

# Graphical Representation of the Generalized Hooke's Law

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*The anisotropic linear elastic behavior of single crystals can be described equivalently by a 4th-order elasticity tensor or two functions  $E(\mathbf{d})$  and  $K(\mathbf{d})$ . These functions represent Young's modulus and a generalized bulk modulus as functions of the tensile direction  $\mathbf{d}$  in a tension test. In the present paper three- and two-dimensional graphical representations of Young's modulus and the generalized bulk modulus are given for single crystals belonging to one of the following symmetry groups: monoclinic, rhombic, trigonal, tetragonal, hexagonal, and cubic symmetry.*

## 1 Introduction

The generalized Hooke's law is the geometrical and physical linear relation between stress and strain of anisotropic elastic solids. It is one of the oldest and best known constitutive relations in continuum mechanics. One dimensional formulations have been discussed first in the 17th century. Over a long time the scientific community agreed to differ about the most general form in linear elasticity. Finally Voigt (1850-1919) answered the open question how many constants have to be determined in the isotropic and anisotropic case. He proved by experiments Green's (1793-1841) hypothesis that in the isotropic case two and in the general anisotropic hyperelastic case 21 constants have to be determined.

Based on Hooke's law structures are analyzed in all branches of mechanical and civil engineering. In most cases the isotropic version of Hooke's law is used. But in the last decades more and more anisotropies have been taken into account, which are especially important if the component parts are laminated or made from single crystals. Also the change of elastic properties of polycrystals during metal forming operations is of importance in order to estimate spring-back effects. Independently from the special application the engineer requires methods to illustrate or to visualize the anisotropic linear elastic properties of materials. In the present paper a visualization based on Young's modulus and a generalized bulk modulus is developed.

The outline of the paper is as follows: In Section 2 the basic properties of Hooke's law are discussed and the elasticity tensor is specified for the eight different symmetry classes relevant in the context of linear elasticity. In Section 3 the harmonic decomposition of elasticity tensors is introduced. This decomposition delivers a tool to decompose a 4th-order elasticity tensor uniquely into isotropic and anisotropic parts. In Section 4 characteristic components of the elasticity tensor are discussed, which are useful scalar functions describing the anisotropic linear elastic behavior (Böhlke, 2001). It is shown that Young's modulus and a generalized bulk modulus depend only on a normalized vector specifying the tensile direction in a tension test. Both scalar functions uniquely determine the elasticity tensor (He and Curnier, 1994). In Section 5 three- and two-dimensional graphical representations of Young's modulus and the generalized bulk modulus are given for single crystals belonging to one of the following symmetry groups: monoclinic, rhombic, trigonal, tetragonal, hexagonal, and cubic symmetry.

**Notation.** Throughout the text a direct tensor notation is preferred. In order to avoid additional formal definitions, the index notation is applied in some cases using the summation convention. A linear mapping of a 2nd-order tensor is written as  $\mathbf{A} = \mathbb{C}[\mathbf{B}]$ . The composition, the scalar product, the dyadic product, and the Frobenius norm of 2nd-order tensors are denoted by  $\mathbf{A}\mathbf{B}$ ,  $\mathbf{A} \cdot \mathbf{B}$ ,  $\mathbf{A} \otimes \mathbf{B}$ , and  $\|\mathbf{A}\| = (\mathbf{A} \cdot \mathbf{A})^{1/2}$ , respectively. Irreducible, i.e., completely symmetric and traceless tensors are designated by a prime, e.g.,  $\mathbf{A}'$  and  $\mathbf{C}'$ . The basic isotropic 2nd-, 4th-, and 6th-order tensors (Zheng and Betten, 1995) are denoted by  $\mathbf{I}$ ,  $\mathbb{I}$ , and  $\mathbb{J}$ , respectively

$$\mathbf{I} = \mathbf{e}_i \otimes \mathbf{e}_i \quad \mathbb{I} = \frac{1}{2} \mathbf{e}_i \otimes \mathbf{e}_j \otimes (\mathbf{e}_i \otimes \mathbf{e}_j + \mathbf{e}_j \otimes \mathbf{e}_i) \quad (1)$$

$$\mathbb{J} = \frac{1}{8} (\mathbf{e}_i \otimes \mathbf{e}_j + \mathbf{e}_j \otimes \mathbf{e}_i) \otimes (\mathbf{e}_j \otimes \mathbf{e}_k + \mathbf{e}_k \otimes \mathbf{e}_j) \otimes (\mathbf{e}_k \otimes \mathbf{e}_i + \mathbf{e}_i \otimes \mathbf{e}_k) \quad (2)$$

where  $\{\mathbf{e}_i\}$  is an arbitrary but fixed orthonormal basis. The Rayleigh product of a 2nd-order tensor  $\mathbf{A}$  and a 4th-order tensor  $\mathbb{C} = C_{ijkl}\mathbf{e}_i \otimes \mathbf{e}_j \otimes \mathbf{e}_k \otimes \mathbf{e}_l$  is defined by

$$\mathbf{A} \star \mathbb{C} = C_{mnop}\mathbf{A}\mathbf{e}_m \otimes \mathbf{A}\mathbf{e}_n \otimes \mathbf{A}\mathbf{e}_o \otimes \mathbf{A}\mathbf{e}_p \quad (3)$$

If (3) is written in components with respect to  $\{\mathbf{e}_i\}$  then one obtains

$$(\mathbf{A} \star \mathbb{C})_{ijkl} = A_{im}A_{jn}A_{ko}A_{lp}C_{mnop} \quad (4)$$

If  $\mathbb{C}$  exhibits a symmetry in the first or second pair of indices (e.g.,  $C_{ijkl} = C_{jikl}$ ) or the major symmetry ( $C_{ijkl} = C_{klij}$ ), then  $\mathbf{A} \star \mathbb{C}$  shows the same symmetry properties for all  $\mathbf{A}$ . Furthermore, the associativity

$$\mathbf{A} \star (\mathbf{B} \star \mathbb{C}) = (\mathbf{A}\mathbf{B}) \star \mathbb{C} \quad (5)$$

holds for all 2nd-order tensors  $\mathbf{A}$  and  $\mathbf{B}$ .

## 2 Hooke's Law: Basic Properties

In classical linear elasticity, the stress tensor  $\mathbf{T}$  is given as a linear map of the (infinitesimal) strain tensor  $\mathbf{E}$ , and vice versa

$$\mathbf{T} = \mathbb{C}[\mathbf{E}] \quad \mathbf{E} = \mathbb{S}[\mathbf{T}] \quad (6)$$

where  $\mathbb{C}$  is the stiffness tensor and  $\mathbb{S}$  is the compliance tensor.  $\mathbb{S} = \mathbb{C}^{-1}$  holds on the space of symmetric 4th-order tensors. This formulation of Hooke's law can be applied if both the strains and rotations are small. For hyperelastic materials a strain energy and a complementary energy exist. They represent potentials for the stresses and strains, respectively. In the hyperelastic case the elasticity tensors possess the major symmetry, i.e.,  $C_{ijkl} = C_{klij}$ . The symmetry in the first and last pair of indices can be assumed for convenience, e.g.  $C_{ijkl} = C_{jikl}$ , since non-symmetric parts do not affect the stress-strain response. For a general discussion of the symmetries of elasticity tensors, see Bertram (1985). If the strain energy density is required to be positive for all non-zero strains, then the elasticity tensors have to be positive definite.

The 4th-order stiffness tensor  $\mathbb{C}$  and the corresponding compliance tensor  $\mathbb{S}$  are specified by the symmetry group  $\mathcal{S}$  of the material being a subgroup of the special orthogonal group, e.g., in terms of stiffnesses

$$\mathbb{C} = \mathbf{H} \star \mathbb{C} \quad \forall \mathbf{H} \in \mathcal{S} \subseteq Orth \quad (7)$$

Two stiffness tensors  $\mathbb{C}_1$  and  $\mathbb{C}_2$  are called equivalent if there is a rotation  $\mathbf{Q} \in Orth$  (proper orthogonal group) such that  $\mathcal{S}(\mathbb{C}_1) = \mathcal{S}(\mathbf{Q} \star \mathbb{C}_2)$  holds. Two stiffness tensors are equivalent if their symmetry groups are conjugate, i.e.  $\mathcal{S}(\mathbb{C}_1) = \mathbf{Q}\mathcal{S}(\mathbb{C}_2)\mathbf{Q}^T$ . Equivalence classes on the space of elasticity tensors are called symmetry classes. To each symmetry transformation  $\mathbf{H} \in Orth$  corresponds a  $-\mathbf{H}$ . Therefore, it is sufficient a priori consider only symmetry transformations with positive determinant.

