k^2 + k^2l^2 + l^2h^2}{(h^2 + k^2 + l^2)^2} \quad (26)$$

When a diffracting beam shines on the Reuss model of a polycrystal, only those grains with planes (hkl) oriented to satisfy the Bragg condition will reflect and so the Reuss average of the apparent or diffraction Young's modulus is given by the same expression as (25). Inserting the fundamental cubic elastic moduli from (20) we get an expression for the *effective diffraction Young's modulus* of the Reuss model, E_{DR} ,

$$\frac{1}{E_{DR}} = \frac{1}{9K} + \frac{1}{3\mu'} - \left(\frac{1}{\mu'} - \frac{1}{\mu''} \right) \Gamma \quad (27)$$

where Γ is now regarded as a diffraction parameter that depends on which (hkl) plane is causing the diffraction for which E_{DR} is measured. The *effective diffraction shear modulus* of the Reuss model, G_{DR} , is then given from the isotropic relation

$$\frac{1}{G_{DR}} = \frac{3}{E_{DR}} - \frac{1}{3K} = \frac{1}{\mu'} - 3 \left(\frac{1}{\mu'} - \frac{1}{\mu''} \right) \Gamma \quad (28)$$

The average of the diffraction parameter Γ over all orientations is $1/5$ and for this value (28) reduces to (22). We say that (28) represents the diffraction average of an *effective diffraction medium*. In general, by analogy with (5), the average properties of the diffracting material can be written

$$\langle \sigma \rangle = C_D \langle e \rangle_D \quad (29)$$

where $\langle e \rangle_D$ is the diffraction average strain and C_D is the *effective diffraction stiffness*. The motivation for this equation is that we apply the diffraction average to the strain because in diffraction experiments the strain is measured selectively by using the Bragg equation and thus depends on the active reflecting plane (hkl), whereas the regular average is applied to the stress because the actual stress is measured by applying a force. The equation can be solved for the diffraction average strain

$$\langle e \rangle_D = \frac{\langle \sigma \rangle}{C_D} = S_D \langle \sigma \rangle \quad (30)$$

where S_D is the *effective diffraction compliance*. In particular, for the Reuss model where σ is constant we find the effective diffraction compliance is the average diffraction compliance

$$S_{DR} = \langle s \rangle_D \quad (31)$$

By writing the decomposition

$$S_{DR} = \frac{J}{3K_{DR}} + \frac{K}{2G_{DR}} \quad (32)$$

and examining (31), (19), and (28) we see that we now also have derived a rule for the diffraction average of a cubic tensor. If the tensor is given by (23) then the diffraction average is

$$\langle t \rangle_D = aJ + [b' - 3(b' - b'')\Gamma]K \quad (33)$$

This rule can be used alternatively to derive equation (28).

The Comparison Medium

In statistical continuum mechanics it is customary to use perturbation theory to approximate the effective medium in terms of its deviation from a *comparison medium*, which is known and chosen arbitrarily. From the equilibrium equations of elasticity Willis⁵ and Kröner⁶ derived the following basic equation for the relationship

$$e = e_0 - E \delta c e \quad (34)$$

which Kröner called the LSD equation after Lippmann-Schwinger and Dyson. Here

$$\delta c = c - C_0 \quad (35)$$

where e and e_0 are the strains and c and C_0 are the stiffnesses of the polycrystal and comparison medium, respectively. Furthermore E is the singular approximation to the modified Green's function, which is derived from the Green's function for the comparison medium. For the isotropic case Kröner⁶ gave it as

$$E = \frac{1}{3K_0 + 4G_0} J + \frac{1}{5} \left(\frac{1}{G_0} + \frac{2}{3K_0 + 4G_0} \right) K \quad (36)$$

where K_0 and G_0 are the bulk and shear modulus of the comparison medium. The comparison medium has the decomposition

$$C_0 = 3K_0 J + 2G_0 K \quad (37)$$

We now solve (34) for the strain e in the polycrystal

$$e = a e_0 \quad (38)$$

where we have defined the operator

$$a \equiv \frac{I}{I + E \delta c} \quad (39)$$

From (3) the stress in the polycrystal is given by

$$\sigma = c a e_0 \quad (40)$$

From the effective diffraction medium equation (29) we then find

$$\langle c a e_0 \rangle = C_D \langle a e_0 \rangle_D \quad (41)$$

Since e_0 is constant, it can be eliminated. Solving we get the basic equation for the *approximate effective diffraction stiffness*

$$C_D = \langle c a \rangle \frac{I}{\langle a \rangle_D} \quad (42)$$

This is a general and formal equation from which explicit results can be derived for special cases. With equations (39), (36), (35), and (33) we see that C_D can be expressed in terms of the single crystal elastic constants, c , the comparison medium elastic constants, C_0 , and the diffraction parameter, Γ .

