Supplementary Information SI1 for the paper
Alexander Platonenko, Marina Konuhova, Dmitry V. Bocharov, Anatoli I. Popov,
"Structural and mechanical properties of Y_2SiO_5-Lu_2SiO_5 solid solutions from *ab initio* calculations"

Stiffness matrices and visualization of spatially dependent mechanical properties

This file contains the following data:

- Notation of compositions
- Visualization of spatially dependent properties
1. Input: stiffness matrix (coefficients in GPa)
2. Direction-dependent properties:
2.1 Young's modulus
2.2 Linear compressibility
2.3 Shear modulus
2.4 Poisson's ratio

Notation of compositions

The compositions are labeled according to the distribution of Y and Lu atoms over the rare-earth sublattice in the 32-atom primitive unit cell.
The end-member compounds correspond to:

LSO (Lu_2SiO_5): all rare-earth sites are occupied by Lu atoms.
LSO: 0 Y + 8 Lu (0% Y, 100% Lu)

YSO (Y_2SiO_5): all rare-earth sites are occupied by Y atoms;
YSO: 8 Y + 0 Lu (100% Y, 0% Lu)

Intermediate solid solutions are denoted as LYSO_nY, where n indicates the number of Y atoms substituting Lu atoms in the primitive unit cell.
Since the primitive cell contains eight rare-earth cation sites, the notation corresponds to the following compositions:
LYSO_1Y: 1 Y + 7 Lu (12.5% Y, 87.5% Lu)
LYSO_2Y: 2 Y + 6 Lu (25% Y, 75% Lu)

LYSO_3Y: 3 Y + 5 Lu (37.5% Y, 62.5% Lu)
LYSO_4Y: 4 Y + 4 Lu (50% Y, 50% Lu)
LYSO_5Y: 5 Y + 3 Lu (62.5% Y, 37.5% Lu)
LYSO_6Y: 6 Y + 2 Lu (75% Y, 25% Lu)
LYSO_7Y: 7 Y + 1 Lu (87.5% Y, 12.5% Lu)

Thus, for example, LYSO_7Y corresponds to a composition with one Lu atom and seven Y atoms in the primitive cell, i.e., a Y-rich solid solution approaching YSO.

Visualization of spatially dependent properties

For each composition, the spatial dependence of the corresponding mechanical property (subsections 2-5) is presented using both three-dimensional representations and their projections onto principal planes.

Specifically, each set of figures includes:
- 2D projections onto xy, xz, and yz planes
- A 3D surface plot illustrating the full directional dependence of the property.

1. Input: stiffness matrix (coefficients in GPa)

LSO

260.7	74.65	89.671	0	-15.42	0
74.65	208.07	14.527	0	-0.406	0
89.671	14.527	235.61	0	26.761	0
0	0	0	62.51	0	17.608
-15.42	-0.406	26.761	0	90.644	0
0	0	0	17.608	0	58.4

LYSO_1Y

252.32	70.791	87.517	-2.585	-14.373	1.227
70.791	204.34	16.156	-4.838	2.058	1.169
87.517	16.156	231.99	-2.737	27.946	0.937
-2.585	-4.838	-2.737	62.215	0.923	16.619
-14.373	2.058	27.946	0.923	89.281	-0.34
1.227	1.169	0.937	16.619	-0.34	57.207

LYSO_2Y

244.41	67.304	83.534	0.014	-14.629	-0.005
67.304	200.49	16.226	-0.022	2.047	-0.021
83.534	16.226	230.02	-0.038	26.532	0.044
0.014	-0.022	-0.038	61.615	-0.004	15.992
-14.629	2.047	26.532	-0.004	87.544	0.013
-0.005	-0.021	0.044	15.992	0.013	56.353

LYSO_3Y

241.18	70.018	83.421	-1.477	-14.48	1.646
70.018	195.31	14.385	-1.939	2.155	1.867
83.421	14.385	223.24	-1.146	25.937	1.4
-1.477	-1.939	-1.146	60.302	1.194	15.541
-14.48	2.155	25.937	1.194	85.784	-0.547
1.646	1.867	1.4	15.541	-0.547	54.703

LYSO_4Y

237.09	70.226	81.838	-0.005	-14.125	0.1
70.226	189.07	14.323	-0.039	3.488	0.014
81.838	14.323	220.3	0.012	25.69	0.091
-0.005	-0.039	0.012	59.525	0.018	15.144
-14.125	3.488	25.69	0.018	84.356	0.021
0.1	0.014	0.091	15.144	0.021	53.684

LYSO_5Y

230.34	69.18	81.731	2.034	-14.023	-1.667
69.18	191.56	17.125	4.477	2.061	-1.578
81.731	17.125	218.8	4.434	25.593	-1.397
2.034	4.477	4.434	60.57	0.152	14.579
-14.023	2.061	25.593	0.152	82.551	-0.181
-1.667	-1.578	-1.397	14.579	-0.181	51.898

LYSO_6Y

226.41	69.779	82.873	0	-13.804	0
69.779	196.78	22.484	0	-0.538	0
82.873	22.484	221.88	0	24.443	0
0	0	0	62.198	0	13.273
-13.804	-0.538	24.443	0	80.985	0
0	0	0	13.273	0	51.451

LYSO_7Y

221.02	65.966	81.258	-0.108	-11.98	-0.577
65.966	183.66	15.864	-0.514	0.451	-0.091
81.258	15.864	215.57	0.569	26.573	-0.377
-0.108	-0.514	0.569	59.794	-0.355	13.307
-11.98	0.451	26.573	-0.355	79.905	0.08
-0.577	-0.091	-0.377	13.307	0.08	49.658

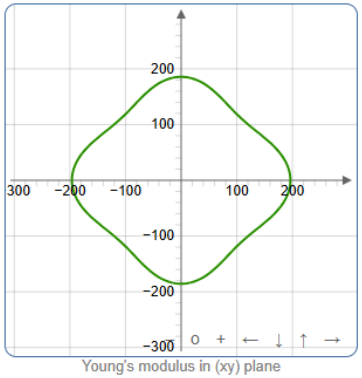
YSO

213.08	59.104	77.147	0	-12.067	0
59.104	161.01	3.355	0	-2.193	0
77.147	3.355	206.48	0	25.539	0
0	0	0	56.149	0	13.948
-12.067	-2.193	25.539	0	78.524	0
0	0	0	13.948	0	47.635

