ElaStr – An Online Tool for Analyzing Elasticity and Crystal Structure Relationships

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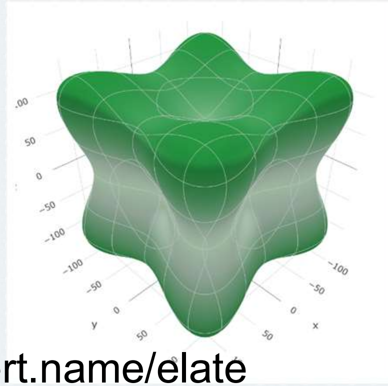
Introduction

$$\sigma_i = \sum_{j=1}^{6} C_{ij}\varepsilon_j$$

- The elastic behavior of a crystal is described by the **second-order stiffness tensor** C_{ij}, linking stress and strain
- Many existing tools (*Elate**, *ElAM*, *MELASA*, *MechElastic*, …) use this tensor to compute and visualize anisotropic properties like:
  - Directional Young's modulus, shear modulus, Poisson's ratio
- These tools typically work in Cartesian coordinates, which are:
  - Effective for high-symmetry lattices (e.g., cubic)
  - Less intuitive for low-symmetry systems

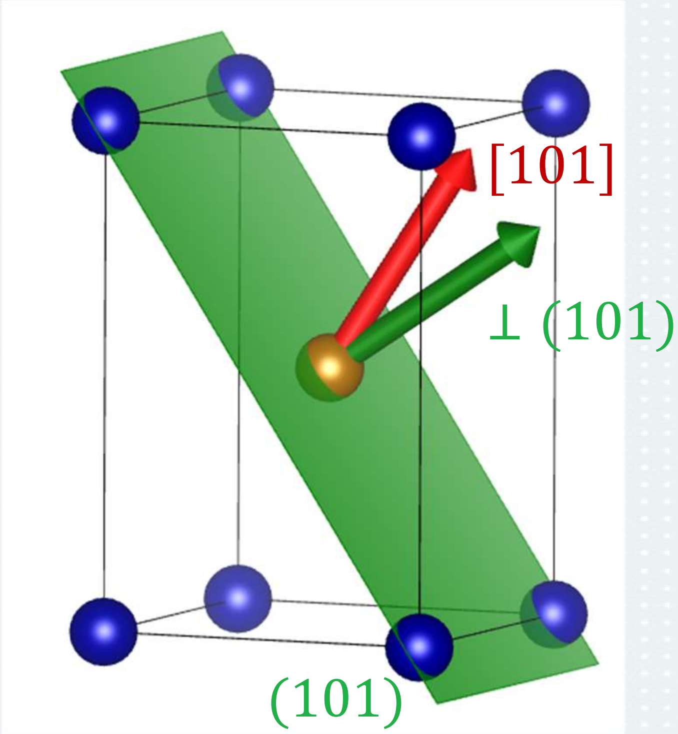
$$\begin{pmatrix} C_{11} & C_{12} & C_{13} & C_{14} & C_{15} & C_{16} \\ & C_{22} & C_{23} & C_{24} & C_{25} & C_{26} \\ & & C_{33} & C_{34} & C_{35} & C_{36} \\ & & & C_{44} & C_{45} & C_{46} \\ & & & & C_{55} & C_{56} \\ & & & & & C_{66} \end{pmatrix}$$



*R. Gaillac *et al.*: *J. Phys. Condens. Matter* **28**, 275201 (2016). https://progs.coudert.name/elate

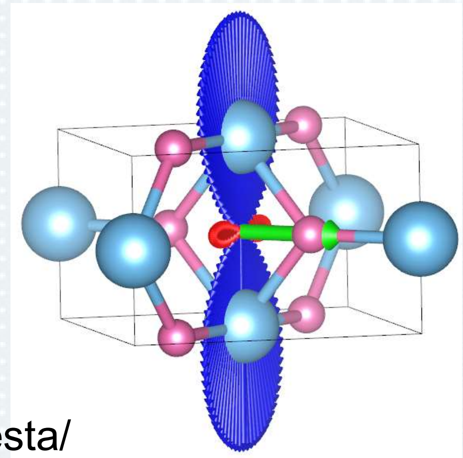
Motivation

- In low-symmetry crystals (e.g. tetragonal), analysis should reflect crystallographic directions and planes
- Miller indices ([*uvw*], (*hkl*)) provide a more natural description of material directions and planes
  - Example: in tetragonal crystals, the [101] direction is not perpendicular to the (101) plane due to $c/a \neq 1$
- A new tool is needed to:
  - Bridge the gap between the elastic tensors and the crystal structure
  - Provide analysis in crystallographic (not just Cartesian) terms