Gairola-Kröner Formula

We now decompose the approximate effective diffraction stiffness as follows

$$C_D = 3K_D J + 2G_D K \quad (43)$$

where K_D and G_D are the approximate effective diffraction bulk and shear modulus. Equation (42) can be written out entirely in terms of κ , μ' , μ'' , Γ , K_0 , and G_0 , by using (18), (39), (36), (37), and calculating the averages from (24) and (33). Equating the coefficients of J we find that $K_D = \kappa$. Equating the coefficients of K we get

$$G_D = \frac{\frac{\frac{2}{5}\mu'}{1 + \frac{2}{5}\left(\frac{1}{G_0} + \frac{2}{3\kappa + 4G_0}\right)(\mu' - G_0)} + \frac{\frac{\frac{3}{5}\mu''}{1 + \frac{2}{5}\left(\frac{1}{G_0} + \frac{2}{3\kappa + 4G_0}\right)(\mu'' - G_0)}}{1 - 3\Gamma}}{\frac{\frac{2}{5}\mu'}{1 + \frac{2}{5}\left(\frac{1}{G_0} + \frac{2}{3\kappa + 4G_0}\right)(\mu' - G_0)} + \frac{\frac{3}{5}\mu''}{1 + \frac{2}{5}\left(\frac{1}{G_0} + \frac{2}{3\kappa + 4G_0}\right)(\mu'' - G_0)}}{3\Gamma}} \quad (44)$$

This equation can be reduced to the following expression for the approximate effective diffraction shear modulus

$$G_D(G_0) = \frac{\alpha_0 + \alpha_1 G_0 + \alpha_2 G_0^2}{\beta_0 + \beta_1 G_0 + \beta_2 G_0^2} \quad (45)$$

where

$$\begin{cases} \alpha_0 = 30\kappa\mu'\mu'' \\ \alpha_1 = 3(6\kappa\mu' + 9\kappa\mu'' + 20\mu'\mu'') \\ \alpha_2 = 8(2\mu' + 3\mu'') \end{cases} \quad \begin{cases} \beta_0 = 30\kappa[\mu'' + 3(\mu' - \mu'')\Gamma] \\ \beta_1 = 15[3\kappa + 4\mu'' + 12(\mu' - \mu'')\Gamma] \\ \beta_2 = 40 \end{cases} \quad (46)$$

For $\Gamma=1/5$ this reduces to the Gairola-Kröner⁷ formula. The shear modulus in (45) is approximate because it is a perturbation from a comparison medium, which may be chosen arbitrarily. If we choose $G_0=\infty$ or $G_0=0$ we get the Voigt or Reuss approximations.

Self-Consistent Moduli

If we choose the comparison medium to be the same as the effective medium

$$G_0 = G_D \quad (47)$$

then there is no deviation between the two media and we get the so-called *self-consistent* moduli. For this case (45) reduces to

$$\gamma_0 + \gamma_1 G_D + \gamma_2 G_D^2 + \gamma_3 G_D^3 = 0 \quad (48)$$

where

$$\begin{cases} \gamma_0 = -30\kappa\mu'\mu'' \\ \gamma_1 = -3 \left[6\kappa\mu' - \kappa\mu'' + 20\mu'\mu'' - 30\kappa(\mu' - \mu'')\Gamma \right] \\ \gamma_2 = 45\kappa - 16\mu' + 36\mu'' + 180(\mu' - \mu'')\Gamma \\ \gamma_3 = 40 \end{cases} \quad (49)$$

For $\Gamma=1/5$ this reduces to the result derived by Kröner⁸ for the original cubic equation of the self-consistent effective shear modulus of a cubic polycrystal.