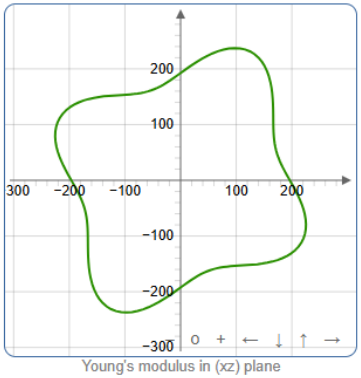
2. Direction-dependent properties

2.1. Spatial dependence of Young's modulus

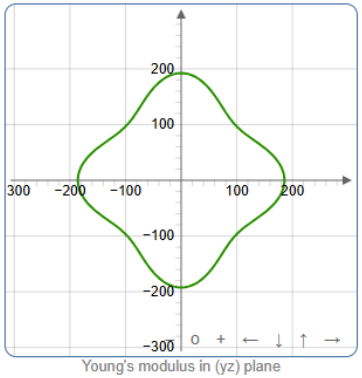
LSO



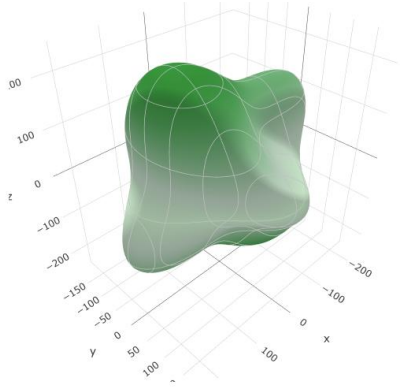
Young's modulus in (xy) plane



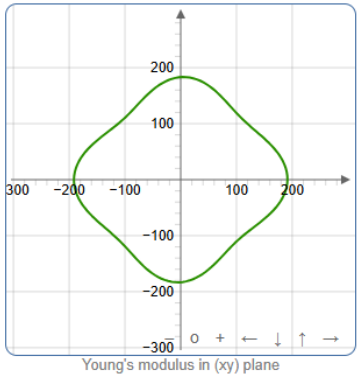
Young's modulus in (xz) plane



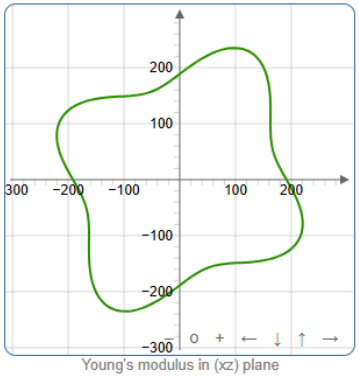
Young's modulus in (yz) plane



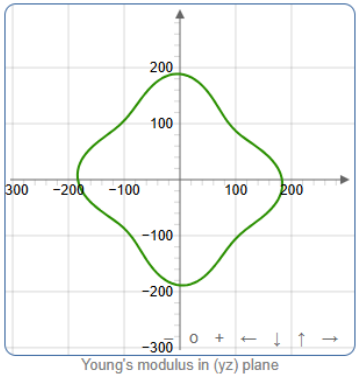
LYSO_1Y



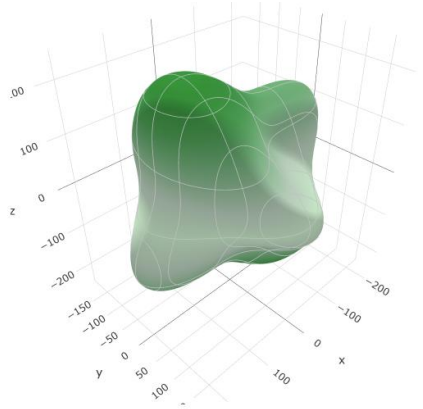
Young's modulus in (xy) plane



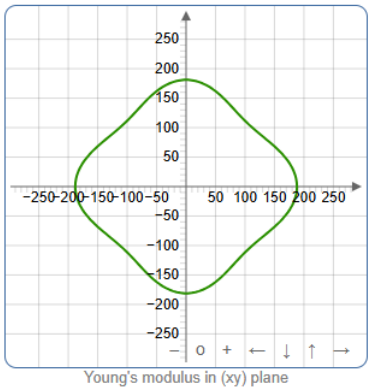
Young's modulus in (xz) plane



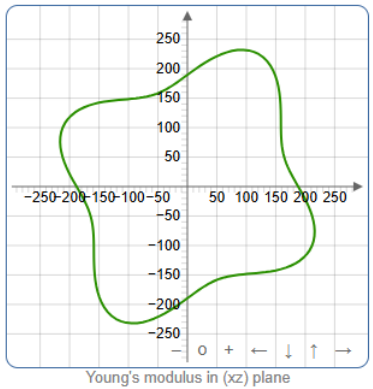
Young's modulus in (yz) plane



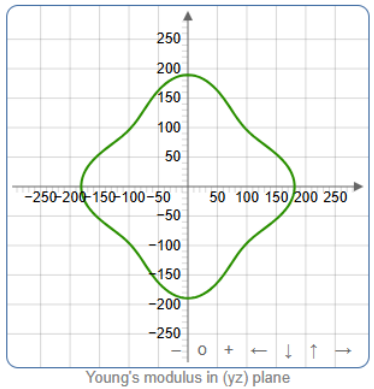
LYSO_2Y



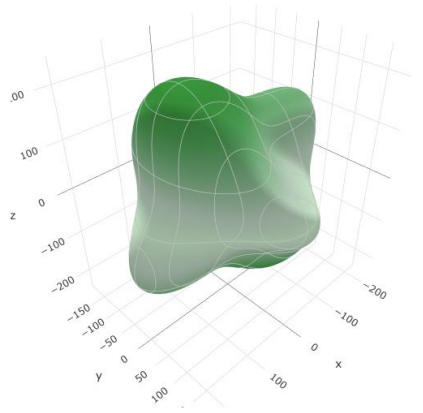
Young's modulus in (xy) plane



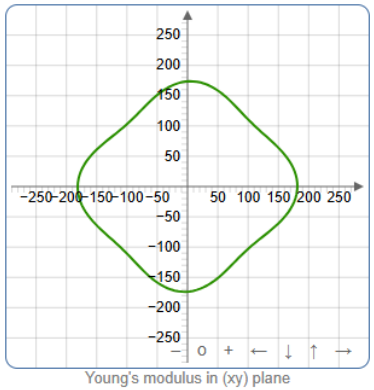
Young's modulus in (xz) plane



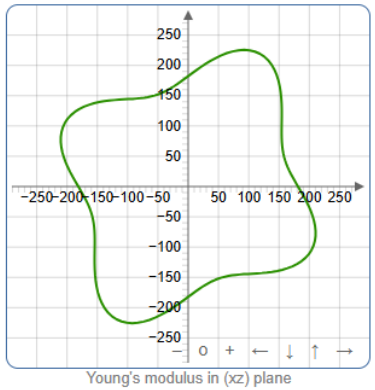
Young's modulus in (yz) plane



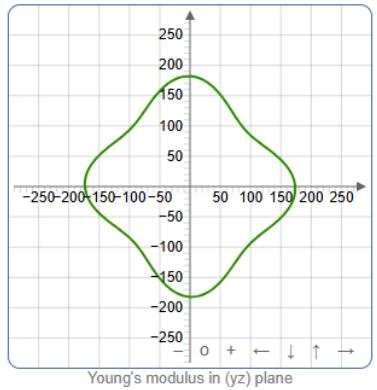
LYSO_3Y



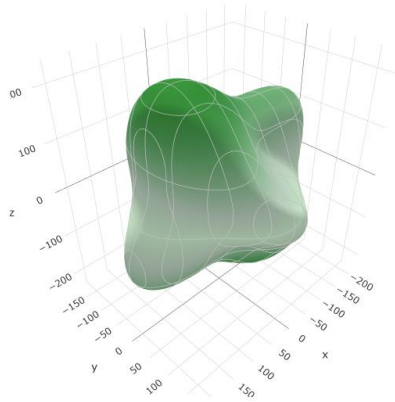
Young's modulus in (xy) plane



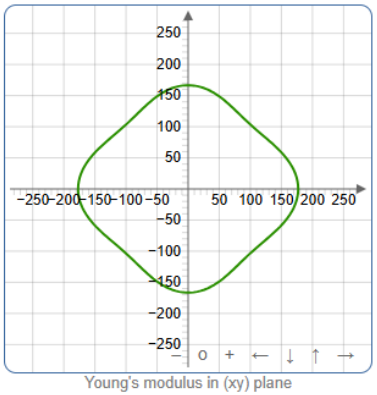
Young's modulus in (xz) plane



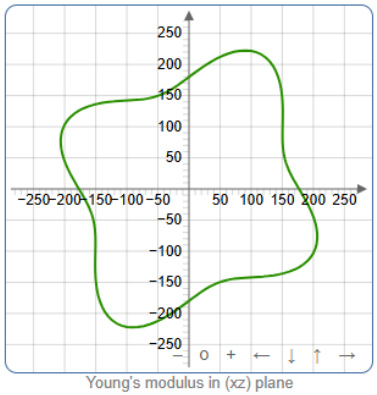
Young's modulus in (yz) plane



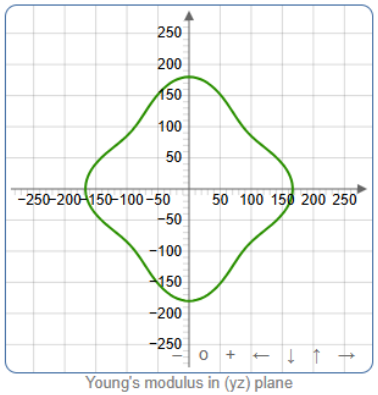
LYSO_4Y



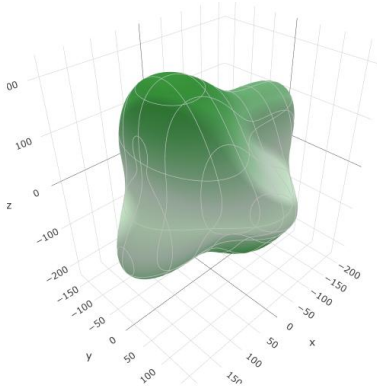
Young's modulus in (xy) plane



