Center for Molecular Modeling

Computational Materials Physics

Department of Materials Science and Engineering

how to predict elastic constants ?

Stefaan.Cottenier@ugent.be

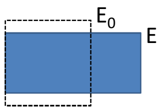
---

total energy   stress tensor

how to predict elastic constants ?

---

total energy



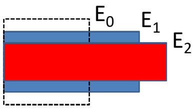
- full geometry optimization (E_0 = ground state total energy)
- deform cell, construct strain tensor
- compute E for deformed cell ($E_{elast} = E - E_0$)

total energy

$$\frac{E_{\mathrm{elast}}}{V} = \frac{1}{2}\begin{bmatrix} \epsilon_{xx} & \epsilon_{yy} & \epsilon_{zz} & 2\epsilon_{yz} & 2\epsilon_{xz} & 2\epsilon_{xy} \end{bmatrix} \begin{bmatrix} C_{11} & C_{12} & C_{13} & C_{14} & C_{15} & C_{16} \\ C_{12} & C_{22} & C_{23} & C_{24} & C_{25} & C_{26} \\ C_{13} & C_{23} & C_{33} & C_{34} & C_{35} & C_{36} \\ C_{14} & C_{24} & C_{34} & C_{44} & C_{45} & C_{46} \\ C_{15} & C_{25} & C_{35} & C_{45} & C_{55} & C_{56} \\ C_{16} & C_{26} & C_{36} & C_{46} & C_{56} & C_{66} \end{bmatrix} \begin{bmatrix} \epsilon_{xx} \\ \epsilon_{yy} \\ \epsilon_{zz} \\ 2\epsilon_{yz} \\ 2\epsilon_{xz} \\ 2\epsilon_{xy} \end{bmatrix}$$

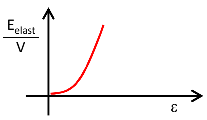
- full geometry optimization (E_0 = ground state total energy)
- deform cell, construct strain tensor
- compute E for deformed cell ($E_{elast} = E - E_0$)

total energy



- full geometry optimization (E_0 = ground state total energy)
- deform cell, construct strain tensor
- compute E for deformed cell ($E_{elast} = E - E_0$)
- repeat for multiple amounts of the same deformation

total energy



- full geometry optimization (E_0 = ground state total energy)
- deform cell, construct strain tensor
- compute E for deformed cell ($E_{elast} = E - E_0$)
- repeat for multiple amounts of the same deformation
- fit suitable expression with C_{ij}
- repeat for other deformations, untill sufficient expressions to know all C_{ij}

total energy

example cubic crystal: C_{11}, C_{44}, C_{12} only

$$\frac{E_{\text{elast}}}{V} = \frac{1}{2}\begin{bmatrix} \epsilon_{xx} & \epsilon_{yy} & \epsilon_{zz} & 2\epsilon_{yz} & 2\epsilon_{xz} & 2\epsilon_{xy} \end{bmatrix} \begin{bmatrix} C_{11} & C_{12} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{11} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{12} & C_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{44} \end{bmatrix} \begin{bmatrix} \epsilon_{xx} \\ \epsilon_{yy} \\ \epsilon_{zz} \\ 2\epsilon_{yz} \\ 2\epsilon_{xz} \\ 2\epsilon_{xy} \end{bmatrix}$$

- full geometry optimization (E_0 = ground state total energy)
- deform cell, construct strain tensor
- compute E for deformed cell ($E_{elast} = E - E_0$)
- repeat for multiple amounts of the same deformation
- fit suitable expression with C_{ij}
- repeat for other deformations, untill sufficient expressions to know all C_{ij}