What ElaStr Does

- **ElaStr** is a user-friendly online tool for analyzing elastic properties in relation to the crystal structure
- Reads inputs:
  - 6×6 stiffness matrix C_{ij}, 3×3 matrix of lattice vectors $\mathbf{R} = [\vec{a}, \vec{b}, \vec{c}]$, or VASP POSCAR
  - Miller indices of a crystallographic direction [*uvw*] and a plane (*hkl*)
- Computes elastic properties for the given [*uvw*] direction and the normal to the (*hkl*) plane
- Visualizes results for the given (*hkl*) plane using:
  - Polar plots
  - Crystal structure in a format suitable for VESTA*
  - Table of raw data



* K. Momma, F. Izumi: *J. Appl. Crystallogr.* **41**, 653 (2008). https://jp-minerals.org/vesta/

What ElaStr Does

- **ElaStr** is primary designed to visualize results from *ab initio* (DFT) calculations, regardless of the specific method used:
  - Energy-strain method
  - Stress-strain method
  - Linea response theory
- Or experimental data can be used
  - Only the stiffness matrix and structural (lattice) information are required
- ⚠**Important:** The stiffness matrix and lattice vectors **must be defined in the same orientation** with respect to the Cartesian coordinate system!!!
  - Your stiffens matrix is dependent on the choice of the computational cell
  - Miller indices are defined with respect to given cell, for example: if you describe *fcc* as *bct* unicell with $c/a = \sqrt{2}$ then $[100]_{bct} = [110]_{fcc}$ and coordination system is rotated about 45°
  - In ElaStr, both the stiffness matrix and lattice vectors can be rotated together as needed

Methodology and Functionality

- First, the direction [*uvw*] and the normal of the (*hkl*) plane are transformed to Cartesian coordinates and normalized:

$$\vec{r}_{cart} = \begin{bmatrix} \alpha_1 \\ \alpha_2 \\ \alpha_3 \end{bmatrix} = \mathbf{R} \cdot \begin{bmatrix} w \\ v \\ w \end{bmatrix}, \vec{n}_{cart} = \begin{bmatrix} \beta_1 \\ \beta_2 \\ \beta_3 \end{bmatrix} = (\mathbf{R}^{-1})^{\mathrm{T}} \cdot \begin{bmatrix} h \\ k \\ l \end{bmatrix}$$

- Then, the members of the stiffness matrix C_{ij} are inverted to obtain the compliance matrix S_{ij}:

$$\mathbf{S} = \mathbf{C}^{-1}$$

- The compliance matrix in Voight notation is expanded to full 4th-order 3×3×3×3 tensor S_{klmn}:

$$S_{klmn} = \frac{1}{f_i f_j} \cdot S_{ij}, \text{ where } f_i = 1 \text{ for } i = 1,2,3 \text{ and } f_i = 2 \text{ for } i = 4,5,6$$