Depending on the number of rotations or reflections of symmetry, Voigt (1910) classified crystals into 32 classes. All kinds of physically possible 2- and 3-dimensional symmetry groups have been classified by Zheng and Boehler (1994). Forte and Vianello (1996) classified all different forms of linear operators  $\mathbb{C}$  due to 3-dimensional symmetry groups and showed that in the context of 4th-order operators only 8 different symmetry classes can be distinguished (see Lemma 2 and the corresponding remarks on pp. 98–99 in the aforementioned article). The same result has been obtained by Khatkevich (1961); Federov (1968); Cowin (1995); Ting (1996). Note that e.g. by Gurtin (1972) ten different matrices have been given, which contain redundancies. Khatkevich (1961) and Cowin (1995) give an explicit proof that two of the matrices given by Gurtin (1972, pp. 88–89) are redundant, whereas Federov (1968) mentioned the redundancies without proof. Forte and Vianello (1996) discuss the redundancies in a group theoretical context and give an historical overview concerning the representation of linear elastic laws due to different types of anisotropy.

It is convenient to represent elasticity tensors by six by six matrices, the components of which refer to the orthonormal basis  $\mathbf{B}_\alpha (\alpha = 1 \dots 6)$  of symmetric 2nd-order tensors, i.e.,  $C_{\alpha\beta} = \mathbf{B}_\alpha \cdot \mathbb{C}[\mathbf{B}_\beta]$ , where

$$\begin{aligned} \mathbf{B}_1 &= \mathbf{e}_1 \otimes \mathbf{e}_1 & \mathbf{B}_4 &= \frac{\sqrt{2}}{2} (\mathbf{e}_2 \otimes \mathbf{e}_3 + \mathbf{e}_3 \otimes \mathbf{e}_2) \\ \mathbf{B}_2 &= \mathbf{e}_2 \otimes \mathbf{e}_2 & \mathbf{B}_5 &= \frac{\sqrt{2}}{2} (\mathbf{e}_1 \otimes \mathbf{e}_3 + \mathbf{e}_3 \otimes \mathbf{e}_1) \\ \mathbf{B}_3 &= \mathbf{e}_3 \otimes \mathbf{e}_3 & \mathbf{B}_6 &= \frac{\sqrt{2}}{2} (\mathbf{e}_1 \otimes \mathbf{e}_2 + \mathbf{e}_2 \otimes \mathbf{e}_1) \end{aligned} \quad (8)$$

This modified Voigt notation has been proposed, e.g., by Federov (1968) and Cowin (1989). The representation of elasticity tensors by six by six matrices with respect to the basis  $\mathbf{B}_\alpha$  has the advantage that invariants, eigenvalues, and eigentensors can be determined by means of the square matrix  $C_{\alpha\beta}$ . Note that this is not the case if Voigt's original notation is used.

In the following we list the component forms of the stiffnesses corresponding to the eight different symmetry classes (Ting, 1996). The matrices are given together with the number of independent elastic constants  $N_c$  and the number of planes of symmetry  $N_p$ :

triclinic symmetry ( $N_c = 21, N_p = 0$ )

$$\mathbb{C} = \begin{bmatrix} C_{1111} & C_{1122} & C_{1133} & \sqrt{2}C_{1123} & \sqrt{2}C_{1113} & \sqrt{2}C_{1112} \\ & C_{2222} & C_{2233} & \sqrt{2}C_{2223} & \sqrt{2}C_{2213} & \sqrt{2}C_{2212} \\ & & C_{3333} & \sqrt{2}C_{3323} & \sqrt{2}C_{3313} & \sqrt{2}C_{3312} \\ & & & 2C_{2323} & 2C_{2313} & 2C_{2312} \\ \text{sym.} & & & & 2C_{1313} & 2C_{1312} \\ & & & & & 2C_{1212} \end{bmatrix} \mathbf{B}_\alpha \otimes \mathbf{B}_\beta \quad (9)$$

monoclinic symmetry ( $N_c = 13, N_p = 1$ )

$$\mathbb{C} = \begin{bmatrix} C_{1111} & C_{1122} & C_{1133} & \sqrt{2}C_{1123} & 0 & 0 \\ & C_{2222} & C_{2233} & \sqrt{2}C_{2223} & 0 & 0 \\ & & C_{3333} & \sqrt{2}C_{3323} & 0 & 0 \\ & & & 2C_{2323} & 0 & 0 \\ \text{sym.} & & & & 2C_{1313} & 2C_{1312} \\ & & & & & 2C_{1212} \end{bmatrix} \mathbf{B}_\alpha \otimes \mathbf{B}_\beta \quad (10)$$

orthotropic or rhombic symmetry ( $N_c = 9, N_p = 3$ )

$$\mathbb{C} = \begin{bmatrix} C_{1111} & C_{1122} & C_{1133} & 0 & 0 & 0 \\ & C_{2222} & C_{2233} & 0 & 0 & 0 \\ & & C_{3333} & 0 & 0 & 0 \\ & & & 2C_{2323} & 0 & 0 \\ \text{sym.} & & & & 2C_{1313} & 0 \\ & & & & & 2C_{1212} \end{bmatrix} \mathbf{B}_\alpha \otimes \mathbf{B}_\beta \quad (11)$$

trigonal symmetry ( $N_c = 6, N_p = 3$ )

$$\mathbb{C} = \begin{bmatrix} C_{1111} & C_{1122} & C_{1133} & \sqrt{2}C_{1123} & 0 & 0 \\ & C_{1111} & C_{1133} & -\sqrt{2}C_{1123} & 0 & 0 \\ & & C_{3333} & 0 & 0 & 0 \\ & & & 2C_{2323} & 0 & 0 \\ \text{sym.} & & & & 2C_{2323} & 2C_{1123} \\ & & & & & C_{1111} - C_{1122} \end{bmatrix} \mathbf{B}_\alpha \otimes \mathbf{B}_\beta \quad (12)$$

tetragonal symmetry ( $N_c = 6, N_p = 5$ )

$$\mathbb{C} = \begin{bmatrix} C_{1111} & C_{1122} & C_{1133} & 0 & 0 & 0 \\ & C_{1111} & C_{1133} & 0 & 0 & 0 \\ & & C_{3333} & 0 & 0 & 0 \\ & & & 2C_{2323} & 0 & 0 \\ \text{sym.} & & & & 2C_{2323} & 0 \\ & & & & & 2C_{1212} \end{bmatrix} \mathbf{B}_\alpha \otimes \mathbf{B}_\beta \quad (13)$$

transversely isotropic or hexagonal symmetry ( $N_c = 5, N_p = 1 + \infty$ )

$$\mathbb{C} = \begin{bmatrix} C_{1111} & C_{1122} & C_{1133} & 0 & 0 & 0 \\ & C_{1111} & C_{1133} & 0 & 0 & 0 \\ & & C_{3333} & 0 & 0 & 0 \\ & & & 2C_{2323} & 0 & 0 \\ \text{sym.} & & & & 2C_{2323} & 0 \\ & & & & & C_{1111} - C_{1122} \end{bmatrix} \mathbf{B}_\alpha \otimes \mathbf{B}_\beta \quad (14)$$

cubic symmetry ( $N_c = 3, N_p = 9$ )

$$\mathbb{C} = \begin{bmatrix} C_{1111} & C_{1122} & C_{1122} & 0 & 0 & 0 \\ & C_{1111} & C_{1122} & 0 & 0 & 0 \\ & & C_{1111} & 0 & 0 & 0 \\ & & & 2C_{2323} & 0 & 0 \\ \text{sym.} & & & & 2C_{2323} & 0 \\ & & & & & 2C_{2323} \end{bmatrix} \mathbf{B}_\alpha \otimes \mathbf{B}_\beta \quad (15)$$

isotropic symmetry ( $N_c = 2, N_p = \infty$ )

$$\mathbb{C} = \begin{bmatrix} C_{1111} & C_{1122} & C_{1122} & 0 & 0 & 0 \\ & C_{1111} & C_{1122} & 0 & 0 & 0 \\ & & C_{1111} & 0 & 0 & 0 \\ & & & C_{1111} - C_{1122} & 0 & 0 \\ \text{sym.} & & & & C_{1111} - C_{1122} & 0 \\ & & & & & C_{1111} - C_{1122} \end{bmatrix} \mathbf{B}_\alpha \otimes \mathbf{B}_\beta \quad (16)$$

The orientation of the crystal is such that its symmetry planes coincide with some of the coordinate

planes. Therefore, in all but the triclinic and isotropic case, in addition to the  $N_c$  coefficients, the orientation of the anisotropy axes has to be supplemented in terms of three parameters. Otherwise the elasticity tensor is not determined uniquely. In the transversely isotropic case only two additional parameters have to be given.

