Elastic constants

2nd rank tensor

Hooke's Law $\sigma_{ij} = \sum_{kl} C_{ijkl}\,\varepsilon_{kl}$ only 36 components required due to symmetries in σ_{ij} and ε_{kl}

4th order tensor

Using the Voigt notation for a symmetric tensors,
to re-write Hooke's Law in matrix-times-vector form

1=xx, 2=yy, 3=zz, 4=yz, 5=zx, 6=xy

compression mixed

$$\begin{pmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \sigma_{zz} \\ \hline \sigma_{yz} \\ \sigma_{zx} \\ \sigma_{xy} \end{pmatrix} = \left(\begin{array}{ccc:ccc} C_{11} & C_{12} & C_{13} & C_{14} & C_{15} & C_{16} \\ C_{21} & C_{22} & C_{23} & C_{24} & C_{25} & C_{26} \\ C_{31} & C_{32} & C_{33} & C_{34} & C_{35} & C_{36} \\ \hdashline C_{41} & C_{42} & C_{43} & C_{44} & C_{45} & C_{46} \\ C_{51} & C_{52} & C_{53} & C_{54} & C_{55} & C_{56} \\ C_{61} & C_{62} & C_{63} & C_{64} & C_{65} & C_{66} \end{array}\right) \begin{pmatrix} \varepsilon_{xx} \\ \varepsilon_{yy} \\ \varepsilon_{zz} \\ \hline \varepsilon_{yz} \\ \varepsilon_{zx} \\ \varepsilon_{xy} \end{pmatrix}$$

compression

shear

stress mixed shear strain

Considering the possibility to exchange indexes $C_{12} = C_{21}$
there are 21 independent elastic constants

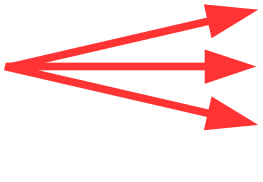
Elastic constants with cubic symmetry

Cubic symmetry: only 3 independent elastic constants C_{11}, C_{12}, C_{44}

$$\begin{pmatrix} C_{11} & C_{12} & C_{12} & & & \\ C_{12} & C_{11} & C_{12} & & 0 & \\ C_{12} & C_{12} & C_{11} & & & \\ & & & C_{44} & 0 & 0 \\ & 0 & & 0 & C_{44} & 0 \\ & & & 0 & 0 & C_{44} \end{pmatrix}.$$

Transformation due to the strain

Lattice vectors of the unit cell



$$\begin{pmatrix} \mathbf{a}_1 \\ \mathbf{a}_2 \\ \mathbf{a}_3 \end{pmatrix} = \begin{pmatrix} a_{1x} & a_{1y} & a_{1z} \\ a_{2x} & a_{2y} & a_{2z} \\ a_{3x} & a_{3y} & a_{3z} \end{pmatrix}$$

Transformation of the lattice vectors due to the strain:

$$\begin{pmatrix} \mathbf{a}'_1 \\ \mathbf{a}'_2 \\ \mathbf{a}'_3 \end{pmatrix} = \begin{pmatrix} \mathbf{a}_1 \\ \mathbf{a}_2 \\ \mathbf{a}_3 \end{pmatrix} \left(\hat{I} + \hat{\varepsilon} \right)$$

where

$$\hat{I} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \qquad \hat{\varepsilon} = \begin{pmatrix} e_1 & e_6/2 & e_5/2 \\ e_6/2 & e_2 & e_4/2 \\ e_5/2 & e_4/2 & e_3 \end{pmatrix}$$

- strain tensor

Total energy of the distorted lattice

$$E = E_0 - P(V_0)\Delta V + \frac{1}{2}V_0 \sum_{i=1}^{6}\sum_{j=1}^{6} C_{ij}e_i e_j$$