Methodology and Functionality

- Young's modulus for loading along [*uvw*]: $$E^{[uvw]} = \sum_{k=1}^{3}\sum_{l=1}^{3}\sum_{m=1}^{3}\sum_{n=1}^{3}\frac{1}{\alpha_k\alpha_l\alpha_m\alpha_n S_{klmn}}$$
- Linear compressibility in [*uvw*]: $$\kappa^{[uvw]} = \sum_{k=1}^{3}\sum_{l=1}^{3}\sum_{m=1}^{3}\alpha_k\alpha_l S_{klmm}$$
- If $\vec{r}_{cart}$ and $\vec{n}_{cart}$ are perpendicular:
- Shear modulus for shearing along [*uvw*] in the (*hkl*) plane: $$G^{[uvw](hkl)} = \sum_{k=1}^{3}\sum_{l=1}^{3}\sum_{m=1}^{3}\sum_{n=1}^{3}\frac{1}{4\alpha_k\beta_l\alpha_m\beta_n S_{klmn}}$$
- Poisson's ratio in the direction normal to (*hkl*) for loading along [*uvw*] direction: $$\nu^{[uvw](hkl)} = \sum_{k=1}^{3}\sum_{l=1}^{3}\sum_{m=1}^{3}\sum_{n=1}^{3}\frac{\alpha_k\alpha_l\beta_m\beta_n S_{klmn}}{\alpha_k\alpha_l\alpha_m\alpha_n S_{klmn}}$$

A. Marmier *et al.*: *Comput. Phys. Commun.* **181**, 2102 (2010).

Methodology and Functionality

- For a given [*uvw*], the lowest and highest shear moduli, $G_{min}^{[uvw]}$ and $G_{max}^{[uvw]}$, as well as lowest and highest Poisson's ratios, $\nu_{min}^{[uvw]}$ and $\nu_{max}^{[uvw]}$, are estimated by scanning of all possible plane normals $\vec{n}_{cart}$ perpendicular to $\vec{r}_{cart}$

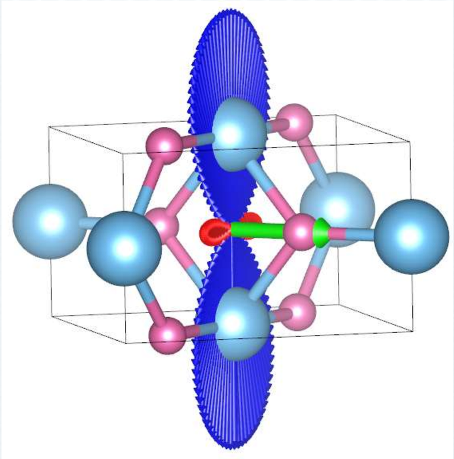
- It is also possible to exchange $\vec{r}_{cart}$ and $\vec{n}_{cart}$ and calculate, e.g., Young's modulus for loading along the normal of the (*hkl*) plane:

$$E^{\perp(hkl)} = \sum_{k=1}^{3}\sum_{l=1}^{3}\sum_{m=1}^{3}\sum_{n=1}^{3}\frac{1}{\beta_k\beta_l\beta_m\beta_n S_{klm}}$$

- and other properties $\kappa^{\perp(hkl)}, G^{\perp(hkl)\perp[uvw]}, \nu^{\perp(hkl)\perp[uvw]}, G_{min}^{\perp(hkl)}, G_{max}^{\perp(hkl)}, \nu_{min}^{\perp(hkl)}, \nu_{max}^{\perp(hkl)}$ in a similar way

Methodology and Functionality

- For a given (*hkl*) plane (or a plane defined by [*uvw*] as its normal,) **ElaStr** also offers to calculate and visualize — via polar plots or in VESTA — the following:
  - Young's moduli for all loading directions lying in the plane
  - Linear compressibilities for all deformation directions in the plane
  - Minimum and maximum shear moduli for all shearing directions in the plane
  - Minimum and maximum Poisson's ratios for all loading directions in the plane
  - Shear moduli for all shearing directions in the plane
  - Poisson's ratios for all directions in the plane, with loading in the direction of the plane normal