Diffraction Elastic Constants

In diffraction experiments it is conventional to measure the two *diffraction elastic constants*, which occur naturally in the diffraction equations. They are given by

$$\begin{cases} S_1 = \frac{1}{9K_D} - \frac{1}{6G_D} \\ S_2 = \frac{1}{G_D} \end{cases} \quad (50)$$

For the self-consistent case it follows from (50), (48), (49), and (20) that the diffraction elastic constants are functions of the diffraction parameter Γ and the elastic constants c_{11} , c_{12} , and c_{44} : $S_1(\Gamma, c_{11}, c_{12}, c_{44})$ and $S_2(\Gamma, c_{11}, c_{12}, c_{44})$.

Experimental Results

If S_1 and S_2 are measured for several diffraction reflections (hkl) in a polycrystal, then we can regard S_1 and S_2 as dependent variables, and Γ as the independent variable in a regression analysis where the elastic constants c_{11} , c_{12} , and c_{44} are the unknown parameters. Recently Gnäupel-Herold, Brand, and Prask⁹ measured the diffraction elastic constants for various cubic polycrystals. Their results are summarized in Table 1.

To do the regression analysis we write chi-square

$$\chi^2(c_{11}, c_{12}, c_{44}) = \sum_r \left[\left(\frac{S_1^{\text{meas}} - S_1^{\text{calc}}}{\sigma(S_1)} \right)^2 + \left(\frac{S_2^{\text{meas}} - S_2^{\text{calc}}}{\sigma(S_2)} \right)^2 \right] \quad (51)$$

and minimize with respect to c_{11} , c_{12} , and c_{44} . The results are given in Table 2. Here A represents the anisotropy factor

$$A = \frac{2c_{44}}{c_{11} - c_{12}} \quad (52)$$

and χ_{red}^2 is χ^2 divided by the degrees of freedom (DoF). A value of $\chi_{\text{red}}^2 = 1$ represents the best fit.

Table 1. *Experimental results for steel, aluminum and copper*

The mass content of elements other than iron in the steel samples was 2.25% Cr and 1% Mo. The aluminum sample contained 0.25% Cu, 0.6% Si, 1.0% Mg, 0.2% Cr. The copper sample was high-conductivity copper with a purity of 99.9%. The values in parentheses represent the standard deviations.

<i>hkl</i>	S_1 [TPa ⁻¹]	$\frac{1}{2}S_2$ [TPa ⁻¹]
Steel		
002	-1.758 (±0.084)	7.522 (±0.150)
011	-1.121 (±0.062)	5.499 (±0.101)
211	-1.010 (±0.103)	5.342 (±0.172)
310	-1.692 (±0.099)	6.852 (±0.166)
Aluminum		
002	-5.081(±0.243)	19.765(±0.437)
022	-5.075(±0.228)	18.793(±0.435)
222	-4.749(±0.287)	18.318(±0.563)
311	-4.742(±0.309)	19.069(±0.638)
331	-4.685(±0.296)	17.808(±0.537)
420	-4.756(±0.260)	18.306(±0.499)
Copper		
002	-3.87(±0.23)	13.66(±0.35)
022	-2.62(±0.37)	9.26(±0.66)
111	-2.32(±0.29)	8.77(±0.39)
311	-2.47(±0.11)	10.51(±0.21)
331	-2.12(±0.35)	8.71(±0.62)

Table 2. *Single-crystal elastic stiffnesses for aluminum, copper and steel*

The quality of each material calculation can be assessed by means of the reduced χ^2 in the last column. The copper sample exhibited some residual texture, which could not be eliminated by repeated cold working and recrystallization. The values in parenthesis are the standard deviations.

Material	c_{11} (GPa)	c_{12} (GPa)	c_{44} (GPa)	A	DoF	χ^2_{red}
Steel	222.8 (±10.6)	123.5 (±10.4)	121.7 (±3.7)	2.45	5	0.96
Aluminum	114.0 (±7.9)	65.3 (±7.6)	28.5 (±0.8)	1.17	9	0.64
Copper	157.7 (±13.7)	104.5 (±13.9)	74.2 (±3.3)	2.79	7	1.70

Graphs of the diffraction elastic constants based in these results for the single crystal elastic constants are shown in Figs. 1, 2 and 3. The experimental values are taken from Table 1 and the error bars represent the standard deviations. The fit is good for steel with a questionable point for S_1 at (310). There is much more error for aluminum, which could be attributed to the fact that aluminum is close

to isotropic, i.e. A is near 1, and that therefore the χ^2 function has a much shallower minimum. The copper results are fair. These results for the single crystal elastic constants agree reasonably well with those in the literature⁹.

