# **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 <u>corresponding paper</u> (*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

### **Summary of the properties (3D material)**



#### Input: stiffness matrix (coefficients in GPa) of

21.692	24.83	13.965	0.2541	-1.0904	-0.1153
24.83	42.576	19.409	0.9002	-1.1102	0.9063
13.965	19.409	274.1	-0.1283	0.7649	-0.0713
0.2541	0.9002	-0.1283	2.9155	-0.216	-0.583
-1.0904	-1.1102	0.7649	-0.216	2.7181	0.2909
-0.1153	0.9063	-0.0713	-0.583	0.2909	2.2818

#### **Average properties**

Averaging scheme	Bulk modulus	Young's modulus	Shear modulus	Poisson's ratio
Voigt	K <sub>V</sub> = 50.53 GPa	<i>E</i> <sub>V</sub> = 53.615 GPa	G <sub>V</sub> = 20.26 GPa	$v_V = 0.32316$
Reuss	K <sub>R</sub> = 20.35 GPa	<i>E</i> <sub>R</sub> = 8.6296 GPa	G <sub>R</sub> = 3.0188 GPa	$v_{R} = 0.42932$
Hill	K <sub>H</sub> = 35.44 GPa	E <sub>H</sub> = 31.473 GPa	G <sub>H</sub> = 11.64 GPa	v <sub>H</sub> = 0.35199

#### Eigenvalues of the stiffness matrix

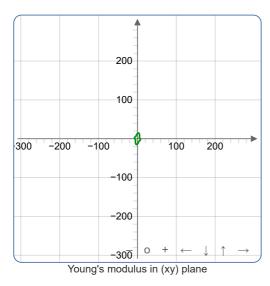
λ <sub>1</sub>	$\lambda_2$	λ <sub>3</sub>	$\lambda_4$	λ <sub>5</sub>	λ <sub>6</sub>	
1 772 GPa	2.5153 GPa	3 384 GPa	5 3663 GPa	56 519 GPa	276 72 GPa	

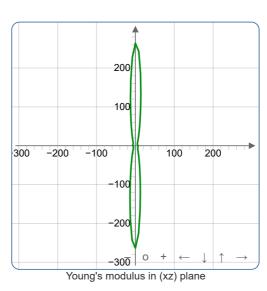
#### Variations of the elastic moduli

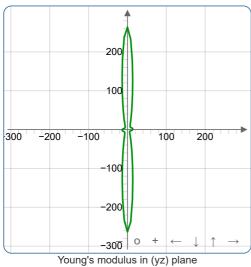
	Young's modulus		Linear compressibility		Shear modulus		Poisson's ratio		
	$E_{min}$	E <sub>max</sub>	$\beta_{\text{min}}$	$\beta_{\text{max}}$	G <sub>min</sub>	G <sub>max</sub>	v <sub>min</sub>	v <sub>max</sub>	
Value	5.345 GPa	264.27 GPa	-11.258 TPa <sup>-1</sup>	60.413 TPa <sup>-1</sup>	1.6871 GPa	13.82 GPa	-0.44725	1.1452	Value
Anisotropy	49	.44	×	o	8.1	92	œ		Anisotropy
Axis	0.8256 0.3951 0.4028	-0.0057 0.0020 -1.0000	-0.0374 0.9993 -0.0041	0.9876 0.0377 0.1524	0.2688 0.9573 -0.1068	0.1206 0.6904 0.7133	-0.0222 0.0905 0.9956	-0.0024 0.9989 0.0466	Axis

## Spatial dependence of Young's modulus

## Visualize in 3D

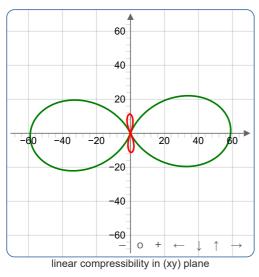


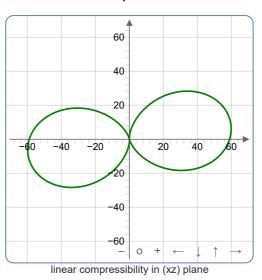


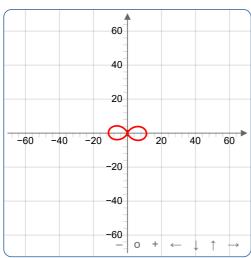


## Spatial dependence of linear compressibility

Visualize in 3D





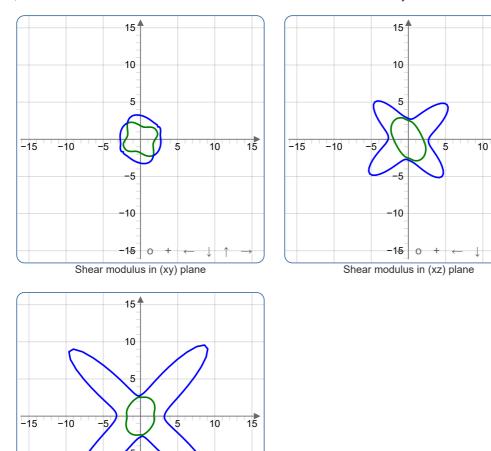


linear compressibility in (yz) plane

# Spatial dependence of shear modulus

Visualize in 3D

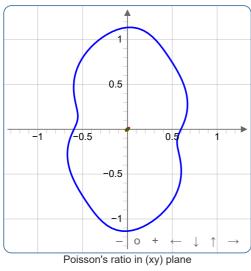
15

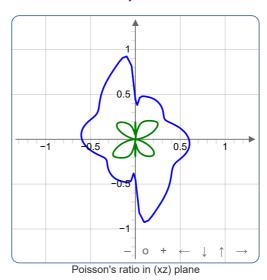


# Spatial dependence of Poisson's ratio

-15 0 + ←
Shear modulus in (yz) plane

Visualize in 3D





0.5 -0.5 0.5 -0.5 0 ↓ ↑

Poisson's ratio in (yz) plane

Code version: 2024.03.15 (running on Python 3.11.2) Execution time: 1.164 seconds