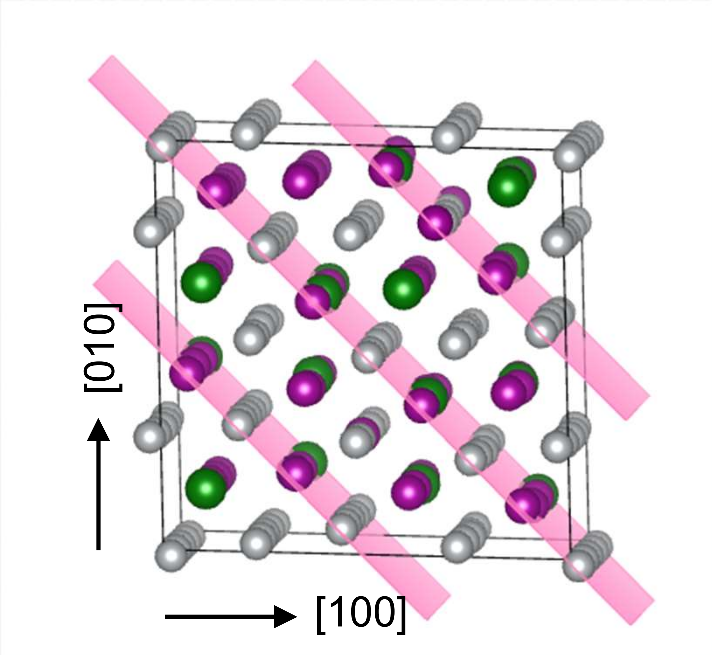


Poisson's ratios ν of the TiO_2 rutile structure in the $(1\bar{1}0)$ plane for loading along the $[1\bar{1}0]$ direction (green arrow). Blue arrows indicate positive ν (transverse contraction), while red arrows indicate negative ν (transverse expansion)

An Example – Ni-Mn-Sn

- Ni-Mn-Sn belongs to the family of magnetic shape memory alloys
- Martensitic structure 4O exhibits modulation of (110) planes with a periodicity of two planes
- Elastic properties were studied with the help of *Density Functional Theory* (VASP)
- Exact composition $Ni_{1.9375}Mn_{1.5625}Sn_{0.5}$
- Lattice constants:
- a = 6.19 Å, b = 6.23 Å, c = 5.34 Å, α = 90.00°, β = 90.00°, γ = 92.53°
- Influence of modulation on elastic properties

A 2×2×2 supercell to describe modulation and off-stoichiometry



M. Friák, M. Zelený *et al.*: *Intermetallics* **151**, 107708 (2022).

An Example – Ni-Mn-Sn

- Input data:

Stiffness matrix

$$\begin{pmatrix} 212 & 128 & 90 & 0 & 0 & 4 \\ & 213 & 92 & 0 & 0 & 2 \\ & & 205 & 1 & 0 & -19 \\ & & & 68 & -2 & 0 \\ & & & & 65 & -1 \\ & & & & & 84 \end{pmatrix}$$