E_0 - total energy of the undistorted lattice

V_0 - volume of the undistorted lattice

$P(V_0)$ - pressure of the undistorted lattice at volume V_0

ΔV - change of the volume due to the strain

C_{ij} - elastic constants of the lattice (21 independent due to symmetry)

e_i - elements of the strain tensor

Strain → volume conserving $\Delta V = 0$

Strain → not volume conserving $\Delta V \neq 0$

Total energy of the distorted lattice

$$E = E_0 - \cancel{P(V_0)\Delta V} + \frac{1}{2} V_0 \sum_{i=1}^{6} \sum_{j=1}^{6} C_{ij} e_i e_j$$

E_0 - total energy of the undistorted lattice

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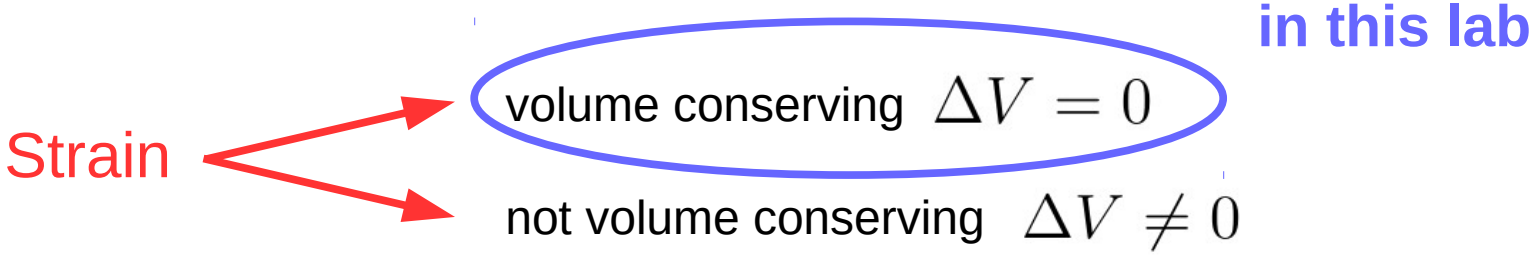
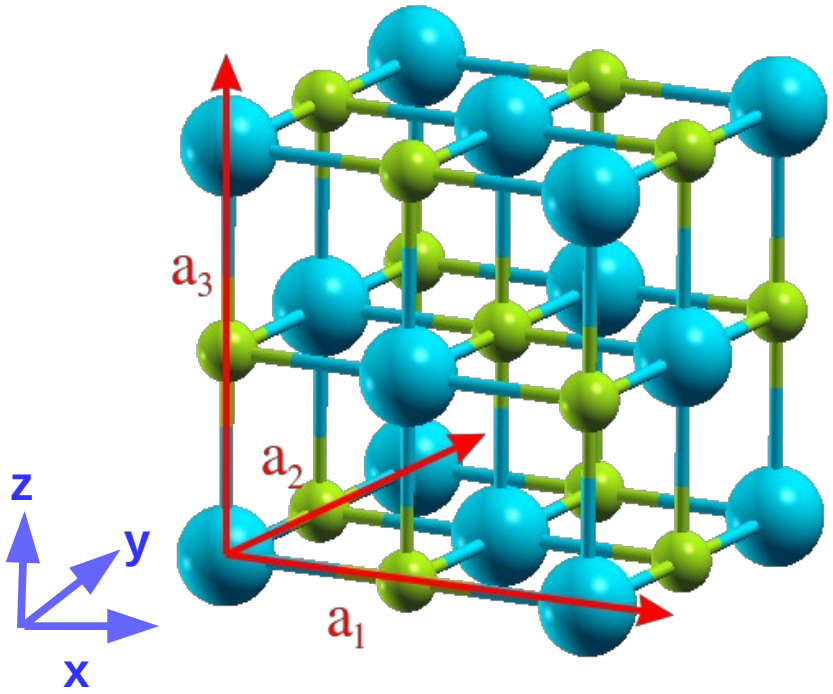