Conclusion

We have shown how the method of statistical continuum mechanics can be used to derive self-consistent expressions for the diffraction elastic constants of a cubic polycrystal in terms of the single crystal elastic constants. The diffraction elastic constants can be measured and a regression analysis can then deduce the single crystal elastic constants. This method has proven to be feasible experimentally. It is possible to use it as an alternative method for determining single crystal elastic constants experimentally. For this simple analysis to work the polycrystal must be homogeneous, isotropic, and disordered, i.e. there must be no texture.

Reference List

1. W. Voigt, "Theoretische Studien über die Elastizitätsverhältnisse der Kristalle," *Abh. Kgl. Ges. Wis. Göttingen, Math. Kl.* **34**, 1 (1887).
2. A. Reuss, "Berechnung der Fließgrenze von Mischkristallen auf Grund der Plastizitätsbedingungen für Einkristalle," *Z. ang. Math. und Mech.* **9**, 49-58 (1929).
3. L. J. Walpole, "Elastic Behavior of Composite Materials: Theoretical Foundations," *Advances in Applied Mechanics* **21**, 169-242 (1981).
4. J. F. Nye, *Physical Properties of Crystals* (Oxford University Press, Oxford, 1960).
5. J. R. Willis, "Variational and Related Methods for the Overall Properties of Composites," *Advances in Applied Mechanics* **21**, 1-78 (1981).
6. E. Kröner, "Statistical Modelling," in *Modelling Small Deformations of Polycrystals*, Chap. 8, J. Gittus and J. Zarka, Eds. (Elsevier Applied Science, London, New York, 1986), pp. 229-291.
7. B. K. D. Gairola and E. Kröner, "A Simple Formula for Calculating the Bounds and the Self-Consistent Value of the Shear Modulus of a Polycrystalline Aggregate of Cubic Crystals," *International Journal of Engineering Science* **19**, 865-869 (1981).
8. E. Kröner, "Berechnung der elastischen Konstanten des Vielkristalls aus dem Konstanten des Einkristalls," *Zeitschrift für Physik* **151**, 504-518 (1958).
9. T. Gnäupel-Herold, P. C. Brand, H. J. Prask, "Calculation of single-crystal elastic constants for cubic crystal symmetry from powder diffraction data," *Journal of Applied Crystallography* **31**, 929-935 (1998).