### 3 Harmonic Decomposition of Elasticity Tensors

It is possible to decompose the 4th-order elasticity tensor of arbitrary symmetry into a direct sum of orthogonal subspaces on which the action of *Orth* is irreducible which means that there are no proper invariant subspaces. The harmonic decomposition has the form

$$\mathbb{C} = h_1 \mathbb{P}_1^I + h_2 \mathbb{P}_2^I + \mathbf{H}'_1 \otimes \mathbf{I} + \mathbf{I} \otimes \mathbf{H}'_1 + 4\mathbb{J}[\mathbf{H}'_2] + \mathbb{H}' \quad (17)$$

where

$$\mathbb{P}_1^I = \frac{1}{3} \mathbf{I} \otimes \mathbf{I} \quad \mathbb{P}_2^I = \mathbb{I} - \mathbb{P}_1^I \quad 4\mathbb{J}[\mathbf{A}] = (A_{im} \delta_{jn} + A_{in} \delta_{jm} + \delta_{im} A_{jn} + \delta_{in} A_{jm}) \mathbf{e}_i \otimes \mathbf{e}_j \otimes \mathbf{e}_m \otimes \mathbf{e}_n \quad (18)$$

(Schouten, 1924; Spencer, 1970; Cowin, 1989; Boehler et al., 1994). A review concerning this representation is given by Forte and Vianello (1996).  $h_1$  and  $h_2$  are called the first and second isotropic parts;  $\mathbf{H}'_1$  and  $\mathbf{H}'_2$  are the first and second deviatoric part, respectively;  $\mathbb{H}'$  is the harmonic part. The symmetry group of  $\mathbb{C}$  is the intersection of the symmetry groups of its deviatoric and harmonic parts. The tensors  $\mathbf{H}'_1$ ,  $\mathbf{H}'_2$ , and  $\mathbb{H}'$  are irreducible, i.e., completely symmetric and traceless

$$H'_{1ij} = H'_{1ji} \quad H'_{1ii} = 0 \quad H'_{2ij} = H'_{2ji} \quad H'_{2ii} = 0 \quad (19)$$

$$H'_{ijkl} = H'_{jikl} = H'_{klij} = H'_{kjl i} = \dots \quad H'_{iikl} = 0 \quad (20)$$

Irreducible 2nd-order tensors have five and irreducible 4th-order tensors have nine independent components.

The first and second isotropic parts  $h_1$  and  $h_2$  are determined by a projection of  $\mathbb{C}$  onto the space of isotropic 4th-order tensors, i.e.

$$h_\gamma = \mathbb{C} \cdot \frac{\mathbb{P}_\gamma^I}{\|\mathbb{P}_\gamma^I\|^2} \quad (21)$$

( $\gamma = 1, 2$ ).  $h_1$  and  $h_2$  are the eigenvalues of the isotropic part of  $\mathbb{C}$ . Hence  $h_1 = 3K$  and  $h_2 = 2G$  hold, where  $K$  and  $G$  are the bulk and shear modulus of the isotropic part of  $\mathbb{C}$ , respectively. The scalars  $h_1$  and  $h_2$  of the stiffness tensor  $\mathbb{C}$  correspond to the (isotropic) Voigt estimate (Voigt, 1910) of the polycrystals bulk modulus  $h_1 = 3K^{VI}$  and shear modulus  $h_2 = 2G^{VI}$ . The isotropic parts of the compliance tensor  $\mathbb{S}$  correspond to the bulk modulus  $1/h_1 = 3K^{RI}$  and shear modulus  $1/h_2 = 2G^{RI}$  of the Reuss estimate (Reuss, 1929). In the following the bulk modulus  $3K^{RI}$  and Young's modulus  $E^{RI} = 9K^{RI}G^{RI}/(3K^{RI} + G^{RI})$  are used to normalize directional dependent quantities.

The deviatoric parts can be computed by

$$\mathbf{H}'_1 = \frac{5}{7} \mathbf{C}'_1 - \frac{4}{7} \mathbf{C}'_2 \quad \mathbf{H}'_2 = \frac{3}{7} \mathbf{C}'_2 - \frac{2}{7} \mathbf{C}'_1 \quad (22)$$

where  $\mathbf{C}_1$  and  $\mathbf{C}_2$  represent the dilatational modulus and the Voigt tensor (Cowin, 1989)

$$\mathbf{C}_1 = C_{iikl} \mathbf{e}_k \otimes \mathbf{e}_l \quad \mathbf{C}_2 = C_{ikil} \mathbf{e}_k \otimes \mathbf{e}_l \quad (23)$$

Based on eqns (21) and (22), the harmonic part  $\mathbb{H}'$  can be determined as

$$\mathbb{H}' = \langle \mathbb{C} \rangle - \frac{2}{7} \langle \hat{\mathbf{C}} \otimes \mathbf{I} \rangle + \frac{1}{35} \text{tr}(\hat{\mathbf{C}}) \langle \mathbf{I} \otimes \mathbf{I} \rangle \quad (24)$$

where

$$\hat{\mathbf{C}} = \mathbf{C}_1 + 2\mathbf{C}_2 \quad (25)$$

The  $\langle \cdot \rangle$  bracket formula is defined by ( $\mathbf{A}, \mathbf{B} \in \text{Sym}$ )

$$\langle A_{ij} B_{kl} \rangle = \frac{1}{6} (A_{ij} B_{kl} + A_{ik} B_{jl} + A_{il} B_{kj} + B_{ij} A_{kl} + B_{ik} A_{jl} + B_{il} A_{kj}) \quad (26)$$

respectively. Note that  $\mathbf{C}$  has the major symmetry. Therefore,  $\langle C_{ijkl} \rangle = C_{ijkl} + C_{ikjl} + C_{iljk}$  holds. The formulae (21)-(24) show that all parts of the harmonic decomposition are linear functions of the components of  $\mathbf{C}$ .

#### 4 Characteristic Components of the Elasticity Tensor

In order to determine the elastic anisotropy experimentally, Young's modulus  $E$  is measured in most cases in tensile tests. A tensile test is defined by an uniaxial stress state, i.e.,  $\mathbf{T} = \sigma \mathbf{d} \otimes \mathbf{d}$  with the tensile direction  $\mathbf{d}$ . The corresponding strain tensor is given by  $\mathbf{E} = \mathbb{S}[\mathbf{T}] = \sigma \mathbb{S}[\mathbf{d} \otimes \mathbf{d}]$ . The tensile stress  $\sigma$  and the corresponding strain  $\varepsilon$  are the components of the stress and strain tensor with respect to the base tensor  $\mathbf{d} \otimes \mathbf{d}$ . Hence we have  $\sigma = \mathbf{T} \cdot \mathbf{d} \otimes \mathbf{d}$  and  $\varepsilon = \mathbf{E} \cdot \mathbf{d} \otimes \mathbf{d}$ , respectively. Young's modulus  $E(\mathbf{d})$  is defined by the ratio of tensile stress  $\sigma$  and tensile strain  $\varepsilon$ , i.e.,  $E = \sigma/\varepsilon$ . Combining the aforementioned facts one derives

$$\begin{aligned} \frac{1}{E(\mathbf{d})} &= \mathbf{d} \otimes \mathbf{d} \cdot \mathbb{S}[\mathbf{d} \otimes \mathbf{d}] \\ &= \frac{1}{3} h_1 + \frac{2}{3} h_2 + 2\mathbf{H}'_1 \cdot \mathbf{d} \otimes \mathbf{d} + 4\mathbf{H}'_1 \cdot \mathbf{d} \otimes \mathbf{d} + \mathbf{d} \otimes \mathbf{d} \cdot \mathbb{H}'[\mathbf{d} \otimes \mathbf{d}] \\ &= \frac{1}{E_{RI}} + (2\mathbf{H}'_1 + 4\mathbf{H}'_1) \cdot \mathbf{d} \otimes \mathbf{d} + \mathbf{d} \otimes \mathbf{d} \cdot \mathbb{H}'[\mathbf{d} \otimes \mathbf{d}] \end{aligned} \quad (27)$$

(Böhlke, 2001). Here and in the following,  $h_1$ ,  $h_2$ ,  $\mathbf{H}'_1$ ,  $\mathbf{H}'_2$ , and  $\mathbb{H}'$  denote the parts of the harmonic decomposition of  $\mathbb{S}$ .