Strain of the system with a cubic symmetry

Cubic symmetry ⟹ Only 3 independent elastic constants: C_{11}, C_{12}, C_{44}

$$B = \frac{1}{3}\left(C_{11} + 2C_{12}\right)$$ - bulk modulus



$$\begin{pmatrix} \mathbf{a}_1 \\ \mathbf{a}_2 \\ \mathbf{a}_3 \end{pmatrix} = \begin{pmatrix} a_0 & 0 & 0 \\ 0 & a_0 & 0 \\ 0 & 0 & a_0 \end{pmatrix}$$

a_0 - equilibrium lattice parameter

Determine the positions of 8 inequivalent C atoms in the *conventional* unit cell of diamond on the figure above and specify them in your input file.
Remember to change the parameter nat.

Determination of the elastic constants C_11 and C_12

Tetragonal strain:

$$\hat{\varepsilon} = \begin{pmatrix} x & 0 & 0 \\ 0 & -x & 0 \\ 0 & 0 & \frac{x^2}{1-x^2} \end{pmatrix}$$

x - unitless parameter

Change of the total energy due to such a strain:

$$\Delta E(x) = \Delta E(-x) = V_0(C_{11} - C_{12})x^2$$

Make a fit with this function,
and use the expression for the bulk modulus in order to determine C_{11}, C_{12}

Determine the change of the lattice parameters due to such a strain:

$$\begin{pmatrix} \mathbf{a}'_1 \\ \mathbf{a}'_2 \\ \mathbf{a}'_3 \end{pmatrix} = \begin{pmatrix} \mathbf{a}_1 \\ \mathbf{a}_2 \\ \mathbf{a}_3 \end{pmatrix} \left(\hat{I} + \hat{\varepsilon}\right) = \ldots$$

POINT [A]

Use the orthorombic unit cell in order to model such a strain:

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ibrav = 8
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$$\texttt{celldm(1)} = |\mathbf{a}'_1|$$
$$\texttt{celldm(2)} = |\mathbf{a}'_2|/|\mathbf{a}'_1|$$
$$\texttt{celldm(3)} = |\mathbf{a}'_3|/|\mathbf{a}'_1|$$

POINT [B]

Set up the system using ibrav = 0
and the CELL_PARAMETERS
card as described online in the input manual.
Can you get the same results?

Relax your structure for every value of x , in order to find the minimum of energy!

Determination of the elastic constant C_44

$$\hat{\varepsilon} = \begin{pmatrix} 0 & \frac{x}{2} & 0 \\ \frac{x}{2} & 0 & 0 \\ 0 & 0 & \frac{x^2}{4-x^2} \end{pmatrix}$$

x - unitless parameter

Determine the change of the lattice parameters due to such a strain:

$$\begin{pmatrix} \mathbf{a}'_1 \\ \mathbf{a}'_2 \\ \mathbf{a}'_3 \end{pmatrix} = \begin{pmatrix} \mathbf{a}_1 \\ \mathbf{a}_2 \\ \mathbf{a}_3 \end{pmatrix} \left(\hat{I} + \hat{\varepsilon} \right) = \dots$$

Change of the total energy due to such a strain:

$$\Delta E(x) = \Delta E(-x) = \frac{1}{2} V_0 C_{44} x^2$$

Make a fit with this function.

POINT [A]

Use the monoclinic unit cell in order to model such a strain:

ibrav = 12

celldm(1) = $|\mathbf{a}'_1|$

celldm(2) = $|\mathbf{a}'_2|/|\mathbf{a}'_1|$

celldm(3) = $|\mathbf{a}'_3|/|\mathbf{a}'_1|$

celldm(4) = $\mathbf{a}'_1 \cdot \mathbf{a}'_2 / (|\mathbf{a}'_1||\mathbf{a}'_2|)$

POINT [B]

As before, use ibrav = 0 and compare the results.

Relax your structure for every value of x , in order to find the minimum of energy!