ELATE: Elastic tensor analysis

Welcome to ELATE, the online tool for analysis of elastic tensors, developed by **Romain Gaillac** and **François-Xavier Coudert** at CNRS / Chimie ParisTech.
If you use the software in published results (paper, conference, etc.), please cite the corresponding paper (*J. Phys. Condens. Matter*, 2016, 28, 275201) and give the website URL.

ELATE is open source software. Any queries or comments are welcome at fx.coudert@chimie-paristech.fr

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Summary of the properties (3D material)

Input: stiffness matrix (coefficients in GPa) of

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22.957   25.725   11.643   0.8413    0.403   0.9571
25.725   47.182   17.221  -0.1469    -0.08   1.6534
11.643   17.221   272.96  -0.7252  -0.2686   0.6772
0.8413  -0.1469  -0.7252   1.9104  -0.2137  -0.5831
 0.403    -0.08  -0.2686  -0.2137   1.8829  -0.0242
0.9571   1.6534   0.6772  -0.5831  -0.0242   2.6824
```

Average properties

Averaging scheme	Bulk modulus	Young's modulus	Shear modulus	Poisson's ratio
Voigt	K_V = 50.253 GPa	E_V = 54.205 GPa	G_V = 20.529 GPa	ν_V = 0.32022
Reuss	K_R = 20.883 GPa	E_R = 7.5648 GPa	G_R = 2.6274 GPa	ν_R = 0.43962
Hill	K_H = 35.568 GPa	E_H = 31.334 GPa	G_H = 11.578 GPa	ν_H = 0.35317

Eigenvalues of the stiffness matrix

λ_1	λ_2	λ_3	λ_4	λ_5	λ_6
1.358 GPa	1.9748 GPa	2.918 GPa	6.7945 GPa	61.523 GPa	275 GPa

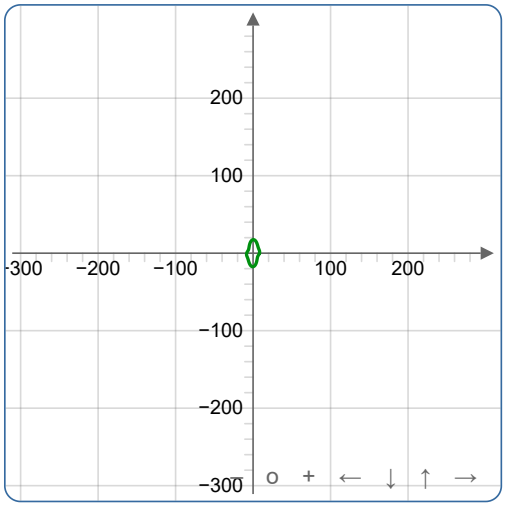
Variations of the elastic moduli

	Young's modulus		Linear compressibility		Shear modulus		Poisson's ratio		
	E_{min}	E_{max}	β_{min}	β_{max}	G_{min}	G_{max}	ν_{min}	ν_{max}	
Value	4.3127 GPa	266.11 GPa	-22.854 TPa^{-1}	57.081 TPa^{-1}	1.4253 GPa	16.86 GPa	-0.9243	1.3757	Value
Anisotropy	61.7		∞		11.83		∞		Anisotropy
Axis	0.4007 0.6700 0.6249	0.0013 0.0034 -1.0000	0.1712 0.7968 0.5796	-0.9852 0.1390 0.0999	-0.1947 0.2389 0.9513	0.0469 0.6782 -0.7333	0.0248 0.0819 -0.9963	0.0324 0.1195 -0.9923	Axis

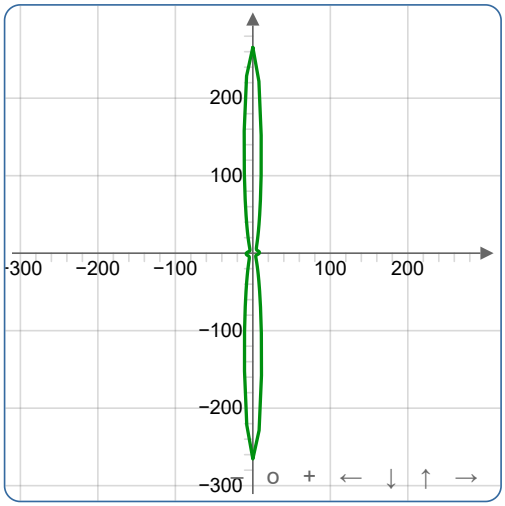
-0.7622	-0.0753	-0.9141	-0.3919	Second axis
-0.6473	-0.7297	0.4054	-0.9118	
0.0065	-0.6796	0.0106	-0.1226	

Spatial dependence of Young's modulus