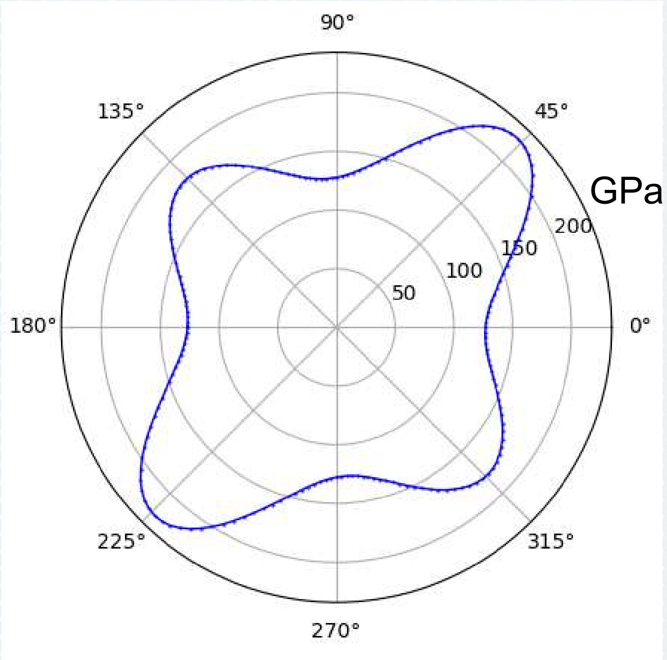
Matrix of lattice vectors

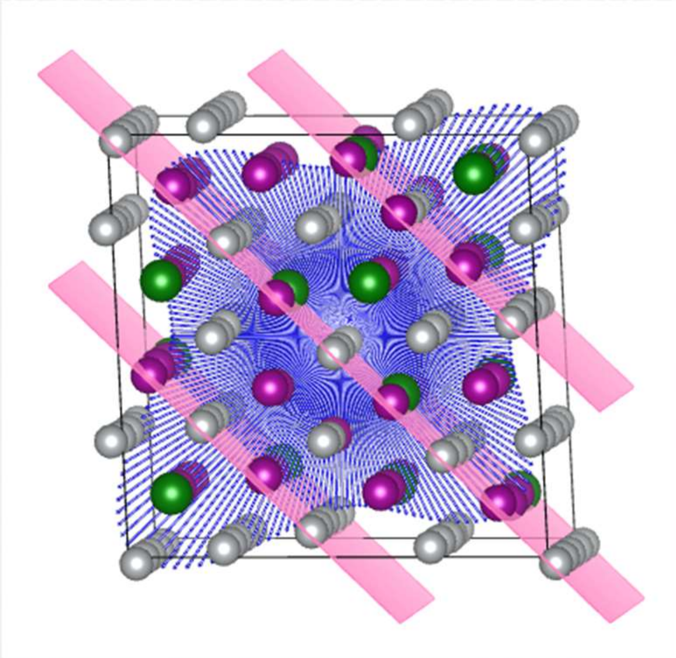
$$\begin{pmatrix} 12.38 & 0 & 0 \\ -0.55 & 12.45 & 0 \\ 0 & 0 & 10.68 \end{pmatrix}$$

- Compared to the work by M. Friák, M. Zelený *et al*.: *Intermetallics* **151**, 107708 (2022), the stiffness matrix was rotated using the rotation matrix: $\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}$. This transformation was applied to align the orientation with the commonly used lattice vectors. In the supercell used in the paper, the shortest lattice constant corresponds to the *b*-axis, rather than the *c*-axis, as is more typical

An Example – Ni-Mn-Sn

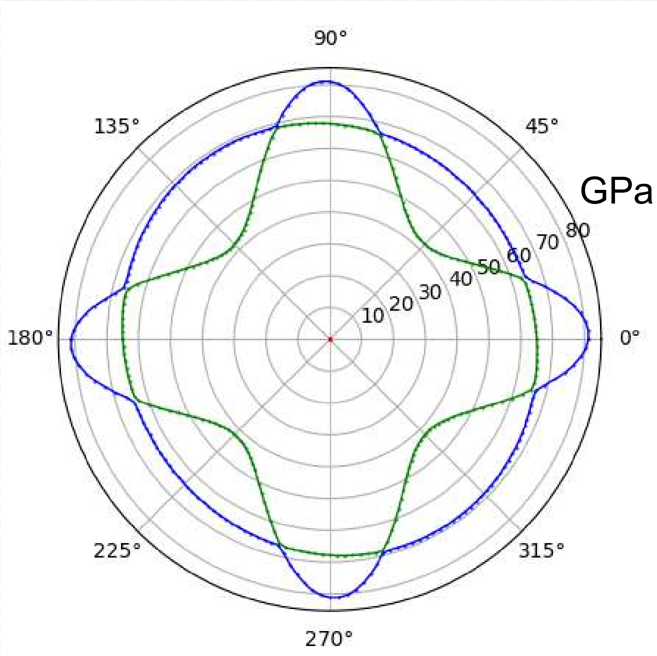
- Young's moduli in the (001) plane (option **1a**):
  - Young's modulus is lower along the modulation planes (179.3 GPa) compared to the direction perpendicular to the modulation planes (222.0 GPa)