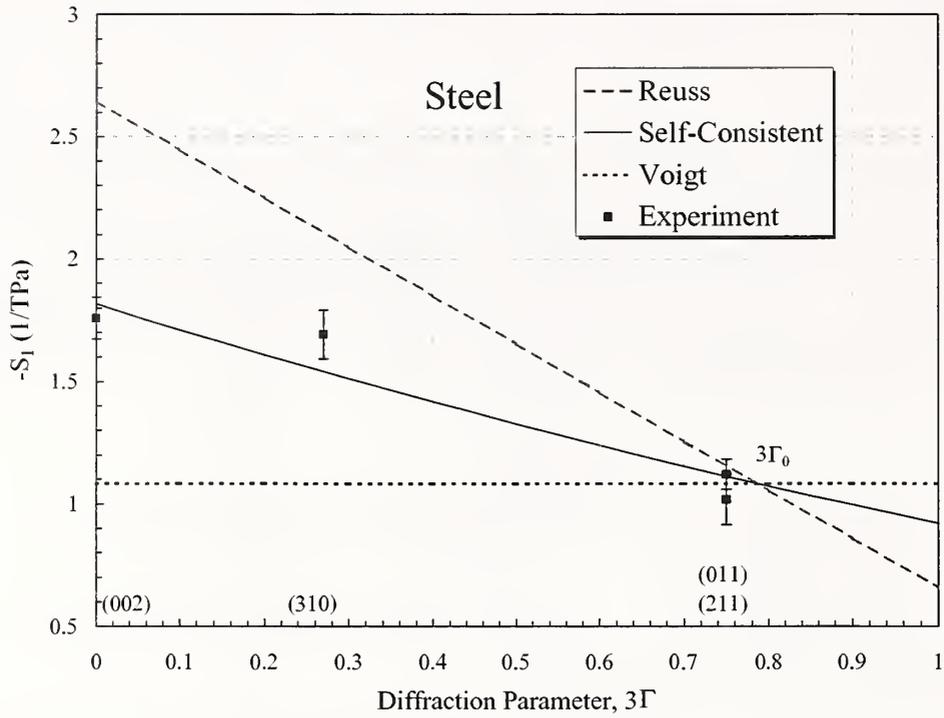


Fig. 1a: Experimental and analytical results for the first diffraction elastic constant of steel

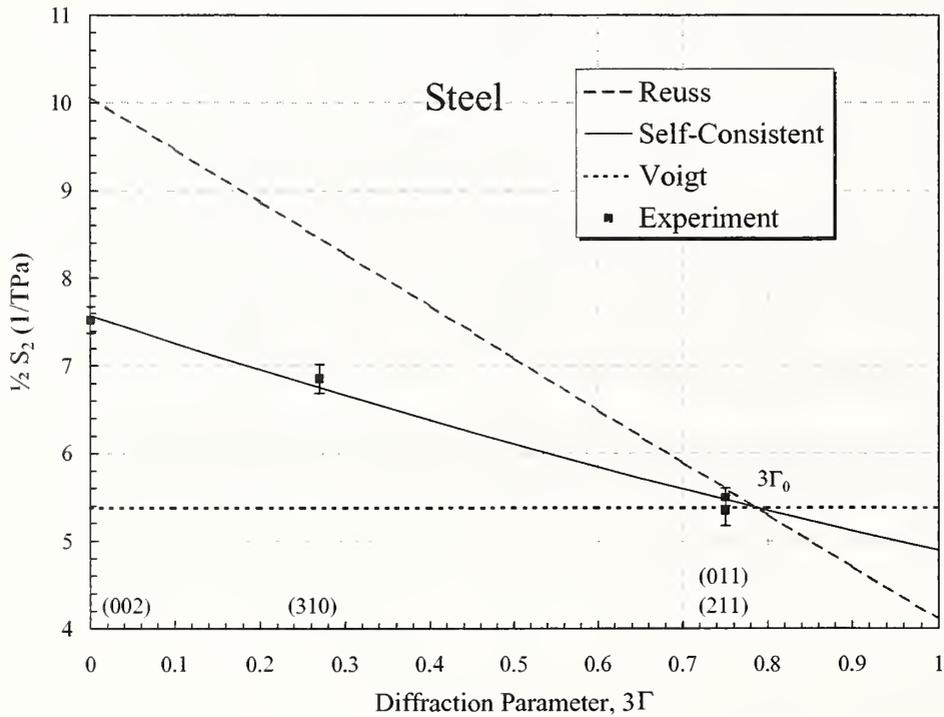


Fig. 1b: Experimental and analytical results for the second diffraction elastic constant of steel