In the isotropic case the bulk modulus is defined by one third of the ratio of the traces of the stress and the strain tensor. He and Curnier (1994) extended the definition of the bulk modulus to the anisotropic case. They defined a generalized bulk modulus by one third of the ratio of the tensile stress and the trace of the strain tensor. Again we have  $\sigma = \mathbf{T} \cdot \mathbf{d} \otimes \mathbf{d}$  and  $\text{tr}(\mathbf{E}) = \mathbf{E} \cdot \mathbf{I}$ , respectively. Note that  $\text{tr}(\mathbf{E})$  represents the relative change of volume  $(dV - dV_0)/dV_0$ . The strain tensor corresponding to  $\mathbf{T} = \sigma \mathbf{d} \otimes \mathbf{d}$  is given by  $\mathbf{E} = \sigma \mathbb{S}[\mathbf{d} \otimes \mathbf{d}]$ . Combining the aforementioned facts one derives

$$\begin{aligned} \frac{1}{3K(\mathbf{d})} &= \mathbf{I} \cdot \mathbb{S}[\mathbf{d} \otimes \mathbf{d}] \\ &= h_1 + \sqrt{3}\mathbf{H}'_1 \cdot \mathbf{d} \otimes \mathbf{d} + \frac{4}{3}\sqrt{3}\mathbf{H}'_2 \cdot \mathbf{d} \otimes \mathbf{d} \\ &= \frac{1}{3K_{RI}} + (\sqrt{3}\mathbf{H}'_1 + \frac{4}{3}\sqrt{3}\mathbf{H}'_2) \cdot \mathbf{d} \otimes \mathbf{d} \end{aligned} \quad (28)$$

(Böhlke, 2001). It is concluded that the quantity  $1/(3K)$  represents the relative change of volume per tensile stress  $\sigma$  in direction  $\mathbf{d}$ . The formula for the generalized bulk modulus shows that  $K(\mathbf{d})$  can exhibit only one of the following symmetries: isotropy, transverse-isotropy or orthotropy. This is due to the fact that it depends only on the 2nd-order deviatoric parts and does not depend on the 4th-order harmonic part. He and Curnier (1994) have shown that  $E(\mathbf{d})$  depends generally on 15 and  $K(\mathbf{d})$  on 6 components of  $\mathbb{S}$ , and that both functions uniquely determine the tensor  $\mathbb{S}$ . As a result, elasticity tensors can be determined from tensile tests alone. For cubic crystals  $K$  is independent of  $\mathbf{d}$  since the deviatoric parts vanish.

Similar to Young's modulus and the bulk modulus other characteristic components of the elasticity

tensors may be expressed by the parts of the harmonic decomposition (He and Curnier, 1994; Rychlewski, 1995) but these quantities are not defined on the unit sphere in  $\mathcal{R}^3$ . The shear modulus  $G$ , in a plane which is specified by the direction  $\mathbf{d}$  and the normal  $\mathbf{n}$  through  $\mathbf{M} = \sqrt{2}(\mathbf{d} \otimes \mathbf{n} + \mathbf{n} \otimes \mathbf{d})/2$  is given by

$$\begin{aligned} \frac{1}{2G(\mathbf{d}, \mathbf{n})} &= \mathbf{M} \cdot \mathbb{S}[\mathbf{M}] \\ &= h_2 + 2\mathbf{H}'_1 \cdot (\mathbf{d} \otimes \mathbf{d} + \mathbf{n} \otimes \mathbf{n}) + \mathbf{M} \cdot \mathbb{H}'[\mathbf{M}] \\ &= \frac{1}{G^{RI}} + 2\mathbf{H}'_1 \cdot (\mathbf{d} \otimes \mathbf{d} + \mathbf{n} \otimes \mathbf{n}) + \mathbf{M} \cdot \mathbb{H}'[\mathbf{M}] \end{aligned} \quad (29)$$

Another characteristic component is Poisson's ratio  $\nu$  in direction  $\mathbf{n}$  under stretch in direction  $\mathbf{d}$

$$\begin{aligned} -\frac{\nu(\mathbf{d}, \mathbf{n})}{E(\mathbf{d})} &= \mathbf{d} \otimes \mathbf{d} \cdot \mathbb{S}[\mathbf{n} \otimes \mathbf{n}] \\ &= \frac{1}{3}(h_1 - h_2) + \mathbf{H}'_1 \cdot (\mathbf{d} \otimes \mathbf{d} + \mathbf{n} \otimes \mathbf{n}) + \mathbf{d} \otimes \mathbf{d} \cdot \mathbb{H}'[\mathbf{n} \otimes \mathbf{n}] \\ &= -\frac{\nu^{RI}}{E^{RI}} + \mathbf{H}'_1 \cdot (\mathbf{d} \otimes \mathbf{d} + \mathbf{n} \otimes \mathbf{n}) + \mathbf{d} \otimes \mathbf{d} \cdot \mathbb{H}'[\mathbf{n} \otimes \mathbf{n}] \end{aligned} \quad (30)$$

## 5 Graphical Representation of $E(\mathbf{d})$ and $K(\mathbf{d})$

Inspection of eqns (27) and (28) shows that in the isotropic case Young's modulus and the generalized bulk modulus are given by

$$\frac{1}{E^{RI}} = \frac{1}{3}h_1 + \frac{2}{3}h_2 \quad \frac{1}{3K^{RI}} = h_1 \quad (31)$$

In the following the quantities  $E(\mathbf{d})$  and  $K(\mathbf{d})$  are normalized by  $E^{RI}$  and  $K^{RI}$ , respectively. The dimensionless quantities  $E(\mathbf{d})/E^{RI}$  and  $K^{RI}/K(\mathbf{d})$  can be computed by the formulae presented in the preceding sections for each direction in  $\mathcal{R}^3$ . All directions in  $\mathcal{R}^3$  can be parameterized by spherical coordinates  $\{r, \varphi, \vartheta\}$  with  $r = 1$ .

For a two-dimensional representation of  $E(\mathbf{d})/E^{RI}$  and  $K^{RI}/K(\mathbf{d})$  it is possible to project these functions by, e.g., a stereographic projection into a plane which contains the point with  $r = 0$ . Note that  $E(\mathbf{d}) = E(-\mathbf{d})$  and  $K(\mathbf{d}) = K(-\mathbf{d})$  hold. The two-dimensional representation could be called quasi pole figure in analogy to the projection technique commonly used in texture analysis (see, e.g., Bunge, 1993; Kocks et al., 1998). The quasi pole figure representation of elastic properties allows for a graphical representation of anisotropic linear elastic properties in two figures. In the following the normal of the projection plane is equal to  $\mathbf{e}_3$ . Then the spherical coordinates  $\{\varphi, \vartheta\}$  can be expressed by the polar coordinates  $\{\bar{r}, \bar{\varphi}\}$

$$\varphi = \bar{\varphi}, \quad \vartheta = 2 \arctan(\bar{r}) \quad (32)$$

The projection is described in Figures 1. Figure 2 shows the function  $E(\mathbf{d})$  for Gold which has a cubic crystal symmetry.

In the Figures 3 - 20 the projections of the functions  $E(\mathbf{d})/E^{RI}$  and  $K^{RI}/K(\mathbf{d})$  are given for different materials belonging to one of the following symmetry groups: monoclinic, rhombic, trigonal, tetragonal, hexagonal, and cubic symmetry. In all Figures lines of equal moduli are plotted. The difference between two lines amounts to  $\Delta(E(\mathbf{d})/E^{RI}) = 0.1$  and  $\Delta(K^{RI}/K(\mathbf{d})) = 0.1$ , respectively. The thick line denotes the ratios of  $E(\mathbf{d})/E^{RI} = 1$  and  $K^{RI}/K(\mathbf{d}) = 1$ . Hence the number of lines allows to quantify the amount of anisotropy in terms of the isotropic parts. For the dark-shadowed areas the ratios are larger than one. For the light-shadowed areas the ratios are less than one.

*Monoclinic symmetry:* In Figures 3 and 4 the three-dimensional and two-dimensional representations of Young's modulus and the bulk modulus are given for Hornblende and Feldspar. Both materials exhibit a

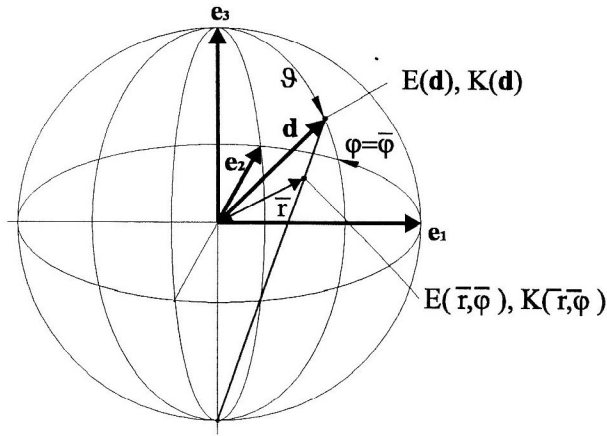


Figure 1: Stereographic Projection of Young's Modulus and the Generalized Bulk Modulus.

