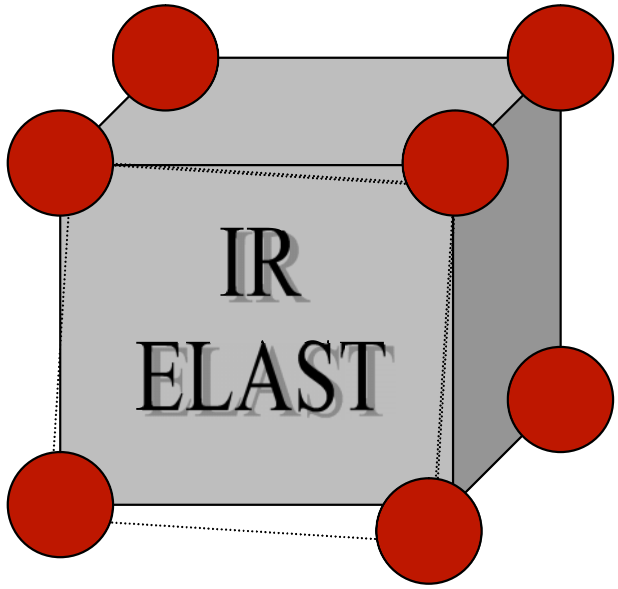

Background theory for calculating elastic constants of orthorhombic phases used in the

ortho-elastic

Package

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Elastic constants are defined by means of a Taylor expansion of the total energy $E(V,\delta)$ for the system, with respect to a small strain (δ) of the lattice. If we consider the bravais lattice vectors of an orthorhombic crystal structure as a matrix form (R) the distortion of the lattice (R') is expressed by multiplying R with a symmetric ($\delta_{xy} = \delta_{yx}$) distortion matrix i.e. ($R' = R * D$), which is written as,

$$D = \begin{pmatrix} 1+\delta_{xx} & \frac{\delta_{xy}}{2} & \frac{\delta_{xz}}{2} \\ \frac{\delta_{yx}}{2} & 1+\delta_{yy} & \frac{\delta_{yz}}{2} \\ \frac{\delta_{zx}}{2} & \frac{\delta_{zy}}{2} & 1+\delta_{zz} \end{pmatrix}$$

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

$$D = \begin{pmatrix} 1+\delta_1 & \frac{\delta_6}{2} & \frac{\delta_5}{2} \\ \frac{\delta_6}{2} & 1+\delta_2 & \frac{\delta_4}{2} \\ \frac{\delta_5}{2} & \frac{\delta_4}{2} & 1+\delta_3 \end{pmatrix}$$

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

$$E(V,\delta) = E(V_0,0) + V_0\left(\sum_{i=1}^{6} \tau_i \delta_i + \frac{1}{2}\sum_{i=1}^{6}\sum_{j=1}^{6} C_{ij}\delta_i\delta_j + O(\delta^3)\right)$$

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

To obtain elastic constants of orthorhombic structure we have used the method developed by Ravindran[1]. In this method elastic constants were calculated by applying small strains to the unstrained lattice.

there are nine independent elastic constants for an orthorhombic symmetry, called C_{11}, C_{22}, C_{33}, C_{44}, C_{55}, C_{66}, C_{12}, C_{13}, and C_{23} . Since we have nine independent elastic constants, we need nine different strains to determine these elastic constants. The nine distortions used in the IR-ELAST Package are described below. The first three distortions are written as

$$D_1 = \begin{pmatrix} 1+\delta & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$D_2 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1+\delta & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

and

$$D_3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1+\delta \end{pmatrix}$$

These three distortions change the lattice parameter in the x, y, and z directions ,respectively. The symmetry of the strained lattice is therefore still orthorhombic, however the volume of the distortion lattice change, and the energy for this distortion can be obtained as

$$E(V,\delta) = E(V_0,0) + V_0\left(\tau_1\delta + \frac{C_{11}}{2}\delta^2\right)$$

$$E(V,\delta) = E(V_0,0) + V_0\left(\tau_2\delta + \frac{C_{22}}{2}\delta^2\right)$$

and

$$E(V,\delta) = E(V_0,0) + V_0\left(\tau_3\delta + \frac{C_{33}}{2}\delta^2\right)$$

respectively.

The second three type of distortions are volume conserved distortion and lead to monoclinic symmetry and written as

$$u = \frac{1}{(1-\delta^2)^{\frac{1}{3}}}$$

$$D_4 = \begin{pmatrix} u & 0 & 0 \\ 0 & u & \delta u \\ 0 & \delta u & u \end{pmatrix}$$

$$D_5 = \begin{pmatrix} u & 0 & \delta u \\ 0 & u & 0 \\ \delta u & 0 & u \end{pmatrix}$$

and

$$D_6 = \begin{pmatrix} u & \delta u & 0 \\ \delta u & u & 0 \\ 0 & 0 & u \end{pmatrix}$$

and the energy for these distortions can be obtained as

$$E(V,\delta) = E(V_0,0) + V_0(2\tau_4\delta + 2C_{44}\delta^2)$$

$$E(V,\delta) = E(V_0,0) + V_0(2\tau_5\delta + 2C_{55}\delta^2)$$

and

$$E(V,\delta) = E(V_0,0) + V_0(2\tau_6\delta + 2C_{66}\delta^2)$$

respectively.

The third three strains we have used are volume conserving orthorhombic distortions and given by

$$D_7 = \begin{pmatrix} (1+\delta)u & 0 & 0 \\ 0 & (1-\delta)u & 0 \\ 0 & 0 & u \end{pmatrix}$$

$$D_8 = \begin{pmatrix} (1+\delta)u & 0 & 0 \\ 0 & u & 0 \\ 0 & 0 & (1-\delta)u \end{pmatrix}$$

and

$$D_9 = \begin{pmatrix} u & 0 & 0 \\ 0 & (1+\delta)u & 0 \\ 0 & 0 & (1-\delta)u \end{pmatrix}$$

The energy for these distortions can be obtained by

$$E(V,\delta) = E(V_0,0) + V_0\left((\tau_1 - \tau_2)\delta + \frac{(C_{11} + C_{22} - 2C_{12})}{2}\delta^2\right)$$

$$E(V,\delta) = E(V_0,0) + V_0\left((\tau_1 - \tau_3)\delta + \frac{(C_{11} + C_{33} - 2C_{13})}{2}\delta^2\right)$$

$$E(V,\delta) = E(V_0,0) + V_0\left((\tau_2 - \tau_3)\delta + \frac{(C_{22} + C_{33} - 2C_{23})}{2}\delta^2\right)$$

respectively.

[1] P. Ravindran, Lars Fast, P. A. Korzhavyi, and B. Johansson, J. Appl. Phys. **84**, (1998).