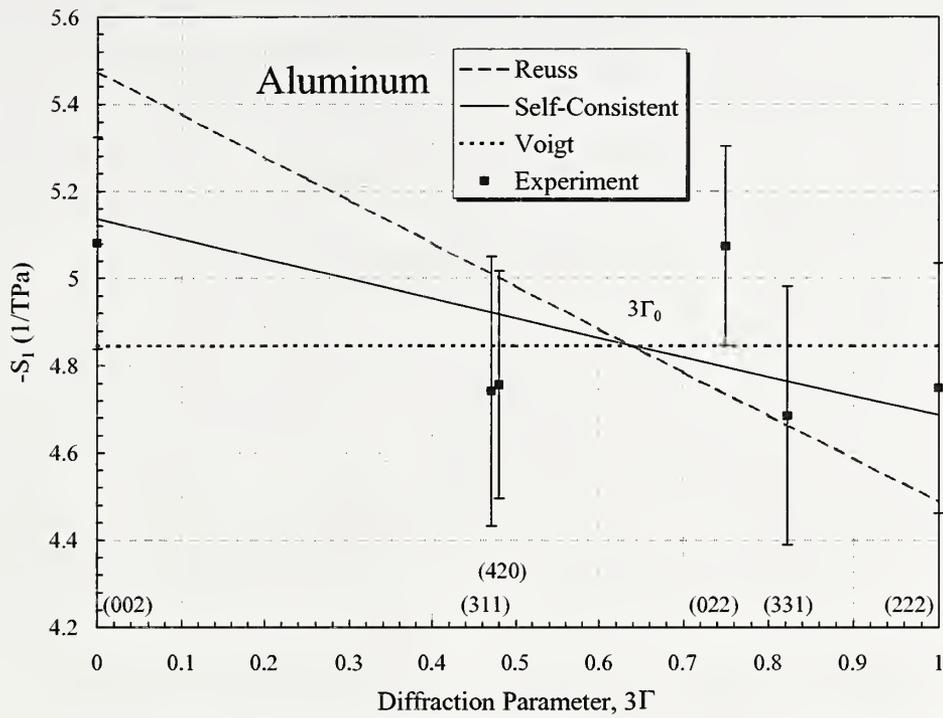


Fig. 2a: Experimental and analytical results for the first diffraction elastic constant of aluminum

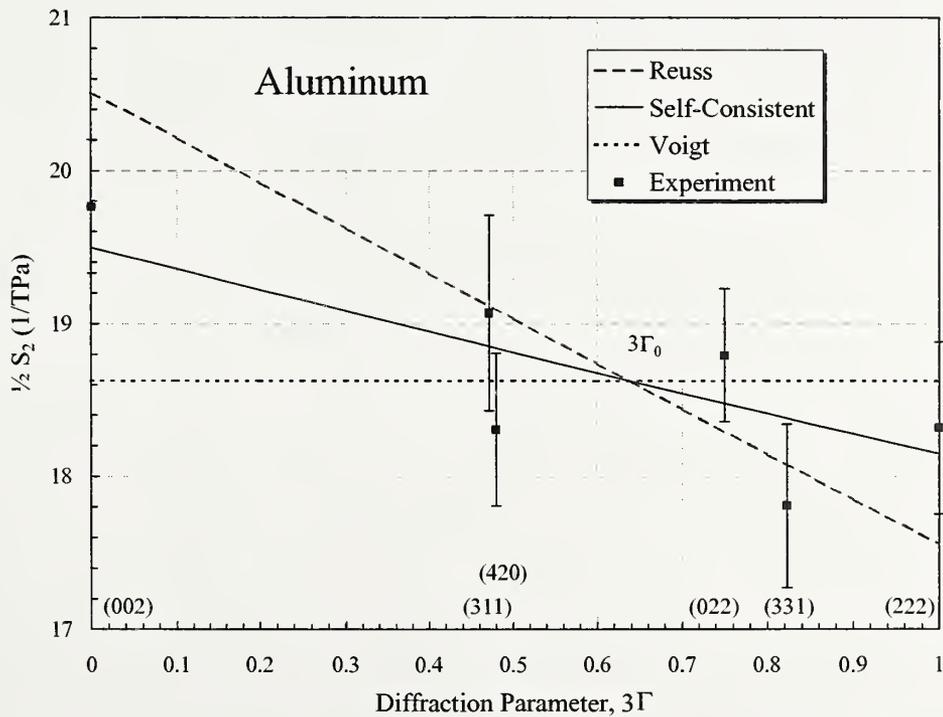


Fig. 2b: Experimental and analytical results for the second diffraction elastic constant of aluminum