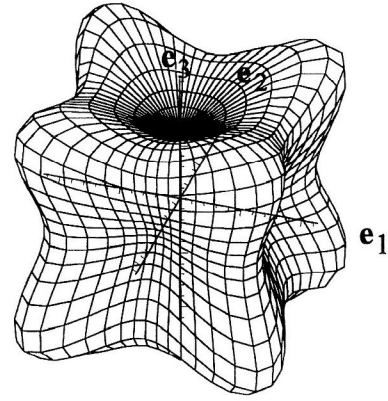


Figure 2: Young's Modulus of Gold (Cubic Symmetry).

significant anisotropy in terms of the functions  $E(\mathbf{d})$  and  $K(\mathbf{d})$ , respectively. In the case of a monoclinic symmetry one plane of symmetry exists ( $N_p = 1$ ). The pole figures indicate that for the considered set of elastic constants the normal of the plane of symmetry is given by  $\mathbf{n} = \mathbf{e}_1$ .

*Rhombic symmetry:* In Figures 5 - 8 the three- and two-dimensional representations are given for Uranium, Olivine, Rochelle Salt, and Topaz. All the materials but Topaz show a significant anisotropy. In the case of a rhombic symmetry three planes of symmetry exist ( $N_p = 3$ ). Their normals are given by the base vectors  $\mathbf{e}_i (i = 1, 2, 3)$ .

*Trigonal symmetry:* For this symmetry group the representations for Aluminium-Phosphate and Quartz are given in Figures 9 and 10. In the trigonal case three planes of symmetry exist ( $N_p = 3$ ). They are given by the base vectors

$$\mathbf{n}_1 = \cos(30^\circ)\mathbf{e}_1 + \sin(30^\circ)\mathbf{e}_2 \quad \mathbf{n}_2 = \mathbf{e}_2 \quad \mathbf{n}_3 = \cos(150^\circ)\mathbf{e}_1 + \sin(150^\circ)\mathbf{e}_2 \quad (33)$$

The pole figure of the bulk modulus shows a transverse isotropic symmetry.

*Tetragonal symmetry:* Here the representations for Weissblech and Zircon are given (Figures 11 and 12). The Figures show the following five planes of symmetry ( $N_p = 5$ )

$$\mathbf{n}_{1,2,3} = \mathbf{e}_{1,2,3} \quad \mathbf{n}_4 = \cos(45^\circ)\mathbf{e}_1 + \sin(45^\circ)\mathbf{e}_2 \quad \mathbf{n}_5 = \cos(135^\circ)\mathbf{e}_1 + \sin(135^\circ)\mathbf{e}_2 \quad (34)$$

Note that similar to the trigonal case the bulk modulus exhibits a transverse isotropic symmetry.

*Hexagonal symmetry:* The Figures 13 and 14 represent the elastic properties of Magnesium and Titanium. In this case the plane with the normal  $\mathbf{n} = \mathbf{e}_3$  is a plane of symmetry. Furthermore all planes which contain the  $\mathbf{e}_3$ -axis are planes of symmetry ( $N_p = 1 + \infty$ ).

*Cubic symmetry:* The Figures 15 - 20 show the elastic properties of Copper, Aluminium, Gold, Iron, Iron-Aluminium, and Pyrite. In the case of a cubic symmetry the material has nine planes of symmetry ( $N_p = 9$ ). Their normals are given by the three base vectors  $\mathbf{e}_i$ . Furthermore all vectors  $\mathbf{n} = (\mathbf{e}_i \pm \mathbf{e}_j)/\sqrt{2}$  with  $i \neq j$  are planes of symmetry. Note that in the cubic case the bulk modulus does not depend on  $\mathbf{d}$ .

## 6 Summary

The anisotropic linear elastic behavior of single crystals has been described by two functions  $E(\mathbf{d})$  and  $K(\mathbf{d})$  defined on the unit sphere in  $\mathcal{R}^3$  which represent Young's modulus and a generalized bulk modulus in the tensile direction  $\mathbf{d}$ .  $E(\mathbf{d})$  is the ratio of tensile stress to tensile strain. The quantity  $1/(3K(\mathbf{d}))$  represents the relative change of volume  $(dV - dV_0)/dV_0$  per tensile stress  $\sigma$  in direction  $\mathbf{d}$ . The elasticity tensors can be uniquely determined if the aforementioned functions are given. Since both functions are defined on the unit sphere in  $\mathcal{R}^3$ , they can be projected into a plane. The resulting plot is called quasi pole figure in analogy to the projection technique commonly used in texture analysis. Three- and two-dimensional representations of Young's modulus and the bulk modulus have been determined for selected single crystals (Kocks et al., 1998; Simmons and Wang, 1971). The figures clearly show the type and the amount of the anisotropy of the linear elastic behavior. The approach discussed in the present paper can be used for a graphical representation of material properties which are described by a fourth-order tensor having the same index symmetries as elasticity tensors.



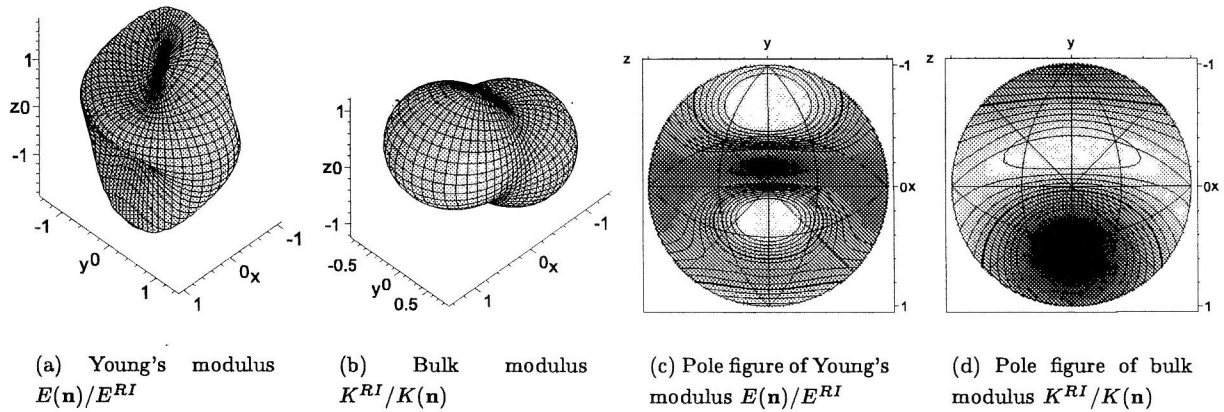


Figure 3: Monoclinic Symmetry: Hornblende 42420 ( $C_{11} = 130.1$ ,  $C_{22} = 187.7$ ,  $C_{33} = 198.4$ ,  $C_{44} = 61.1$ ,  $C_{55} = 38.7$ ,  $C_{66} = 45$ ,  $C_{12} = 61.1$ ,  $C_{13} = 59.5$ ,  $C_{23} = 61.4$ ,  $C_{15} = 9.5$ ,  $C_{25} = -6.9$ ,  $C_{35} = -40.6$ ,  $C_{46} = -0.9$  [GPa] (Simmons and Wang, 1971))

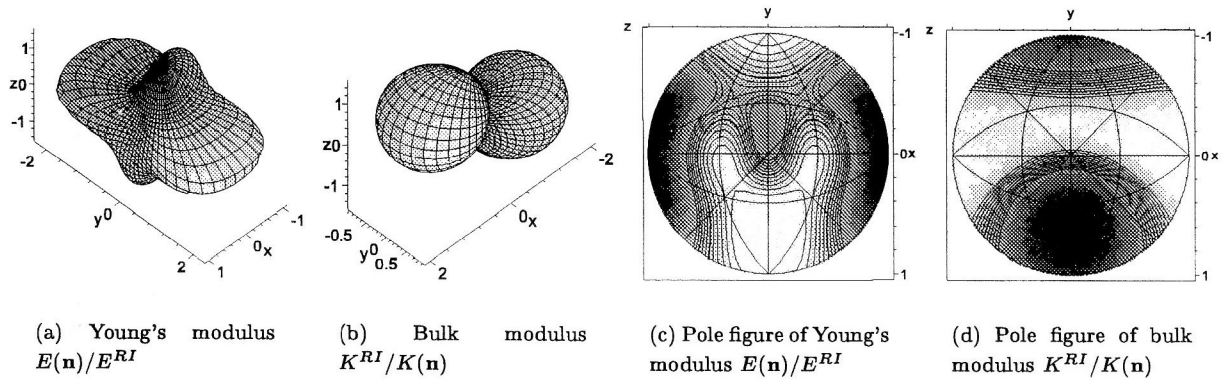


Figure 4: Monoclinic Symmetry: Feldspar (74% or-19.4%Ab-1.95% An) 42414 ( $C_{11} = 61.9$ ,  $C_{22} = 158.3$ ,  $C_{33} = 100.2$ ,  $C_{44} = 14.1$ ,  $C_{55} = 20.3$ ,  $C_{66} = 36$ ,  $C_{12} = 43.4$ ,  $C_{13} = 36.8$ ,  $C_{23} = 21.8$ ,  $C_{15} = -10$ ,  $C_{25} = -1.8$ ,  $C_{35} = -12.1$ ,  $C_{46} = -2.3$  [GPa] (Simmons and Wang, 1971))