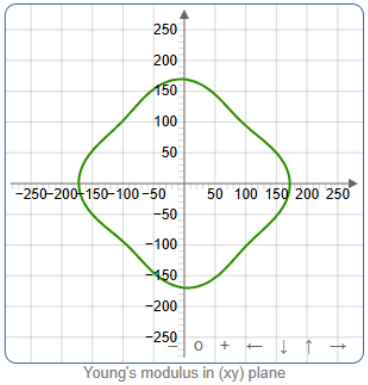
Young's modulus in (xz) plane



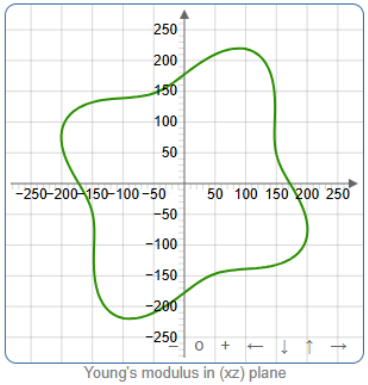
Young's modulus in (yz) plane



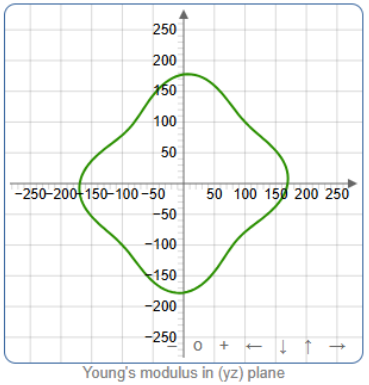
LYSO_5Y



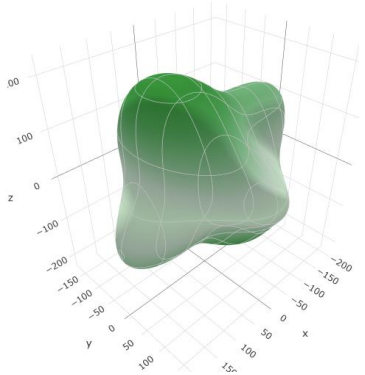
Young's modulus in (xy) plane



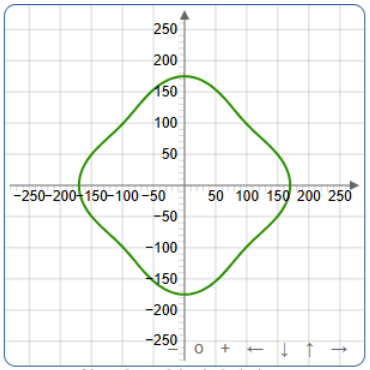
Young's modulus in (xz) plane



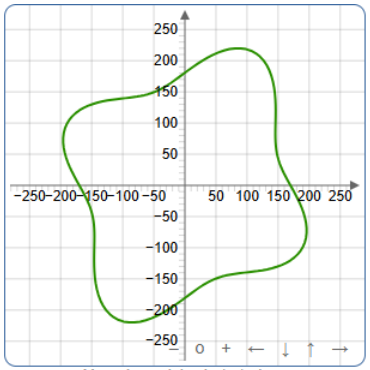
Young's modulus in (yz) plane



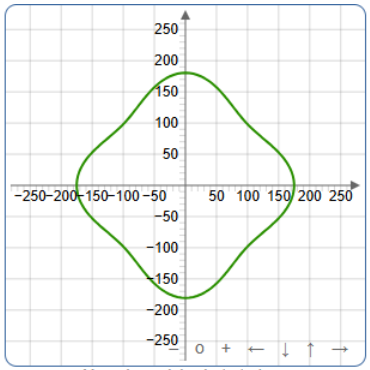
LYSO_6Y



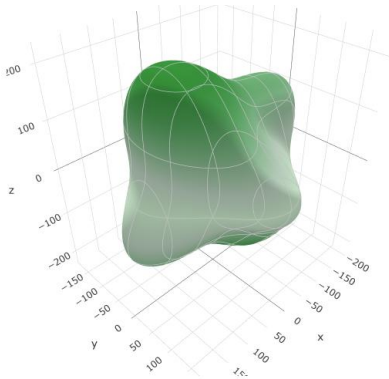
Young's modulus in (xy) plane



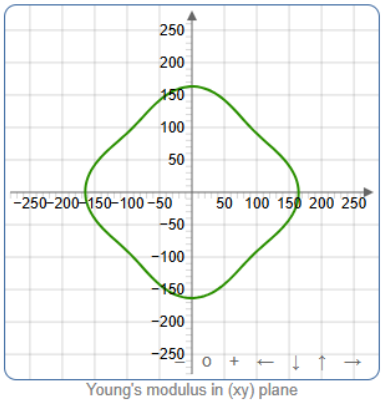
Young's modulus in (xz) plane



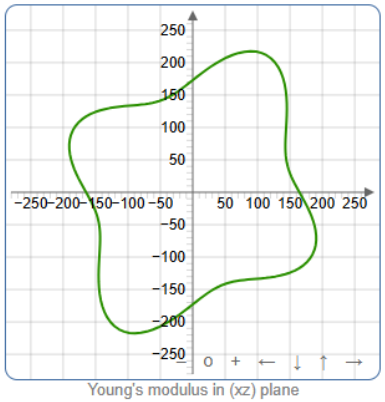
Young's modulus in (yz) plane



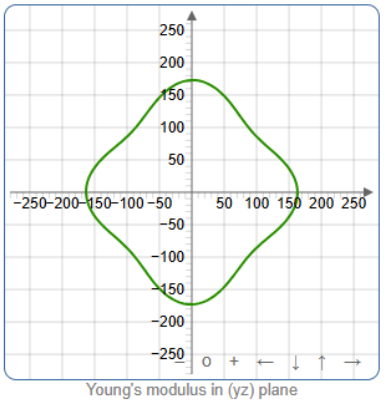
LYSO_7Y



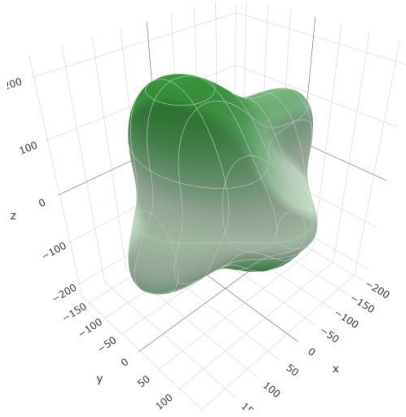
Young's modulus in (xy) plane



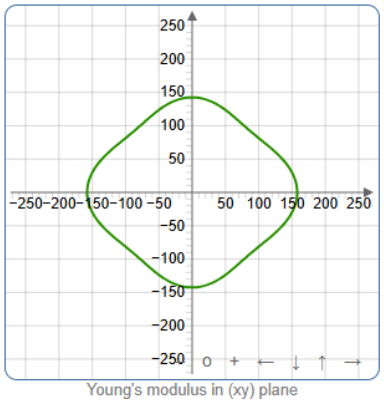
Young's modulus in (xz) plane



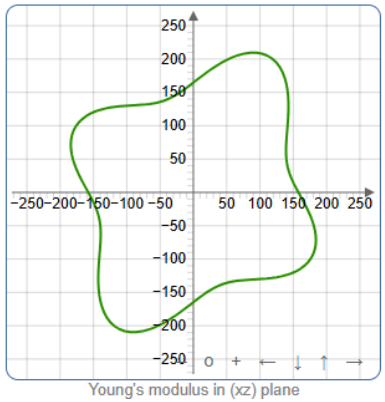
Young's modulus in (yz) plane



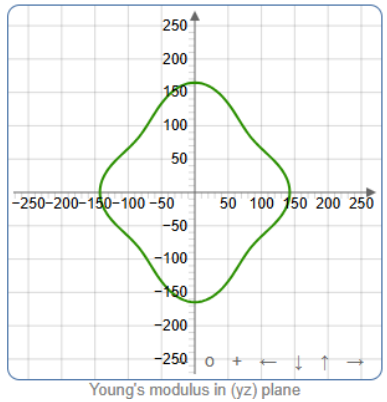
YSO



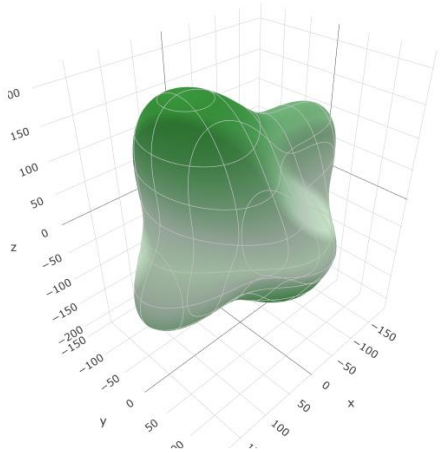
Young's modulus in (xy) plane



Young's modulus in (xz) plane

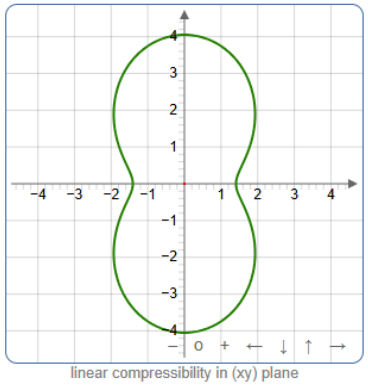


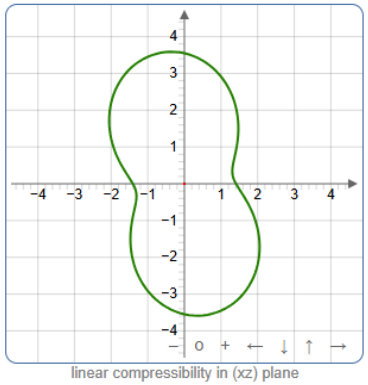
Young's modulus in (yz) plane

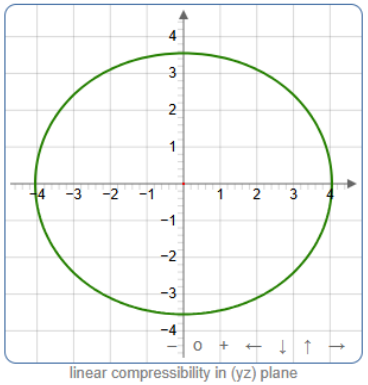


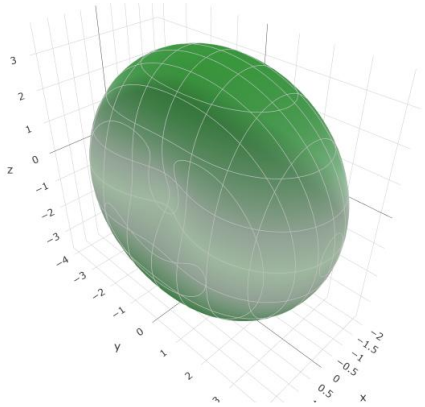
2.2. Spatial dependence of linear compressibility