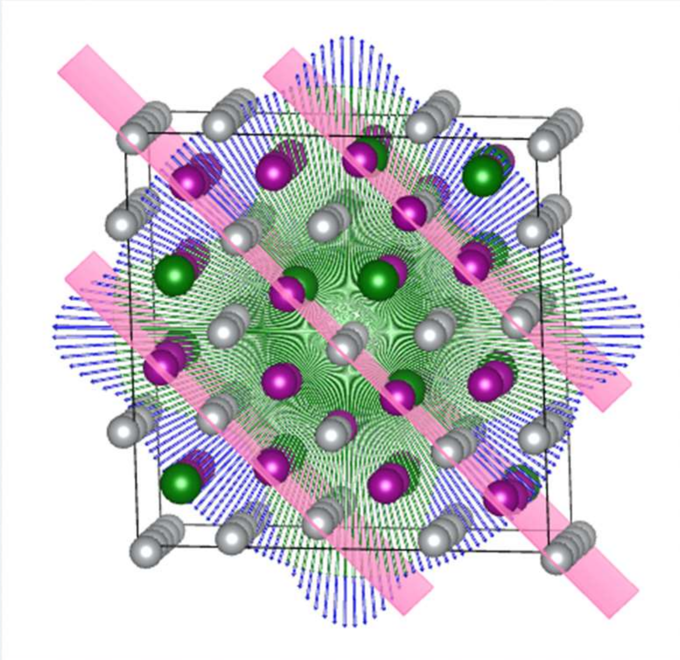




An Example – Ni-Mn-Sn

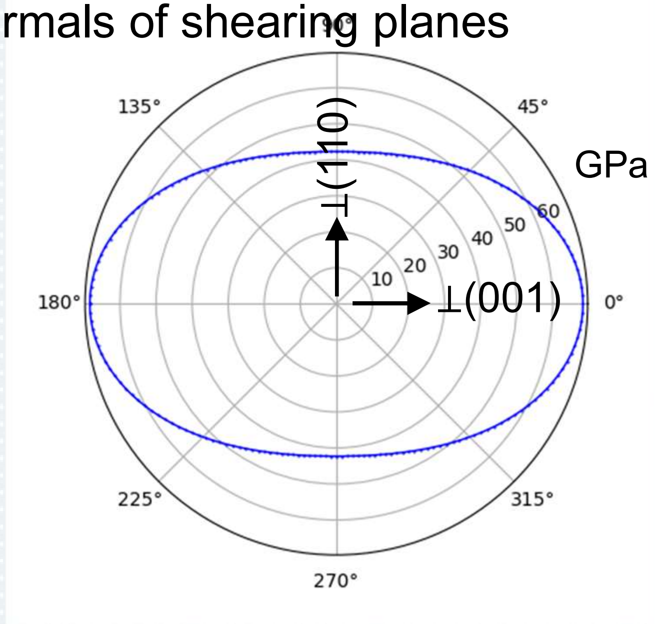
- Min. (green) and max. (blue) shear moduli in the (001) plane (option **3a**):
  - The lowest shear moduli (42.3 GPa) occurs along the (110) plane and perpendicular to the (110) plane