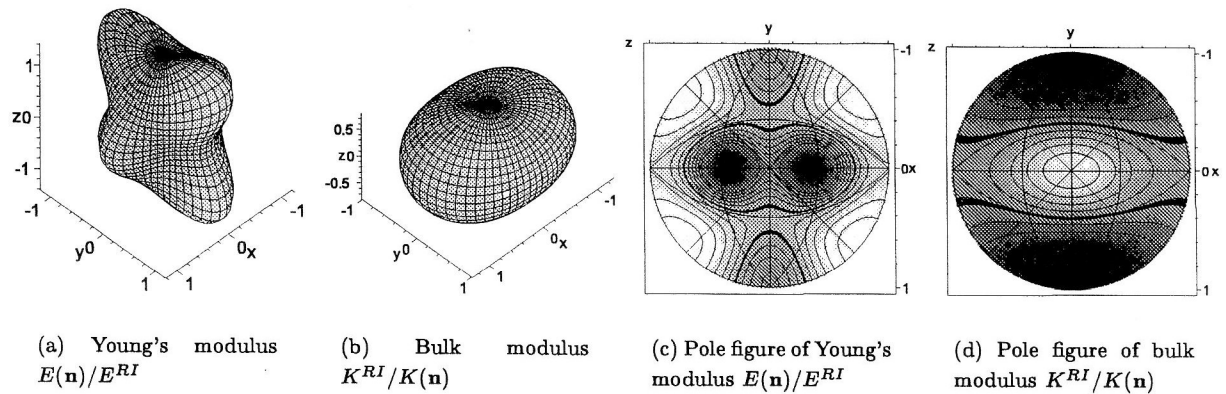


Figure 5: Rhombic Symmetry: Uranium ( $C_{11} = 214.8$ ,  $C_{22} = 198.6$ ,  $C_{33} = 267.1$ ,  $C_{44} = 124.4$ ,  $C_{55} = 73.4$ ,  $C_{66} = 44.3$ ,  $C_{12} = 46.5$ ,  $C_{13} = 21.8$ ,  $C_{23} = 107.6$  [GPa] (Kocks et al., 1998))

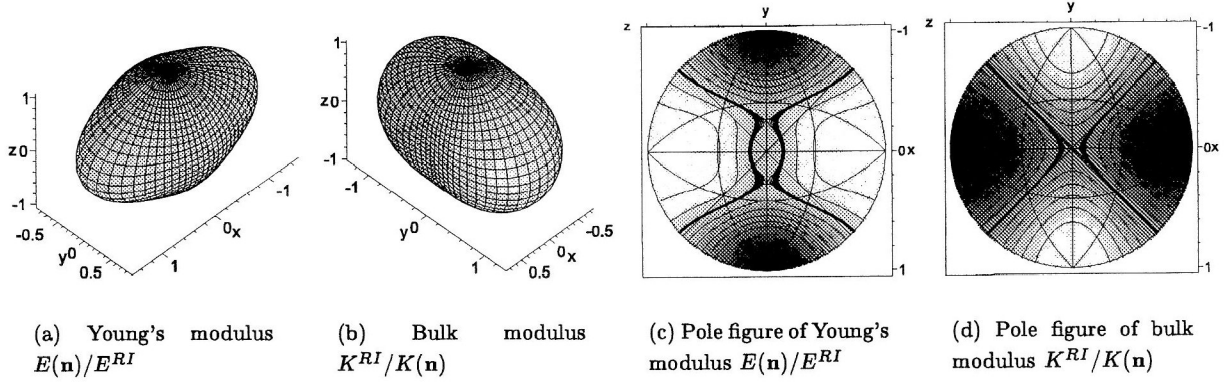


Figure 6: Rhombic Symmetry: Olivine 32294 ( $C_{11} = 323.7$ ,  $C_{22} = 197.6$ ,  $C_{33} = 235.1$ ,  $C_{44} = 64.62$ ,  $C_{55} = 78.05$ ,  $C_{66} = 79.04$ ,  $C_{12} = 66.4$ ,  $C_{13} = 71.6$ ,  $C_{23} = 75.6$  [GPa] (Simmons and Wang, 1971))

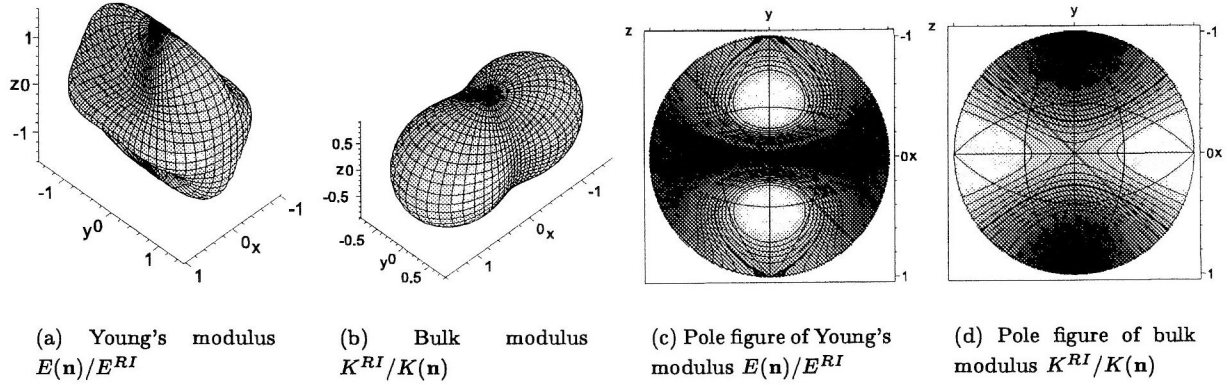


Figure 7: Rhombic Symmetry: Rochelle Salt 32301 ( $C_{11} = 25.5$ ,  $C_{22} = 38.1$ ,  $C_{33} = 37.1$ ,  $C_{44} = 13.4$ ,  $C_{55} = 3.21$ ,  $C_{66} = 9.79$ ,  $C_{12} = 14.1$ ,  $C_{13} = 11.6$ ,  $C_{23} = 14.6$  [GPa] (Simmons and Wang, 1971))

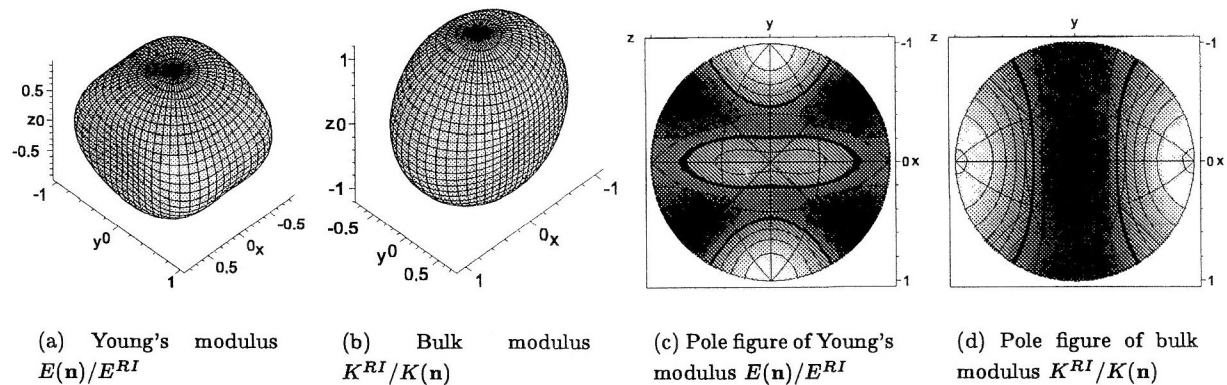


Figure 8: Rhombic Symmetry: Topaz 32310 ( $C_{11} = 281.36$ ,  $C_{22} = 348.95$ ,  $C_{33} = 294.52$ ,  $C_{44} = 108.11$ ,  $C_{55} = 132.98$ ,  $C_{66} = 130.89$ ,  $C_{12} = 125.82$ ,  $C_{13} = 84.64$ ,  $C_{23} = 88.15$  [GPa] (Simmons and Wang, 1971))