LSO

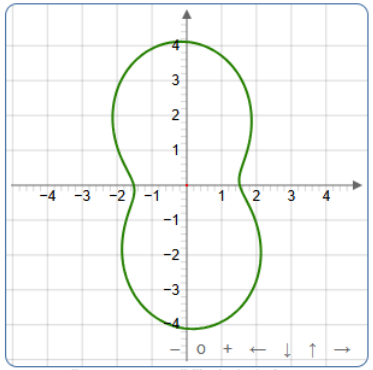

linear compressibility in (xy) plane

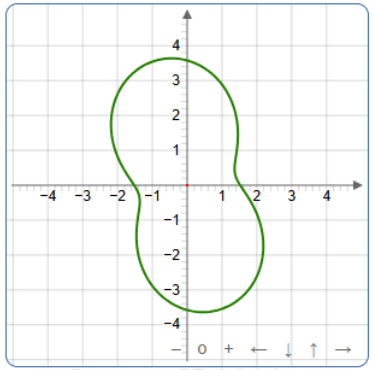

linear compressibility in (xz) plane

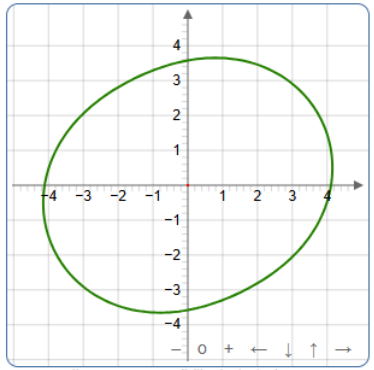

linear compressibility in (yz) plane

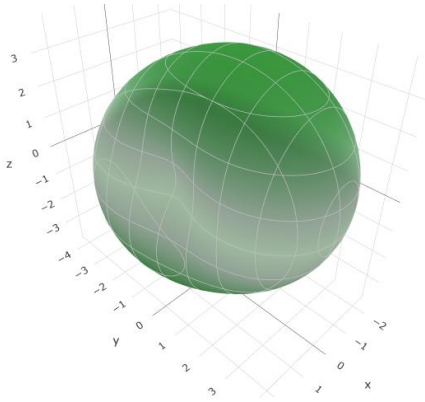


LYSO_1Y

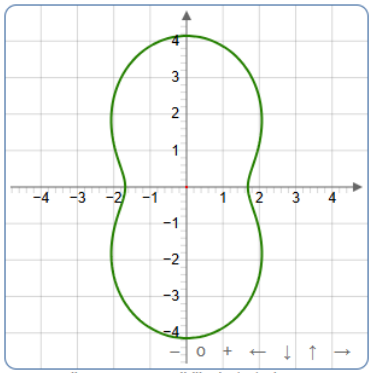

linear compressibility in (xy) plane

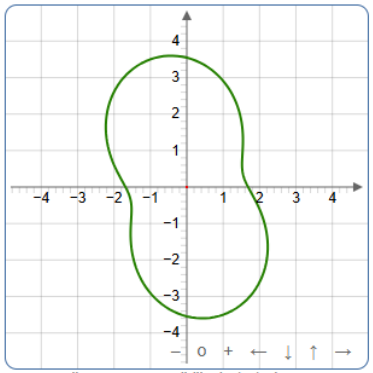

linear compressibility in (xz) plane

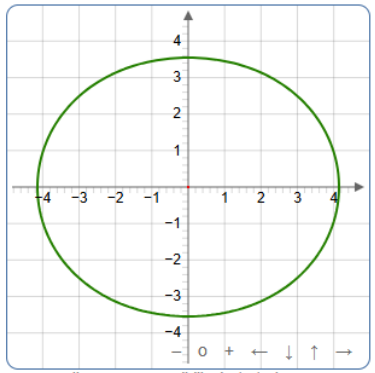

linear compressibility in (yz) plane

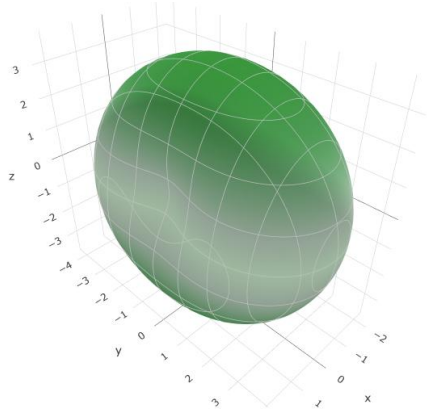


LYSO_2Y

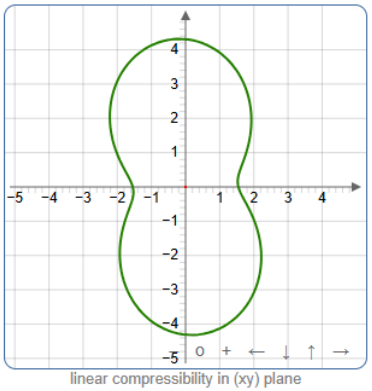


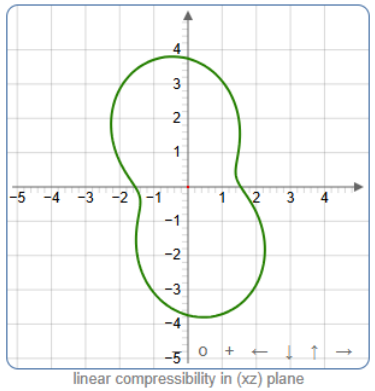


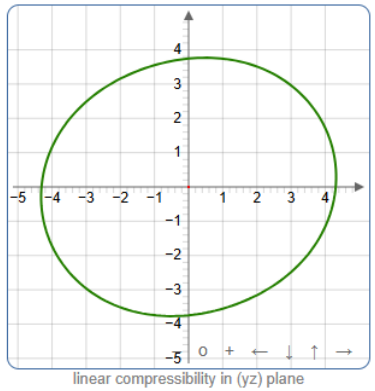


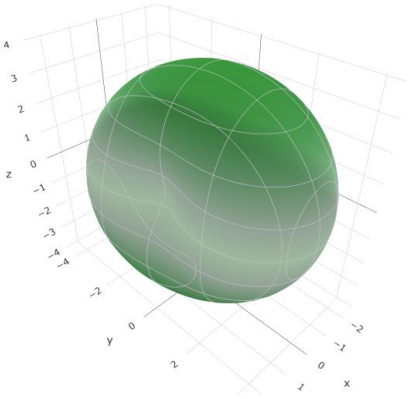


LYSO_3Y

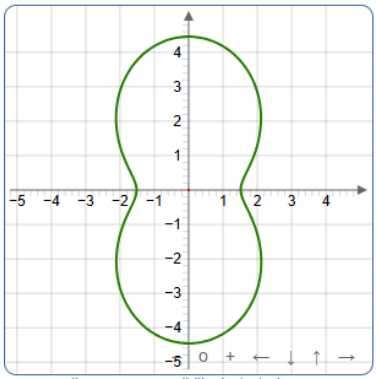


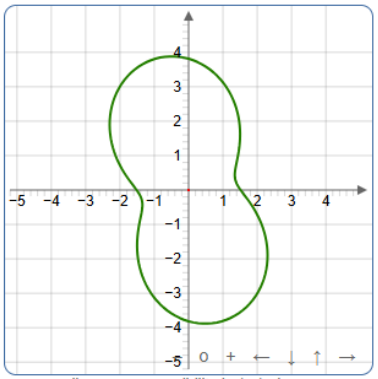


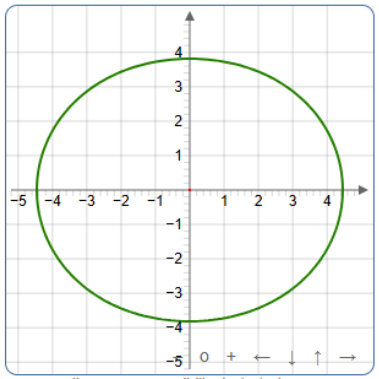


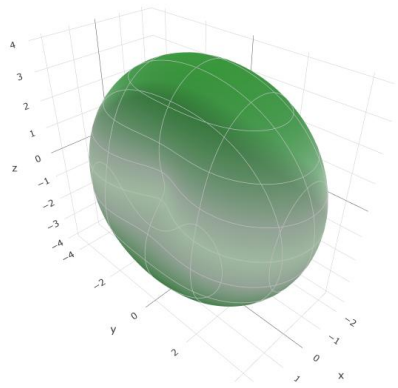