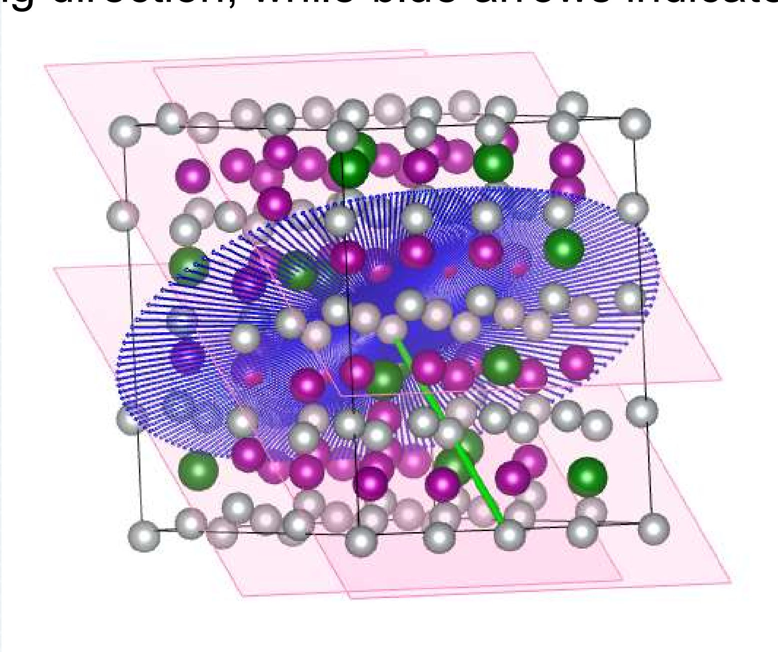




An Example – Ni-Mn-Sn

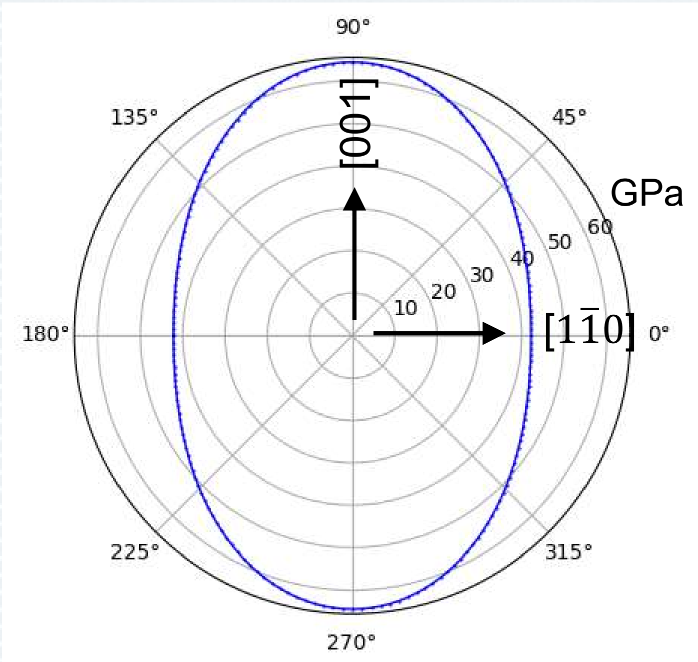
- Does the lowest shear moduli (42.3 GPa) really corresponds to the $[1\bar{1}0](110)$ shear system? Check all shearing planes for the $[1\bar{1}0]$ direction (option **7b**)
  - Shear moduli for all shearing planes corresponding to the $[1\bar{1}0]$ direction
  - The green arrow corresponds to the shearing direction, while blue arrows indicates normals of shearing planes