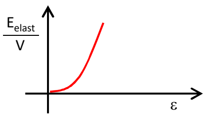
total energy

example cubic crystal: C_{11}, C_{44}, C_{12} only

$$\frac{E_{\text{elast}}}{V} = \frac{1}{2}C_{11}\left(\epsilon_{xx}^2+\epsilon_{yy}^2+\epsilon_{zz}^2\right) + C_{12}\left(\epsilon_{xx}\epsilon_{yy}+\epsilon_{xx}\epsilon_{zz}+\epsilon_{yy}\epsilon_{zz}\right) + 2C_{44}\left(\epsilon_{xy}^2+\epsilon_{xz}^2+\epsilon_{yz}^2\right)$$

- deformation with only $\varepsilon_{xx} \neq 0$:

$$\frac{E_{\text{elast}}}{V} = \frac{1}{2}C_{11}\,\epsilon_{xx}^2$$



- deformation with only $\varepsilon_{xx} = \varepsilon_{yy} \neq 0$:

$$\frac{E_{\text{elast}}}{V} = \left(C_{11}+C_{12}\right)\epsilon_{xx}^2$$

- deformation with only $\varepsilon_{xy} \neq 0$:

$$\frac{E_{\text{elast}}}{V} = 2C_{44}\,\epsilon_{xy}^2$$

total energy

$$\frac{E_{\text{elast}}}{V} = \frac{1}{2}\begin{bmatrix} \epsilon_{xx} & \epsilon_{yy} & \epsilon_{zz} & 2\epsilon_{yz} & 2\epsilon_{xz} & 2\epsilon_{xy} \end{bmatrix} \begin{bmatrix} C_{11} & C_{12} & C_{13} & C_{14} & C_{15} & C_{16} \\ C_{12} & C_{22} & C_{23} & C_{24} & C_{25} & C_{26} \\ C_{13} & C_{23} & C_{33} & C_{34} & C_{35} & C_{36} \\ C_{14} & C_{24} & C_{34} & C_{44} & C_{45} & C_{46} \\ C_{15} & C_{25} & C_{35} & C_{45} & C_{55} & C_{56} \\ C_{16} & C_{26} & C_{36} & C_{46} & C_{56} & C_{66} \end{bmatrix} \begin{bmatrix} \epsilon_{xx} \\ \epsilon_{yy} \\ \epsilon_{zz} \\ 2\epsilon_{yz} \\ 2\epsilon_{xz} \\ 2\epsilon_{xy} \end{bmatrix}$$

- advantage
  only total energy needed
- disadvantage
  many DFT calculations

total energy

stress tensor

how to predict elastic constants ?

---

stress tensor

$$\begin{bmatrix} \sigma_{11} & \sigma_{12} & \sigma_{13} & \sigma_{14} & \sigma_{15} & \sigma_{16} \\ \sigma_{21} & \sigma_{22} & \sigma_{23} & \sigma_{24} & \sigma_{25} & \sigma_{26} \\ \sigma_{31} & \sigma_{32} & \sigma_{33} & \sigma_{34} & \sigma_{35} & \sigma_{36} \\ \sigma_{41} & \sigma_{42} & \sigma_{43} & \sigma_{44} & \sigma_{45} & \sigma_{46} \\ \sigma_{51} & \sigma_{52} & \sigma_{53} & \sigma_{54} & \sigma_{55} & \sigma_{56} \\ \sigma_{61} & \sigma_{62} & \sigma_{63} & \sigma_{64} & \sigma_{65} & \sigma_{66} \end{bmatrix} = \begin{bmatrix} C_{11} & C_{12} & C_{13} & C_{14} & C_{15} & C_{16} \\ C_{12} & C_{22} & C_{23} & C_{24} & C_{25} & C_{26} \\ C_{13} & C_{23} & C_{33} & C_{34} & C_{35} & C_{36} \\ C_{14} & C_{24} & C_{34} & C_{44} & C_{45} & C_{46} \\ C_{15} & C_{25} & C_{35} & C_{45} & C_{55} & C_{56} \\ C_{16} & C_{26} & C_{36} & C_{46} & C_{56} & C_{66} \end{bmatrix} \begin{bmatrix} \epsilon_{11} & \epsilon_{12} & \epsilon_{13} & \epsilon_{14} & \epsilon_{15} & \epsilon_{16} \\ \epsilon_{21} & \epsilon_{22} & \epsilon_{23} & \epsilon_{24} & \epsilon_{25} & \epsilon_{26} \\ \epsilon_{31} & \epsilon_{32} & \epsilon_{33} & \epsilon_{34} & \epsilon_{35} & \epsilon_{36} \\ 2\epsilon_{41} & 2\epsilon_{42} & 2\epsilon_{4}3 & 2\epsilon_{44} & 2\epsilon_{45} & 2\epsilon_{46} \\ 2\epsilon_{51} & 2\epsilon_{52} & 2\epsilon_{53} & 2\epsilon_{54} & 2\epsilon_{55} & 2\epsilon_{56} \\ 2\epsilon_{61} & 2\epsilon_{62} & 2\epsilon_{63} & 2\epsilon_{64} & 2\epsilon_{65} & 2\epsilon_{66} \end{bmatrix}$$