LYSO_4Y

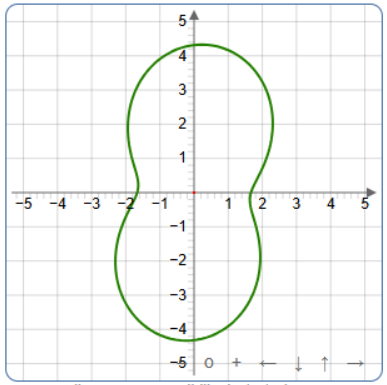


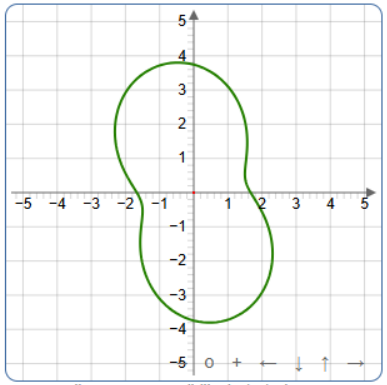


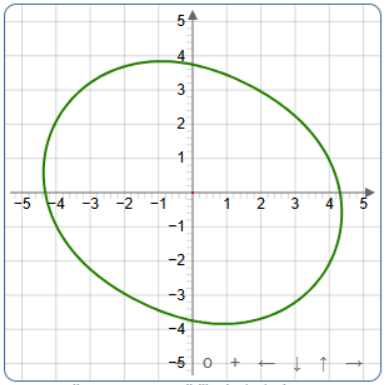


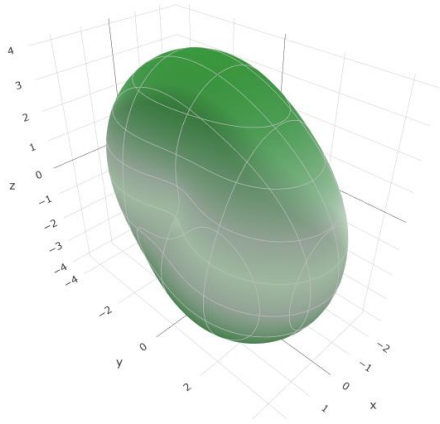


LYSO_5Y

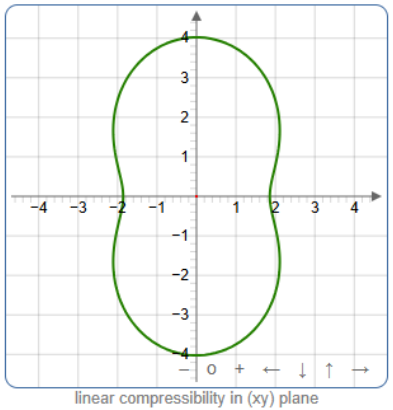


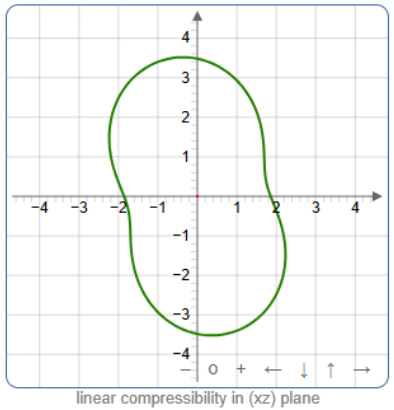


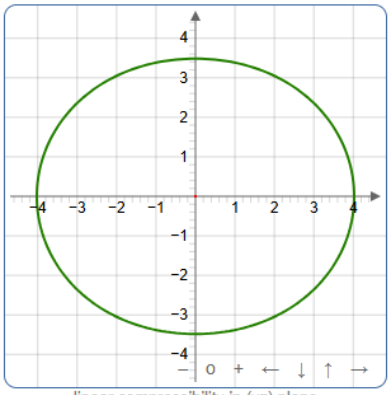


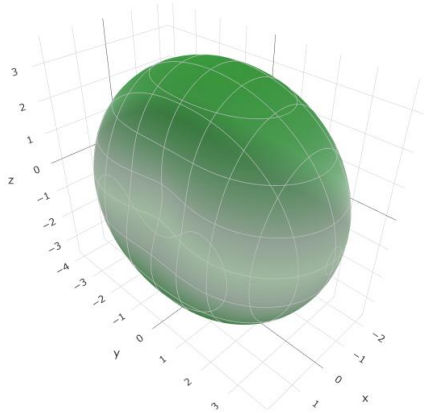


LYSO_6Y

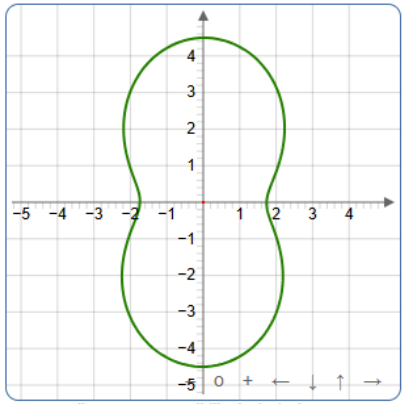


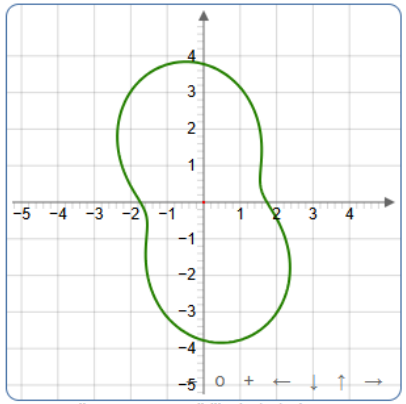


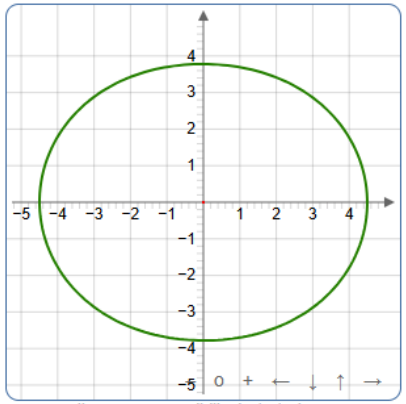


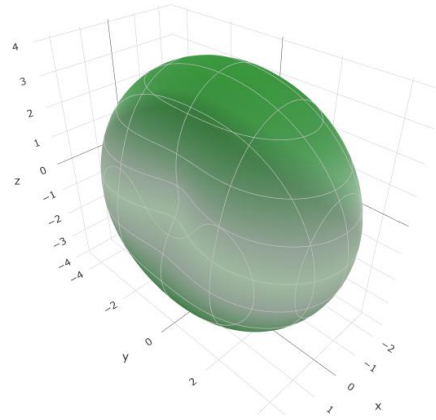


LYSO_7Y

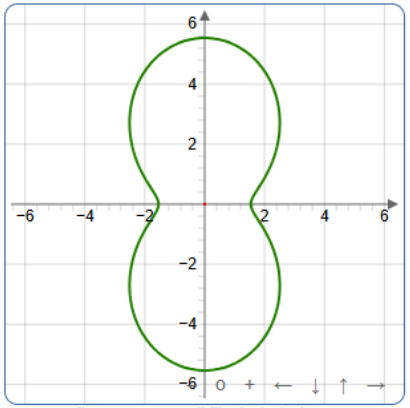




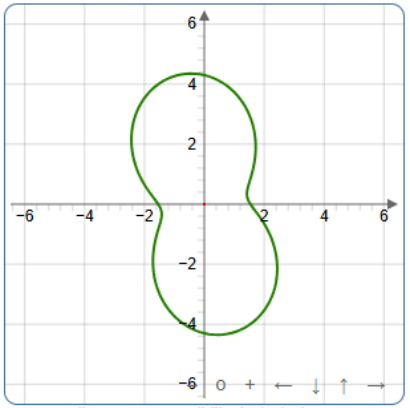




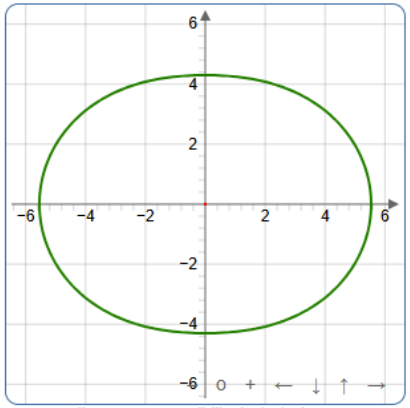
YSO



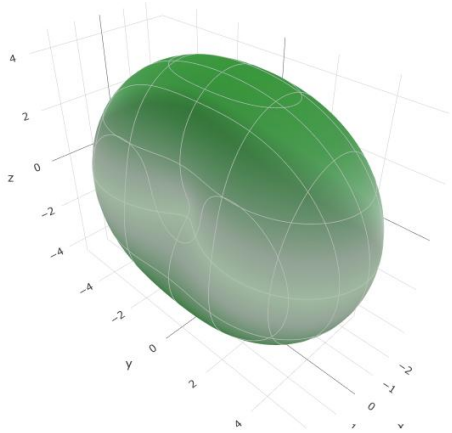
linear compressibility in (xy) plane



linear compressibility in (xz) plane

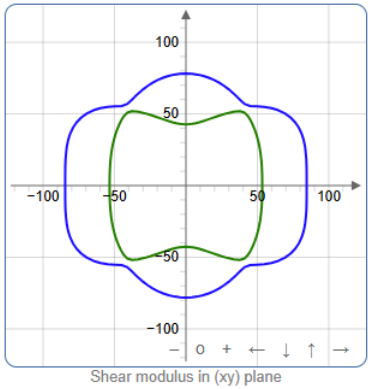


linear compressibility in (yz) plane

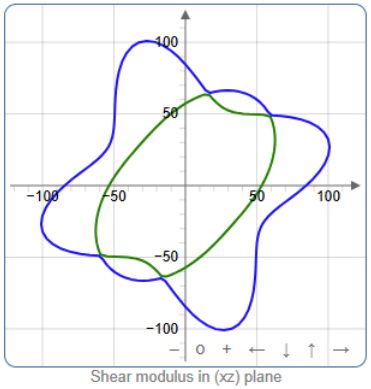