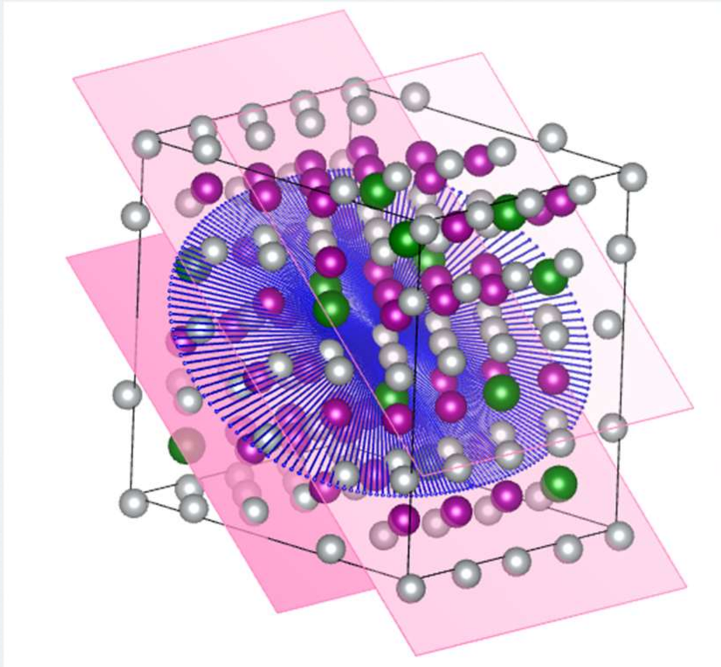




An Example – Ni-Mn-Sn

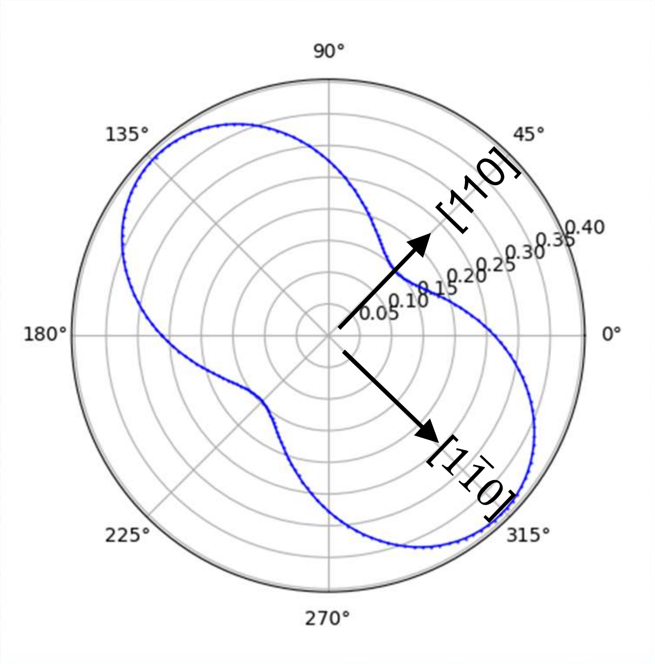
- Or check all shearing directions in the (110) planes (option **5a**)
  - Shear moduli for all shearing directions in the (110) planes

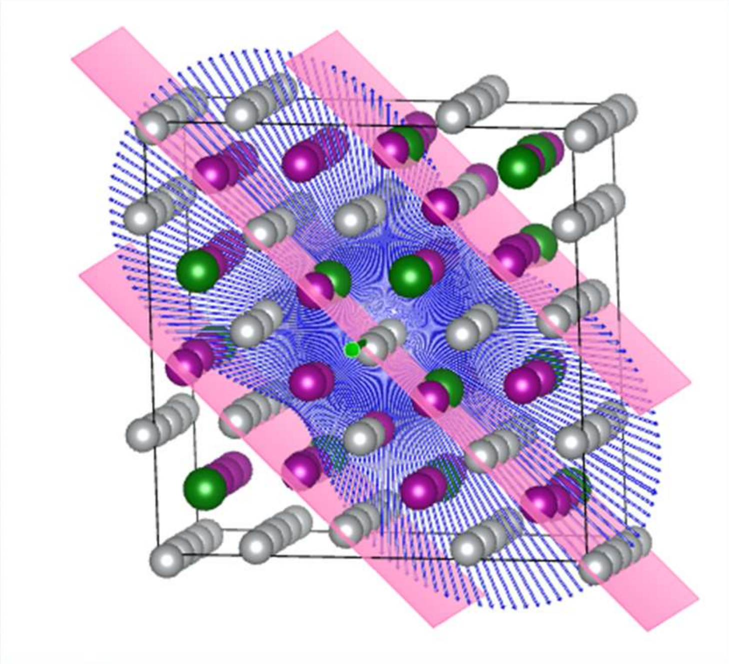




An Example – Ni-Mn-Sn

- Poisson's rations in the (001) plane for loading along the [001] direction (option **8a**):
  - The highest contraction along the (110) planes (0.39), the lowest for the direction perpendicular to the (110) planes (0.15)

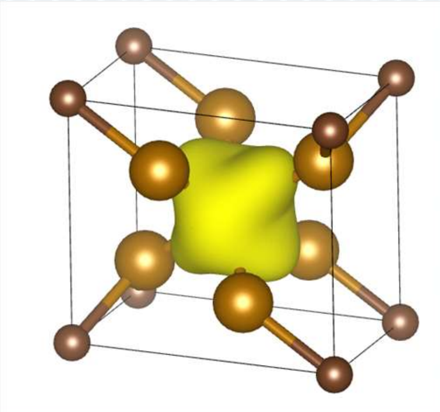




Outlook

- Searching for the lowest and highest $E^{[uvw]}$, $\kappa^{[uvw]}$, $G^{[uvw](hkl)}$, $\nu^{[uvw](hkl)}$ and corresponding [*uvw*] and (*hkl*)
- 3D visualization in VESTA

https://elastr.fme.vutbr.cz



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