Background theory for calculating elastic constants of hexagonal phases [1]

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elastic constants are defined by means of a Taylor expansion of the total energy E(v,e) for the system, with respect to a small strain "e" of the lattice (v is the volume). In this Package we consider the hcp crystal structure, which is spanned by three vectors (√3a/2, -a/2, 0), (0, a, 0), and (0, 0, c). The Bravais lattice vectors are normally written in a matrix form, i.e.,

$$R = \begin{pmatrix} \sqrt{3}a/2 & -a/2 & 0 \\ 0 & a & 0 \\ 0 & 0 & c \end{pmatrix}$$

The distortion of the lattice (R') is expressed by multiplying R with a symmetric ($e_{xy} = e_{yx}$) distortion matrix e (R' = R*e), which is written as,

$$e = \begin{pmatrix} 1+e_{xx} & e_{xy} & e_{xz} \\ e_{yx} & 1+e_{yy} & e_{yz} \\ e_{zx} & e_{zy} & 1+e_{zz} \end{pmatrix}$$

And in Voiget notation (It is often convenient to change to the Voigt notation in order to reduce the number of indices. The Voigt notation replaces xx by 1, yy by 2, zz by 3, zy (and yz) by 4, xz (and zx) by 5, xy (and yx) by 6)

$$e = \begin{pmatrix} 1+e_1 & e_6 & e_5 \\ e_6 & 1+e_2 & e_4 \\ e_5 & e_4 & 1+e_3 \end{pmatrix}$$

we express the energy of the strained system by means of a Taylor expansion in the distortion parameters,

$$E(v,e) = E(v_0,0) + v_0 \left(\sum \Delta_i e_i + 1/2 \sum \sum C_{ij} e_i e_j + o(e^3)\right) \qquad i, j = 1,\ldots,6$$

The linear terms vanish if the strain causes no changes in the volume of the crystal. Otherwise, Δ are related to the strain on the crystal and C_{ij} are elastic constants and V_0 is the volume of unstrained hexagonal system and we use it to evaluate the elastic constants.

there are five independent elastic constants for a hexagonal material, called C11, C12, C13, C33 and C55 [2]. Since we have five independent elastic constants, we need five different strains to determine these. The five distortions used in the present Package are described below. The first distortion is written as

$$\begin{pmatrix} 1+e & 0 & 0 \\ 0 & 1+e & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

and it changes the size of the basal plane, while keeping the z axis constant. The symmetry of the strained lattice is therefore still hexagonal and the energy for this distortion can be obtained as

$$E(v,e) = E(v_0,0) + v_0 \left[(\Delta_1 + \Delta_2)\, e + (C_{11} + C_{12})\, e^2 + o(e^3)\right]$$

The second type of distortion is a volume conserved distortion and lead to Orthorhombic symmetry and written as

$$\begin{pmatrix} 1+e_1 & 0 & 0 \\ 0 & 1+e_2 & 0 \\ 0 & 0 & 1 \end{pmatrix} \qquad \begin{matrix} 1+e_1=(1+x/1-x)^{1/2} \\ 1+e_2=(1-x/1+x)^{1/2} \end{matrix}$$

and the energy for this distortion can be obtained as

$$E(v,e) = E(v_0,0) + v_0 \left[(C_{11} - C_{12})\, x^2 + o(x^3)\right]$$

The third strain we have used is given by

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1+e \end{pmatrix}$$

This strain changes C lattice parameter and keep the symmetry of the strained lattice hexagonal and the energy for this distortion can be obtained by

$$E(v,e) = E(v_0,0) + v_0 [(\Delta_3) e + (C_{33}) e^2 /2 + o(e^3)]$$

The fourth elastic constant, C55, is determined by means of a deformation of the lattice, which produces an object with low symmetry. The deformation is written as

$$\begin{pmatrix} 1 & 0 & e \\ 0 & 1 & 0 \\ e & 0 & 1 \end{pmatrix}$$

And it leads to triclinic symmetry and the energy for this deformation can be written as

$$E(v,e) = E(v_0,0) + v_0 [(\Delta_5) e + (2 C_{55}) e^2 + o(e^3)]$$

Finally, the last strain we have used is volume conserved and keeps the symmetry of the strained lattice hexagonal and can be written as

$$\begin{pmatrix} 1+e_1 & 0 & 0 \\ 0 & 1+e_2 & 0 \\ 0 & 0 & 1+e_3 \end{pmatrix} \qquad \begin{aligned} 1+e_1 &= (1+x)^{-1/3} \\ 1+e_2 &= (1+x)^{-1/3} \\ 1+e_3 &= (1+x)^{2/3} \end{aligned}$$

And the energy for this strain is given by

$$E(v,e) = E(v_0,0) + v_0 [(C_{zz})/9\, x^2 + o(x^3)]$$

And

$$C_{zz} = C_{11} + C_{12} + 2C_{33} - 4C_{13}$$

In practice, to calculate elastic constants we fit E(v,e) to a polynomial of degree N , N is number of data, and then elastic constants is computed by using second order derivative (E”(e)) of Polynomial fit (E=E(v,e)) of Energy vs. strains (e) at zero strain (e=0).

1) L. Fast, J. M. Wills, B. Johansson and O. Eriksson, Phys. Rev. B **51**, (1995).
2) D.C. Wallace, Solid State Phys. 25, 301 (1970)