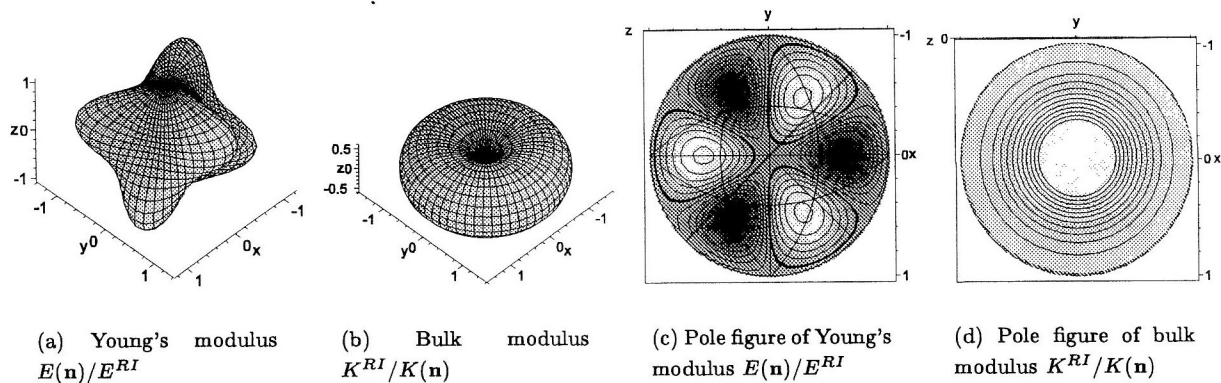


Figure 9: Trigonal Symmetry: Aluminium-Phosphate 62835 ( $C_{11} = 105.03$ ,  $C_{33} = 133.53$ ,  $C_{44} = 23.14$ ,  $C_{12} = 29.34$ ,  $C_{13} = 69.27$ ,  $C_{14} = -12.71$  [GPa] (Simmons and Wang, 1971))

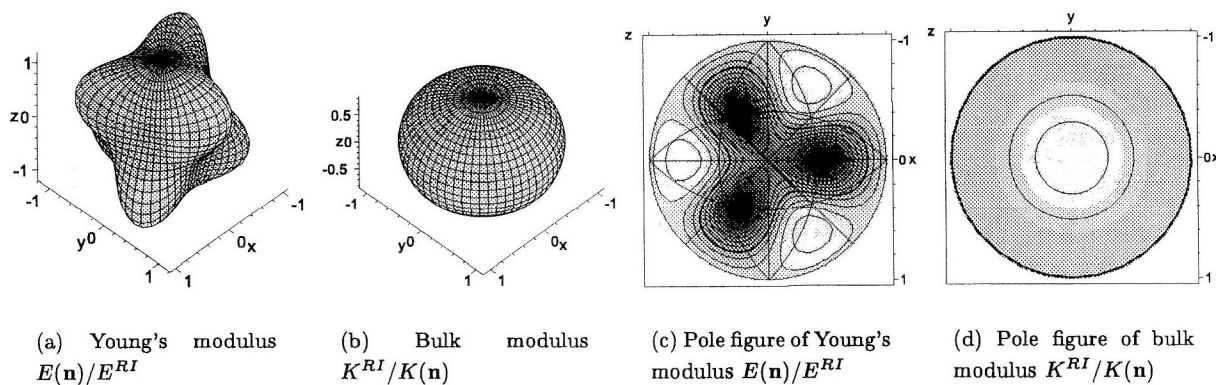


Figure 10: Trigonal Symmetry: Quartz 62894 ( $C_{11} = 86.8$ ,  $C_{33} = 105.75$ ,  $C_{44} = 58.2$ ,  $C_{12} = 7.04$ ,  $C_{13} = 11.91$ ,  $C_{14} = -18.04$  [GPa] (Simmons and Wang, 1971))

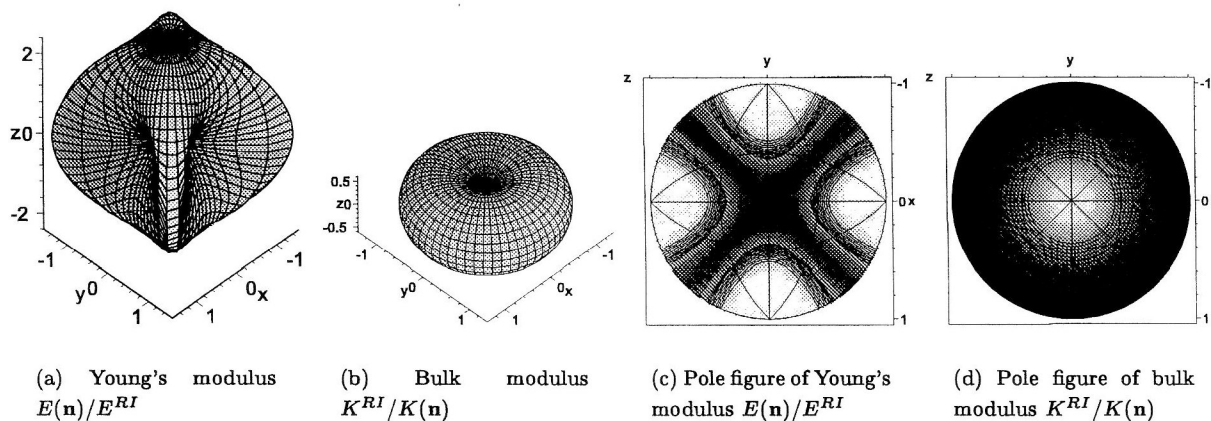


Figure 11: Tetragonal Symmetry: Weissblech 22251 ( $C_{11} = 76.19$ ,  $C_{33} = 116.24$ ,  $C_{44} = 17.04$ ,  $C_{66} = 19.8$ ,  $C_{12} = 71.1$ ,  $C_{13} = 67.68$  [GPa] (Kocks et al., 1998))

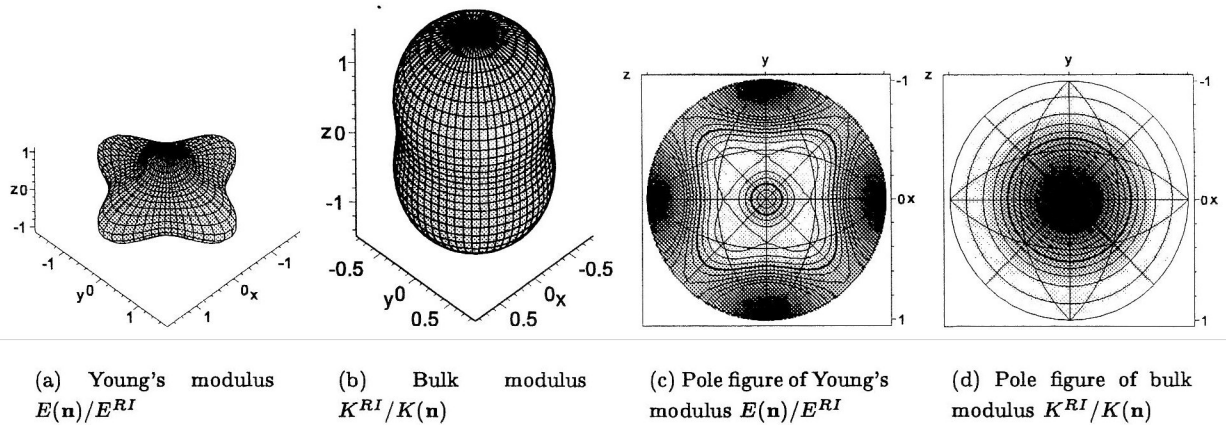


Figure 12: Tetragonal Symmetry: Zircon 22251 ( $C_{11} = 73.5$ ,  $C_{33} = 46$ ,  $C_{44} = 13.8$ ,  $C_{66} = 16$ ,  $C_{12} = 9$ ,  $C_{13} = -5.4$  [GPa] (Simmons and Wang, 1971))

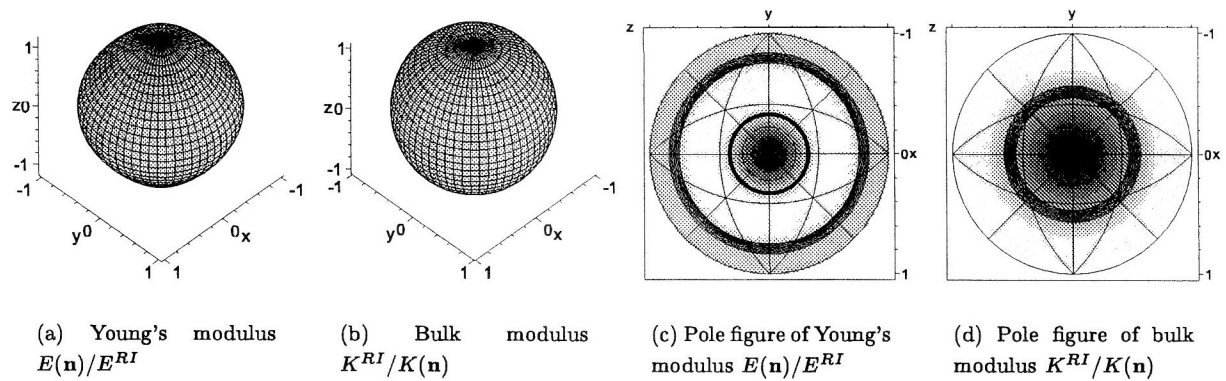


Figure 13: Hexagonal Symmetry: Magnesium 52582 ( $C_{11} = 56.49$ ,  $C_{33} = 58.73$ ,  $C_{44} = 16.81$ ,  $C_{12} = 23.16$ ,  $C_{13} = 18.1$  [GPa] (Simmons and Wang, 1971))