$\Sigma = CE$

- full geometry optimization (E_0 = ground state total energy)
- deform cell, construct strain tensor
- compute stress tensor for deformed cell
- repeat for 6 types of deformation
- all C_{ij} follow from matrix equation

$\Sigma E^{-1} = C$

---

stress tensor

$$\begin{bmatrix} \sigma_{11} & \sigma_{12} & \sigma_{13} & \sigma_{14} & \sigma_{15} & \sigma_{16} \\ \sigma_{21} & \sigma_{22} & \sigma_{23} & \sigma_{24} & \sigma_{25} & \sigma_{26} \\ \sigma_{31} & \sigma_{32} & \sigma_{33} & \sigma_{34} & \sigma_{35} & \sigma_{36} \\ \sigma_{41} & \sigma_{42} & \sigma_{43} & \sigma_{44} & \sigma_{45} & \sigma_{46} \\ \sigma_{51} & \sigma_{52} & \sigma_{53} & \sigma_{54} & \sigma_{55} & \sigma_{56} \\ \sigma_{61} & \sigma_{62} & \sigma_{63} & \sigma_{64} & \sigma_{65} & \sigma_{66} \end{bmatrix} = \begin{bmatrix} C_{11} & C_{12} & C_{13} & C_{14} & C_{15} & C_{16} \\ C_{12} & C_{22} & C_{23} & C_{24} & C_{25} & C_{26} \\ C_{13} & C_{23} & C_{33} & C_{34} & C_{35} & C_{36} \\ C_{14} & C_{24} & C_{34} & C_{44} & C_{45} & C_{46} \\ C_{15} & C_{25} & C_{35} & C_{45} & C_{55} & C_{56} \\ C_{16} & C_{26} & C_{36} & C_{46} & C_{56} & C_{66} \end{bmatrix} \begin{bmatrix} \epsilon_{11} & \epsilon_{12} & \epsilon_{13} & \epsilon_{14} & \epsilon_{15} & \epsilon_{16} \\ \epsilon_{21} & \epsilon_{22} & \epsilon_{23} & \epsilon_{24} & \epsilon_{25} & \epsilon_{26} \\ \epsilon_{31} & \epsilon_{32} & \epsilon_{33} & \epsilon_{34} & \epsilon_{35} & \epsilon_{36} \\ 2\epsilon_{41} & 2\epsilon_{42} & 2\epsilon_{4}3 & 2\epsilon_{44} & 2\epsilon_{45} & 2\epsilon_{46} \\ 2\epsilon_{51} & 2\epsilon_{52} & 2\epsilon_{53} & 2\epsilon_{54} & 2\epsilon_{55} & 2\epsilon_{56} \\ 2\epsilon_{61} & 2\epsilon_{62} & 2\epsilon_{63} & 2\epsilon_{64} & 2\epsilon_{65} & 2\epsilon_{66} \end{bmatrix}$$

$\Sigma E^{-1} = C$

- advantage
  only 6 DFT calculations needed
- disadvantage
  requires DFT code that can compute stress tensor