2.3. Spatial dependence of shear modulus

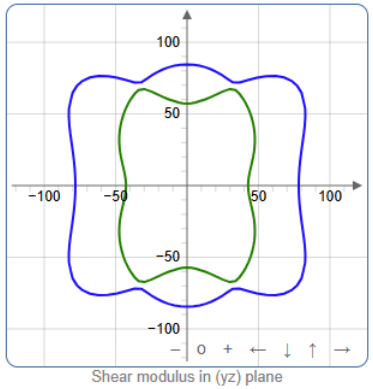
LSO



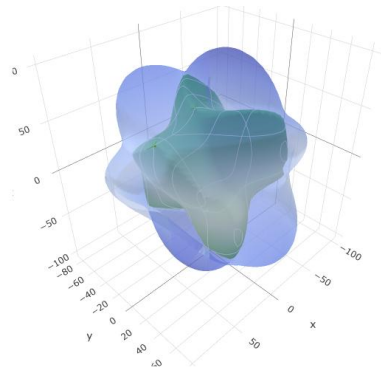
Shear modulus in (xy) plane



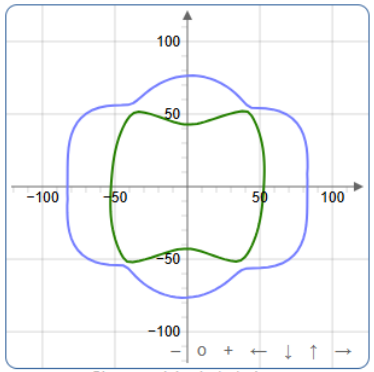
Shear modulus in (xz) plane



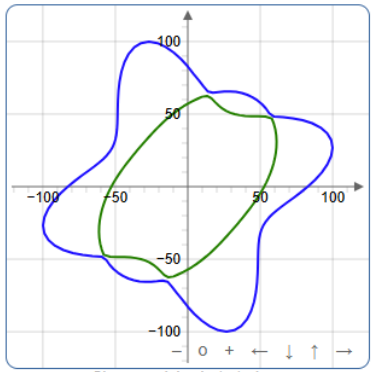
Shear modulus in (yz) plane



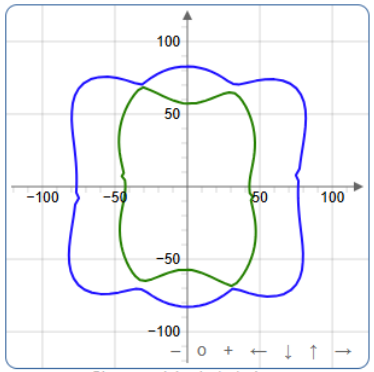
LYSO_1Y



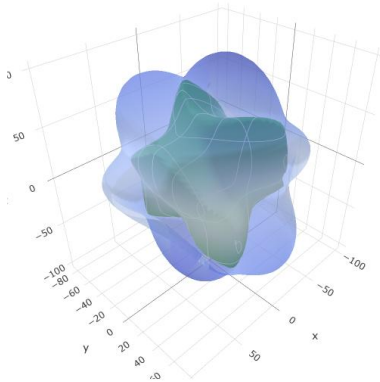
Shear modulus in (xy) plane



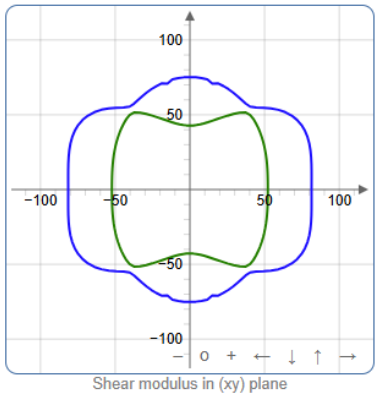
Shear modulus in (xz) plane



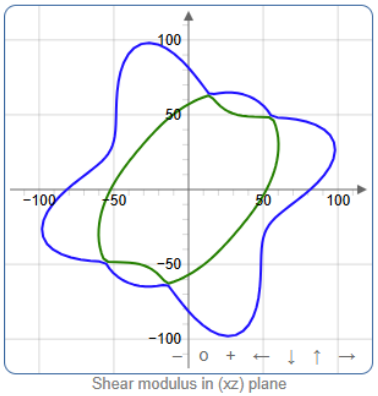
Shear modulus in (yz) plane



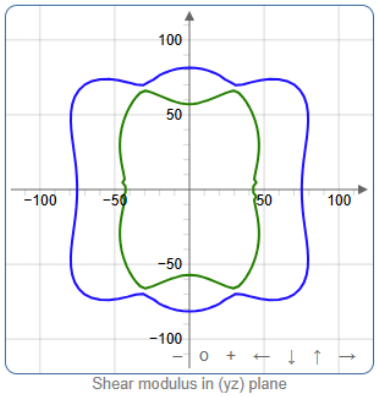
LYSO_2Y



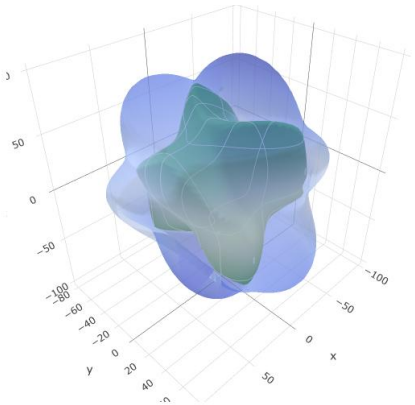
Shear modulus in (xy) plane



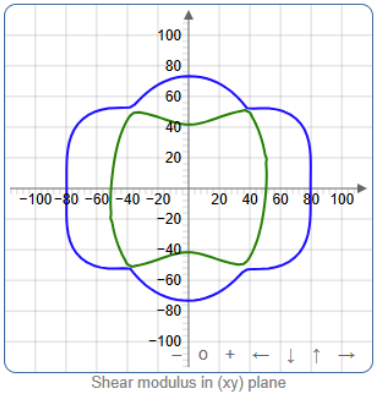
Shear modulus in (xz) plane



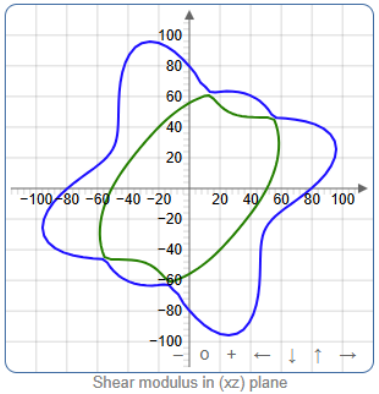
Shear modulus in (yz) plane



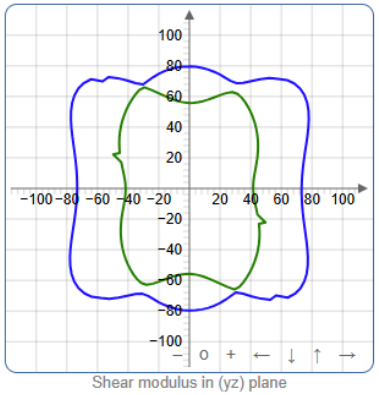
LYSO_3Y



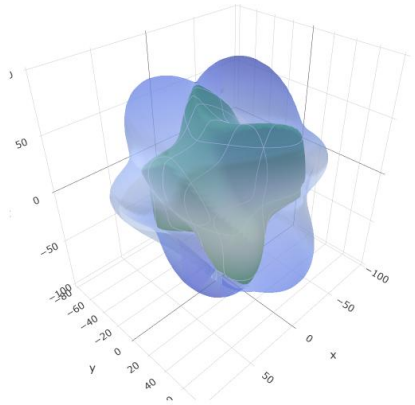