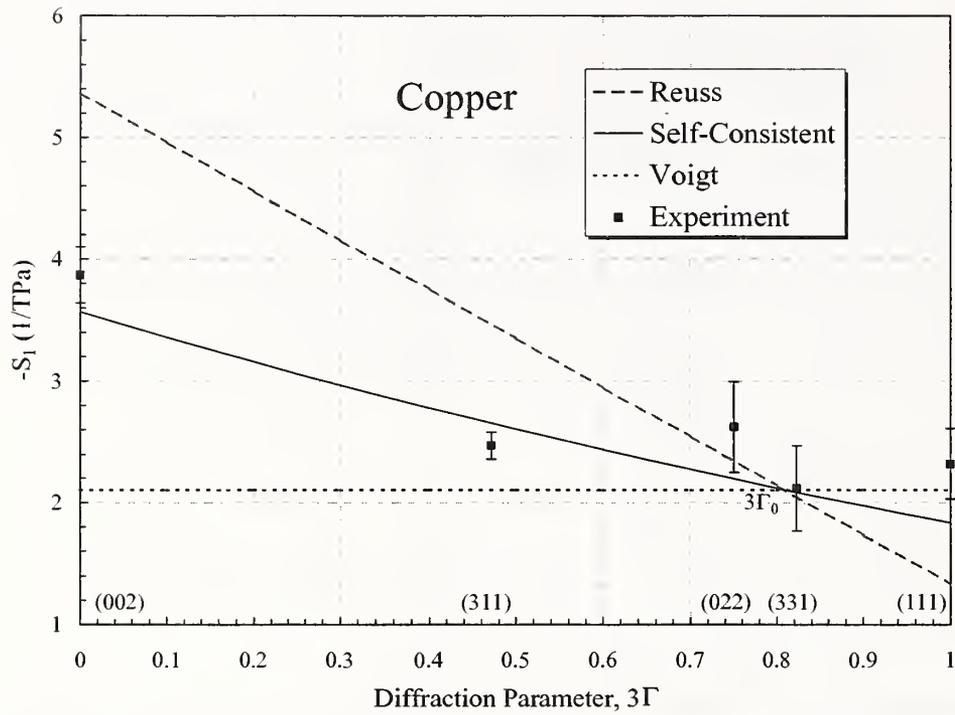


Fig. 3a: Experimental and analytical results for the first diffraction elastic constant of copper

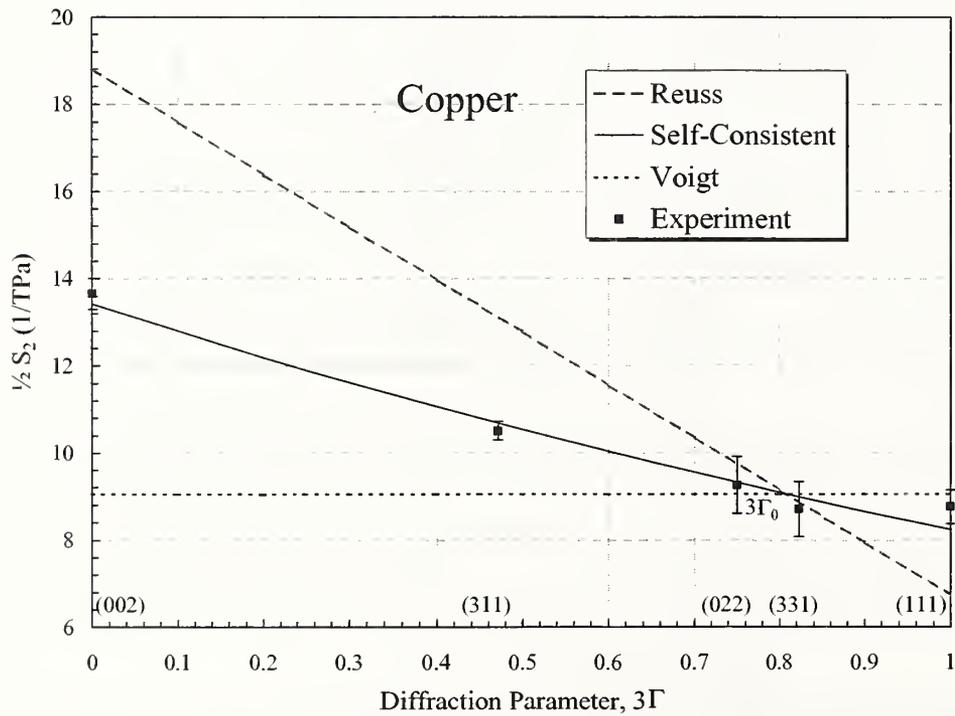


Fig. 3a: Experimental and analytical results for the second diffraction elastic constant of copper