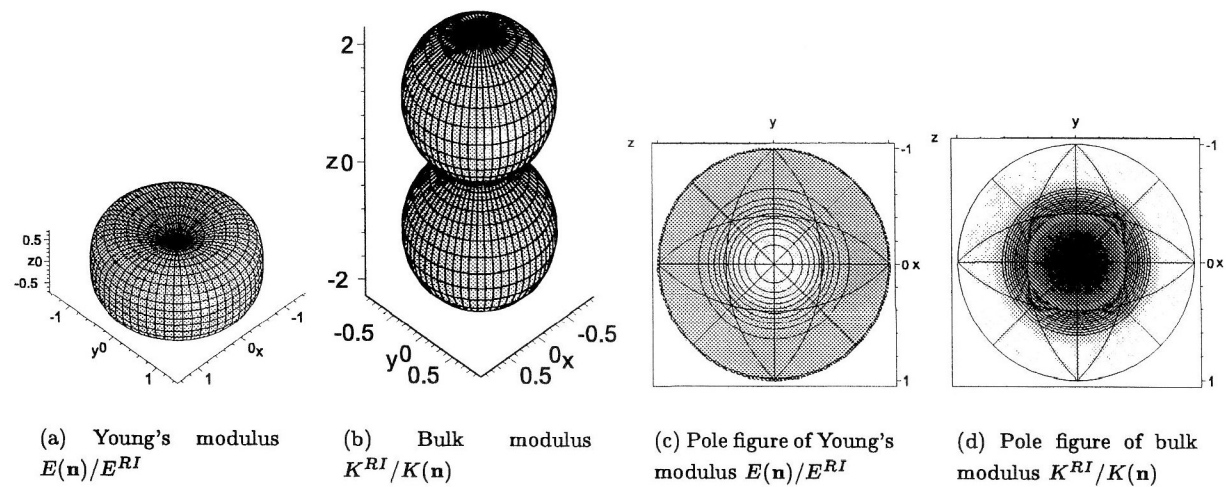
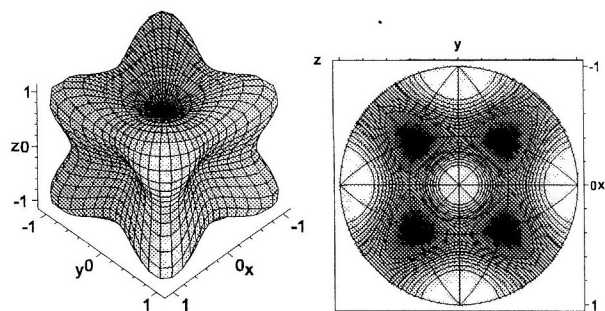
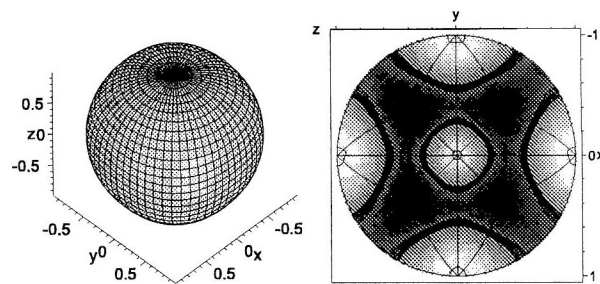


Figure 14: Hexagonal Symmetry: Titanium 52743 ( $C_{11} = 123.1$ ,  $C_{33} = 152.9$ ,  $C_{44} = 30.7$ ,  $C_{12} = 99.6$ ,  $C_{13} = 68.8$  [GPa] (Simmons and Wang, 1971))



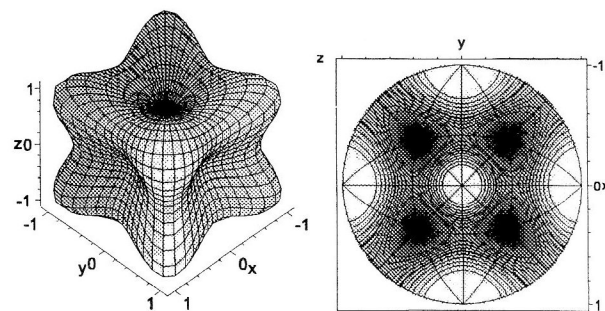
(a) Young's modulus  $E(\mathbf{n})/E^{RI}$  (b) Pole figure of Young's modulus  $E(\mathbf{n})/E^{RI}$



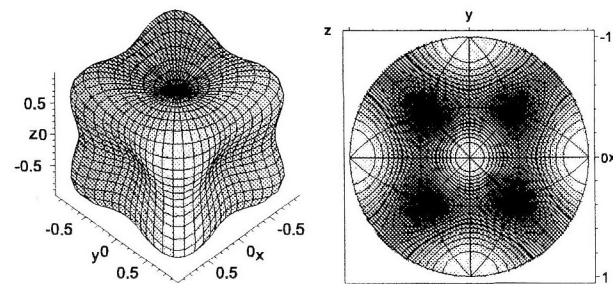
(a) Young's modulus  $E(\mathbf{n})/E^{RI}$  (b) Pole figure of Young's modulus  $E(\mathbf{n})/E^{RI}$

Figure 15: Cubic Symmetry: Copper ( $C_{11} = 168$ ,  $C_{12} = 121.4$ ,  $C_{44} = 75.4$  [GPa] (Kocks et al., 1998))

Figure 16: Cubic Symmetry: Aluminium 10001 ( $C_{11} = 25$ ,  $C_{12} = 10.6$ ,  $C_{44} = 8$  [GPa] (Simmons and Wang, 1971))



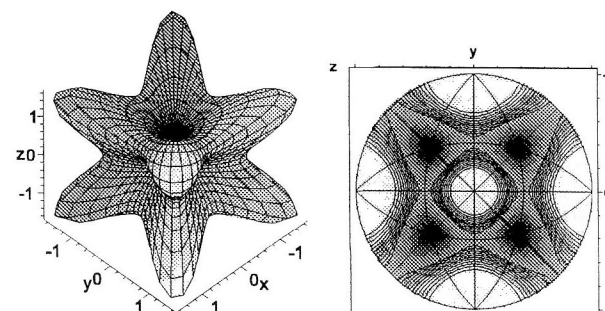
(a) Young's modulus  $E(\mathbf{n})/E^{RI}$  (b) Pole figure of Young's modulus  $E(\mathbf{n})/E^{RI}$



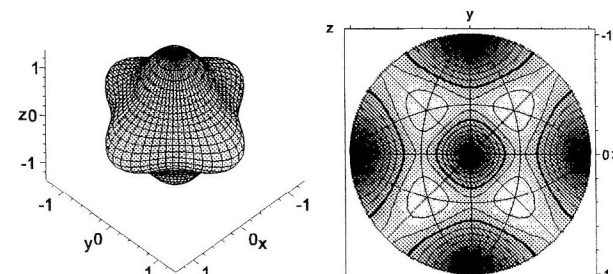
(a) Young's modulus  $E(\mathbf{n})/E^{RI}$  (b) Pole figure of Young's modulus  $E(\mathbf{n})/E^{RI}$

Figure 17: Cubic Symmetry: Gold 10575 ( $C_{11} = 185$ ,  $C_{12} = 158$ ,  $C_{44} = 39.7$  [GPa] (Simmons and Wang, 1971))

Figure 18: Cubic Symmetry: Iron 10627 ( $C_{11} = 228.09$ ,  $C_{12} = 133.48$ ,  $C_{44} = 110.86$  [GPa] (Simmons and Wang, 1971))



(a) Young's modulus  $E(\mathbf{n})/E^{RI}$  (b) Pole figure of Young's modulus  $E(\mathbf{n})/E^{RI}$



(a) Young's modulus  $E(\mathbf{n})/E^{RI}$  (b) Pole figure of Young's modulus  $E(\mathbf{n})/E^{RI}$

Figure 19: Cubic Symmetry: Iron-Aluminium 10676 ( $C_{11} = 170.99$ ,  $C_{12} = 130.61$ ,  $C_{44} = 131.7$  [GPa] (Simmons and Wang, 1971))

Figure 20: Cubic Symmetry: Pyrite 11391 ( $C_{11} = 361.88$ ,  $C_{12} = -47.96$ ,  $C_{44} = 105.49$  [GPa] (Simmons and Wang, 1971))

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