Shear modulus in (xy) plane



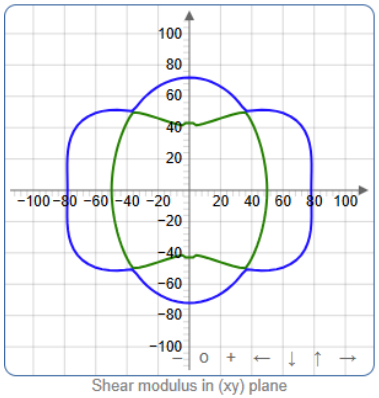
Shear modulus in (xz) plane



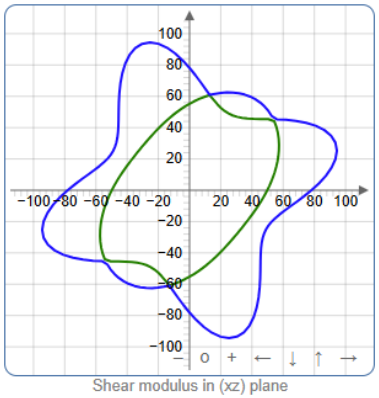
Shear modulus in (yz) plane



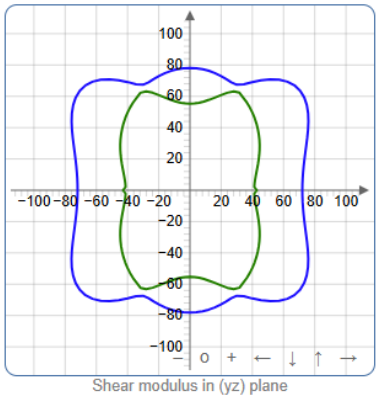
LYSO_4Y



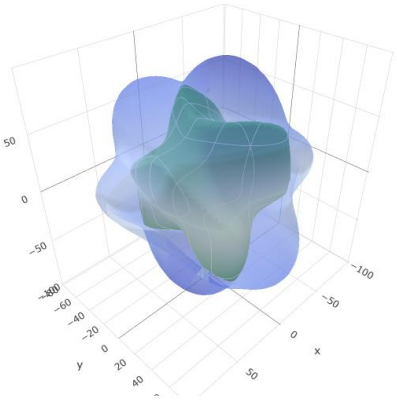
Shear modulus in (xy) plane



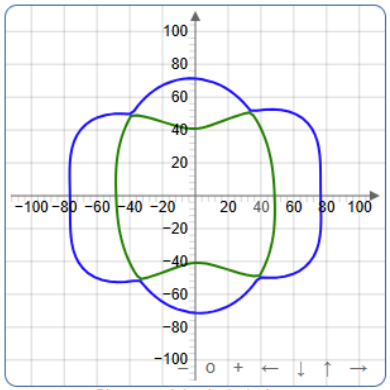
Shear modulus in (xz) plane



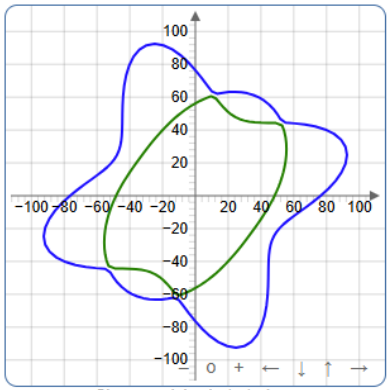
Shear modulus in (yz) plane



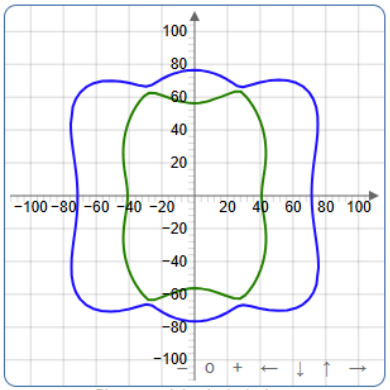
LYSO_5Y



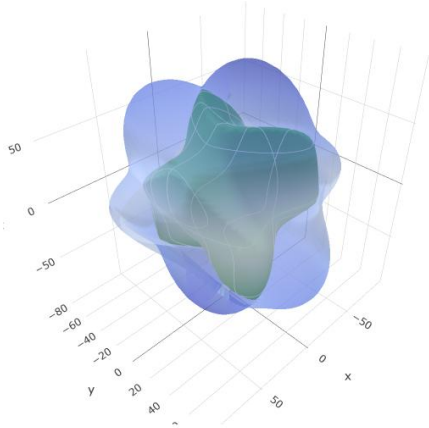
Shear modulus in (xy) plane



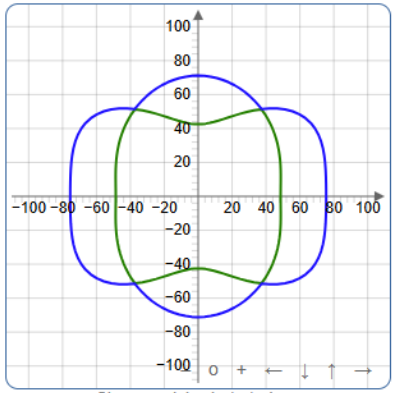
Shear modulus in (xz) plane



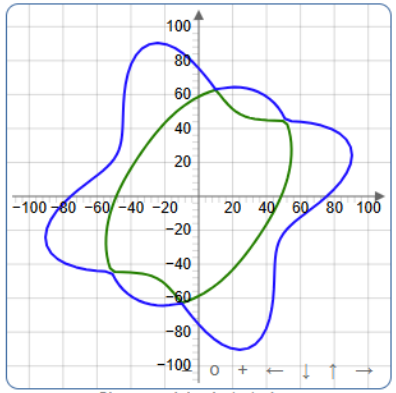
Shear modulus in (yz) plane



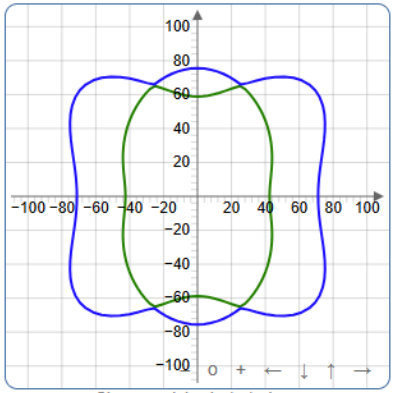
LYSO_6Y



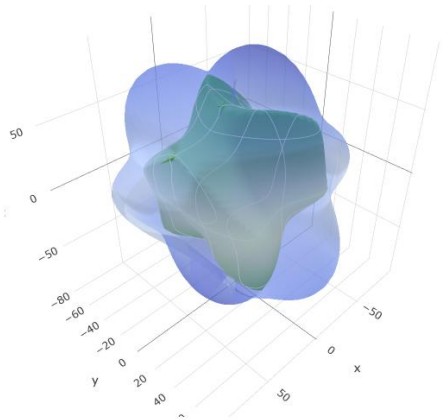
Shear modulus in (xy) plane



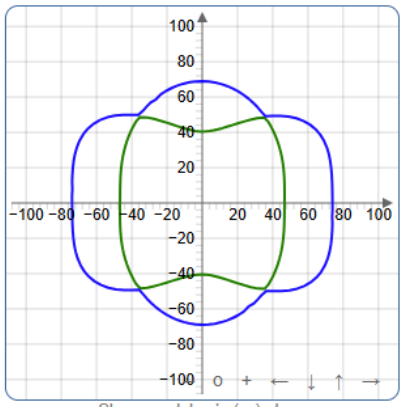
Shear modulus in (xz) plane



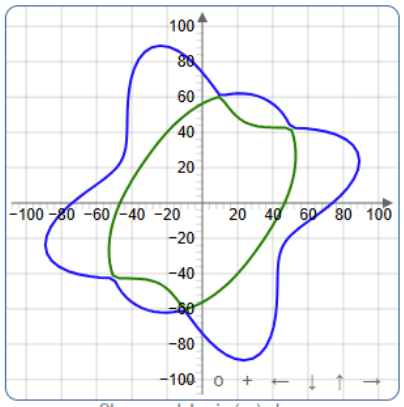