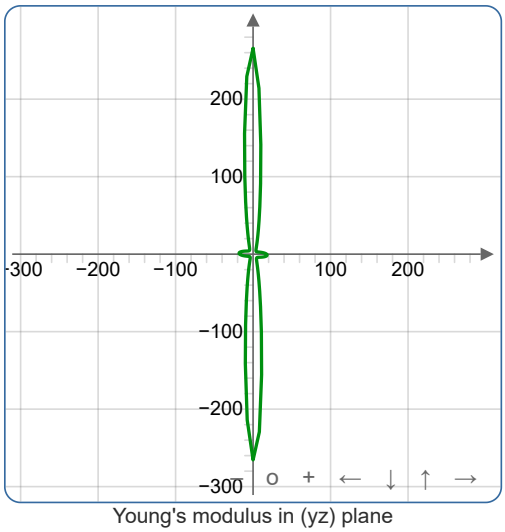
Visualize in 3D



Young's modulus in (xy) plane



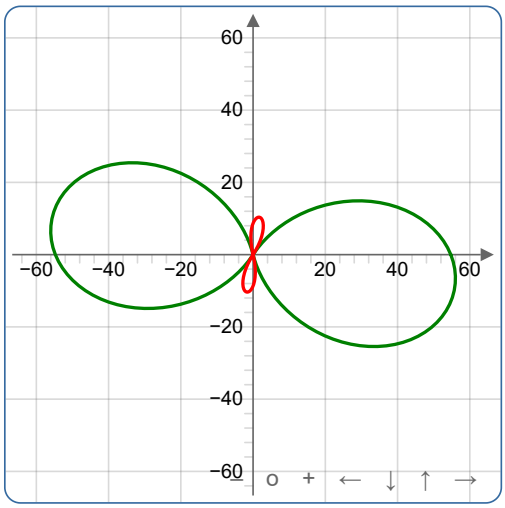
Young's modulus in (xz) plane



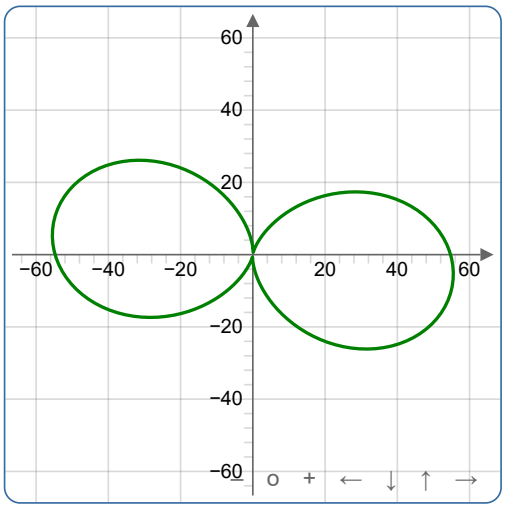
Young's modulus in (yz) plane

Spatial dependence of linear compressibility

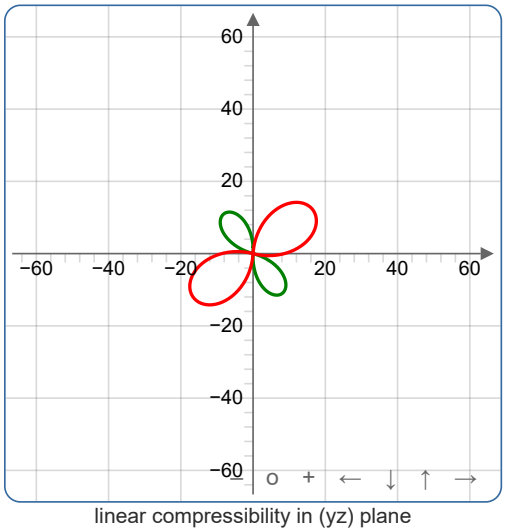
Visualize in 3D



linear compressibility in (xy) plane



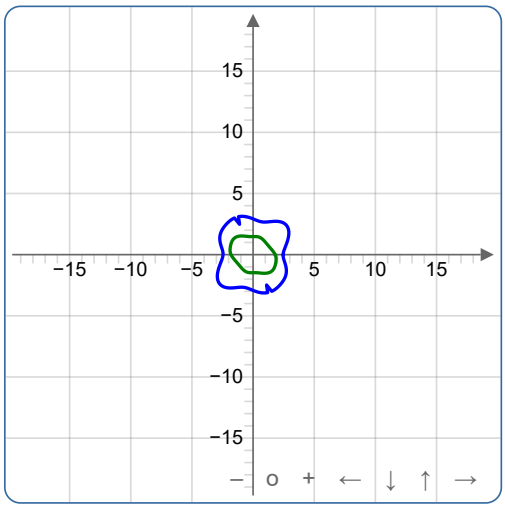
linear compressibility in (xz) plane



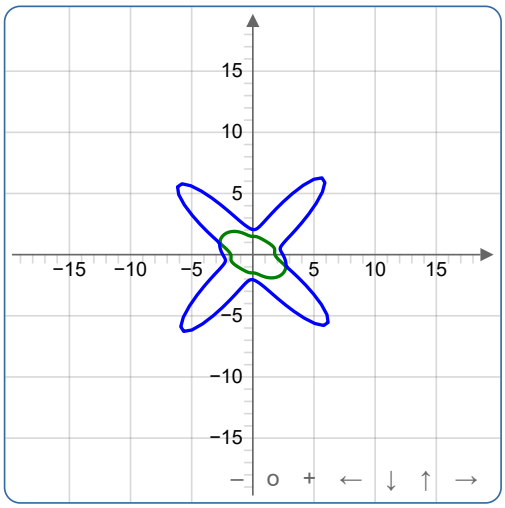
linear compressibility in (yz) plane

Spatial dependence of shear modulus

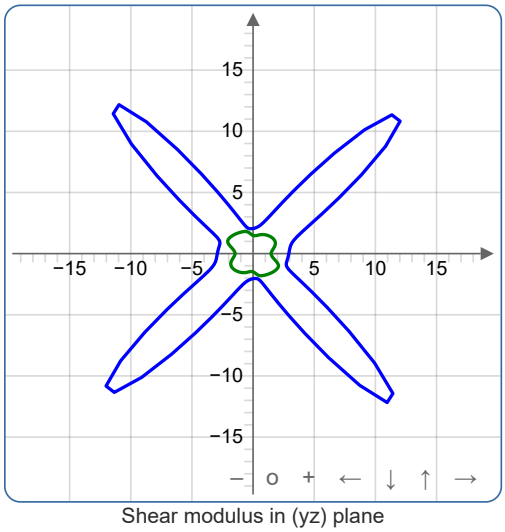
Visualize in 3D



Shear modulus in (xy) plane



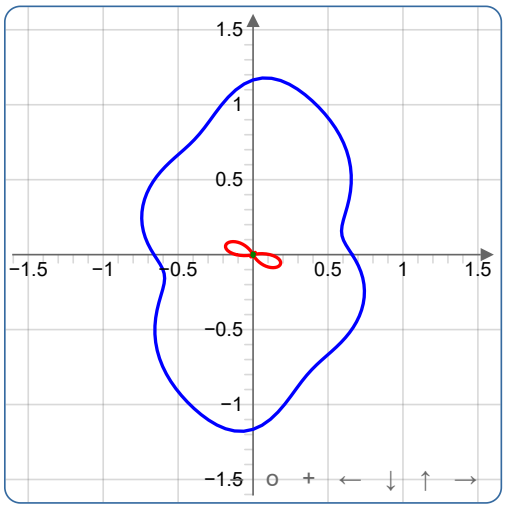
Shear modulus in (xz) plane



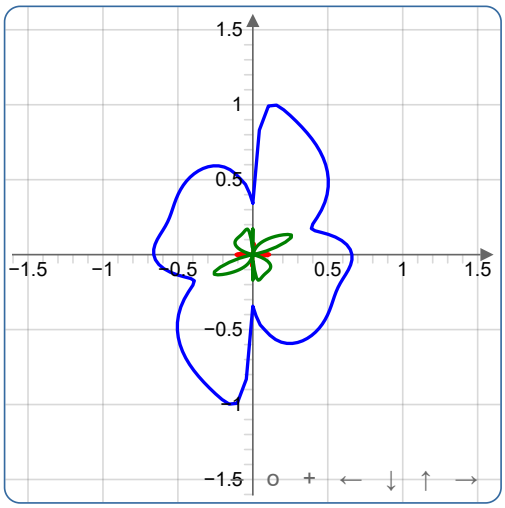
Shear modulus in (yz) plane

Spatial dependence of Poisson's ratio

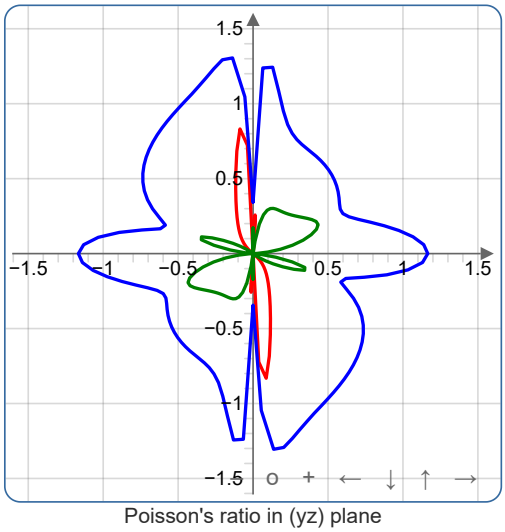
Visualize in 3D



Poisson's ratio in (xy) plane



Poisson's ratio in (xz) plane



Poisson's ratio in (yz) plane

Code version: 2024.03.15 (running on Python 3.11.2)
Execution time: 1.167 seconds