# **ELATE: Elastic tensor analysis**

Welcome to ELATE, the online tool for analysis of elastic tensors, developed by **Romain Gaillac** and **François-Xavier Coudert** at <u>CNRS / Chimie ParisTech</u>.

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

49.089	24.2	15.792	-0.0121	-0.0207	6.9446
24.2	21.049	9.9717	0.1428	0.3205	2.7049
15.792	9.9717	279.05	1.1616	0.031	3.2918
-0.0121	0.1428	1.1616	1.0992	0.8919	0.2544
-0.0207	0.3205	0.031	0.8919	3.756	-0.1076
6.9446	2.7049	3.2918	0.2544	-0.1076	5.7735

#### Average properties

Averaging scheme	Bulk modulus	Young's modulus	Shear modulus	Poisson's ratio
Voigt	K <sub>V</sub> = 49.902 GPa	<i>E</i> <sub>V</sub> = 57.712 GPa	G <sub>V</sub> = 22.074 GPa	$v_{V} = 0.30725$
Reuss	K <sub>R</sub> = 19.199 GPa	<i>E</i> <sub>R</sub> = 7.1586 GPa	G <sub>R</sub> = 2.4893 GPa	$v_{R} = 0.43786$
Hill	K <sub>H</sub> = 34.55 GPa	E <sub>H</sub> = 32.942 GPa	G <sub>H</sub> = 12.282 GPa	v <sub>H</sub> = 0.34109

#### 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>
0.80348 GPa	3.9871 GPa	4.4102 GPa	7.5851 GPa	62.318 GPa	280.71 GPa

### Variations of the elastic moduli

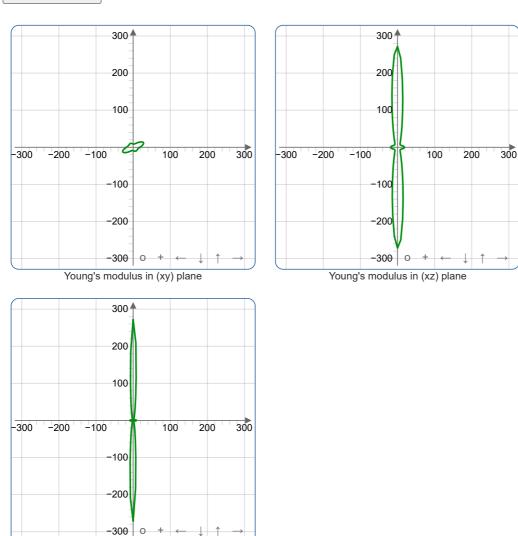
	Young's modulus		Linear compressibility		Shear modulus		Poisson's ratio		
	$\textit{E}_{min}$	E <sub>max</sub>	$\beta_{\text{min}}$	$\beta_{\text{max}}$	G <sub>min</sub>	G <sub>max</sub>	v <sub>min</sub>	v <sub>max</sub>	
Value	2.9356 GPa	273.14 GPa	-6.4246 TPa <sup>–1</sup>	55.605 TPa <sup>–1</sup>	0.80311 GPa	26.109 GPa	-0.26389	1.1429	Value
Anisotropy	93	.04	c	0	32.	.51	∞		Anisotropy
Axis	-0.2511 0.6955 0.6732	-0.0000 0.0039 1.0000	0.9417 0.1731 0.2886	-0.1839 0.9829 0.0104	-0.0763 -0.0170 0.9969	0.6417 0.2864 -0.7115	0.7771 0.5952 -0.2046	0.2040 0.1885 0.9607	Axis

13/09/2024, 16:43 Elastic analysis of

-0.2893 -0.6545 -0.5025 0.3977 0.9572 -0.2790 0.3910 0.8807 Second -0.0058 -0.7027 -0.7711 -0.2572

## Spatial dependence of Young's modulus

### Visualize in 3D

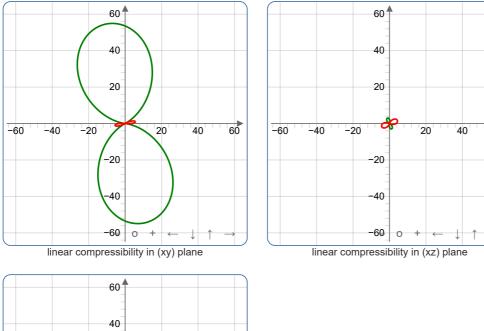


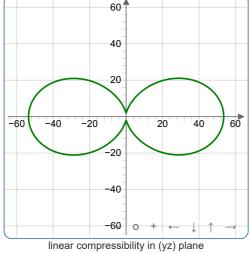
### Spatial dependence of linear compressibility

Young's modulus in (yz) plane

Visualize in 3D

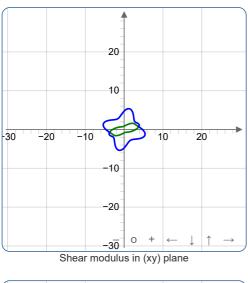
60

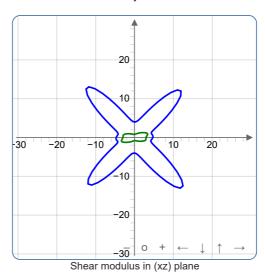


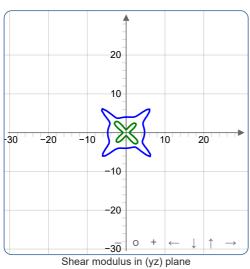


## Spatial dependence of shear modulus

Visualize in 3D

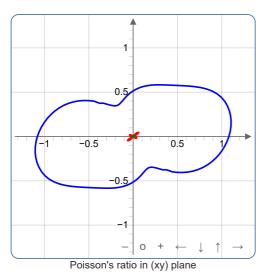


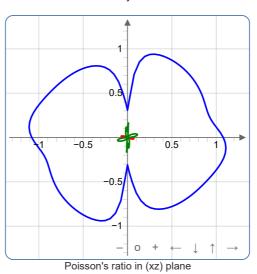


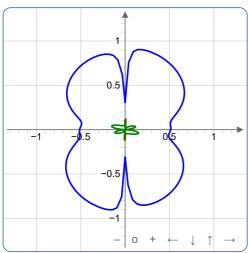


## Spatial dependence of Poisson's ratio

Visualize in 3D







Poisson's ratio in (yz) plane

Code version: 2024.03.15 (running on Python 3.11.2) Execution time: 1.180 seconds