Shear modulus in (yz) plane



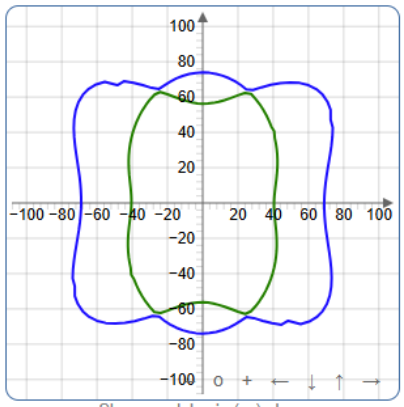
LYSO_7Y



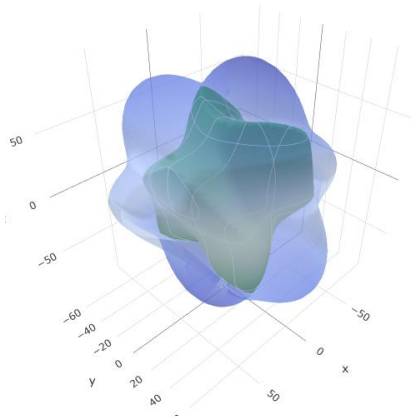
Shear modulus in (xy) plane



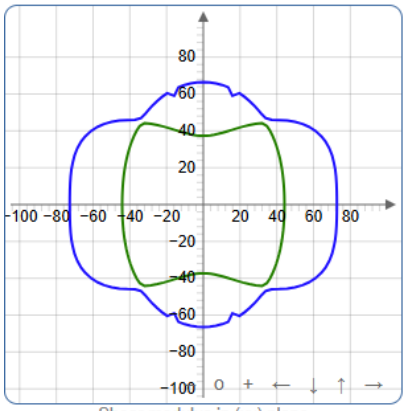
Shear modulus in (xz) plane



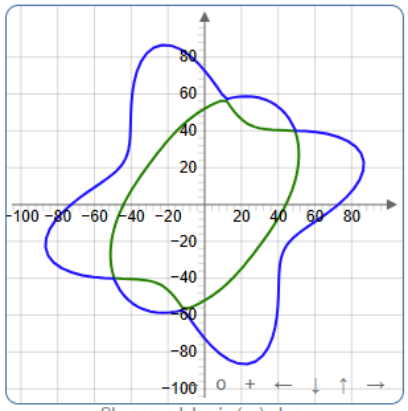
Shear modulus in (yz) plane



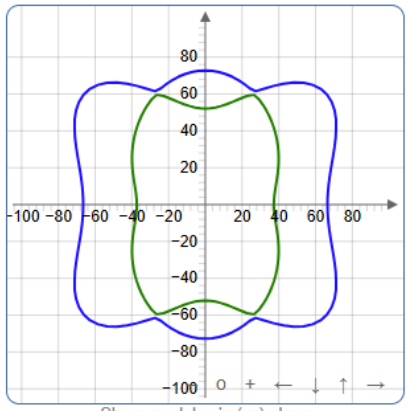
YSO



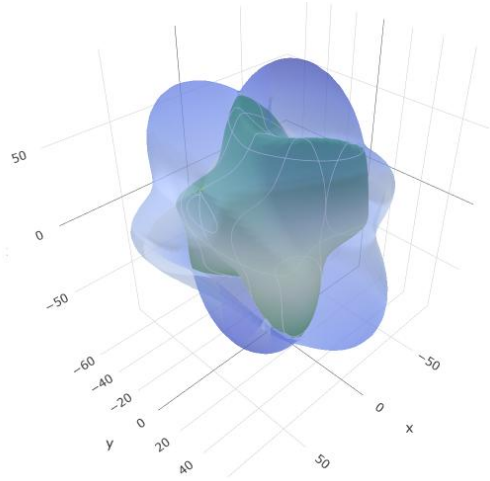
Shear modulus in (xy) plane



Shear modulus in (xz) plane

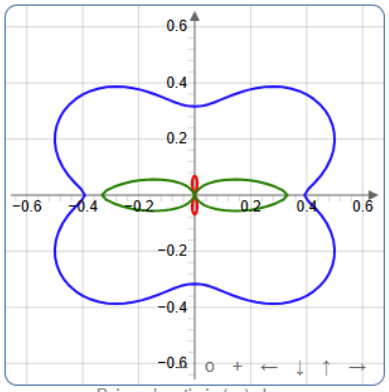


Shear modulus in (yz) plane

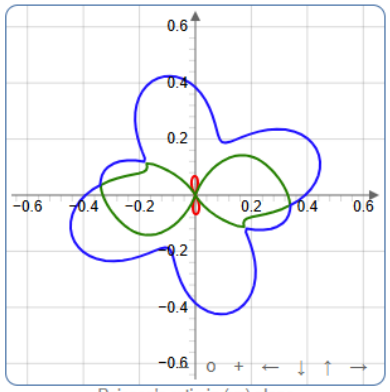


2.4. Spatial dependence of Poisson's ratio

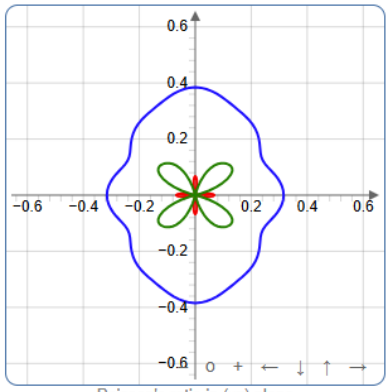
LSO



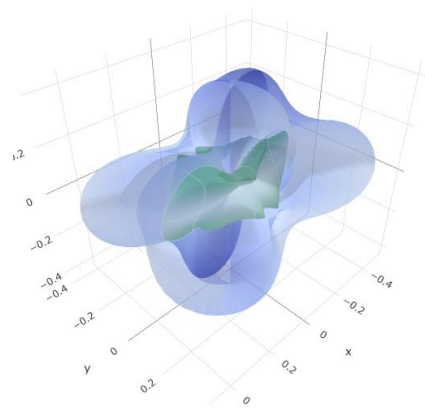
Poisson's ratio in (xy) plane



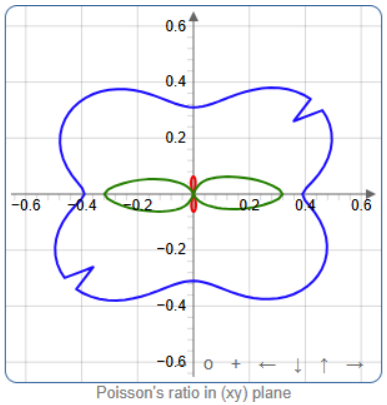
Poisson's ratio in (xz) plane



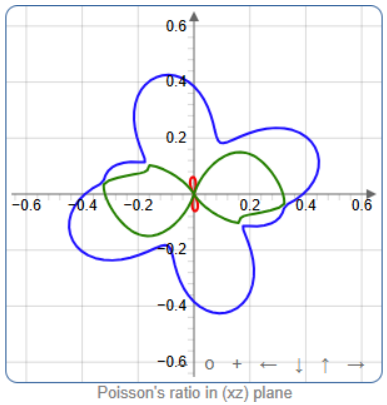
Poisson's ratio in (yz) plane



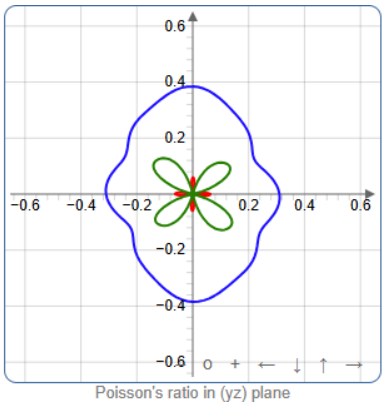
LYSO_1Y



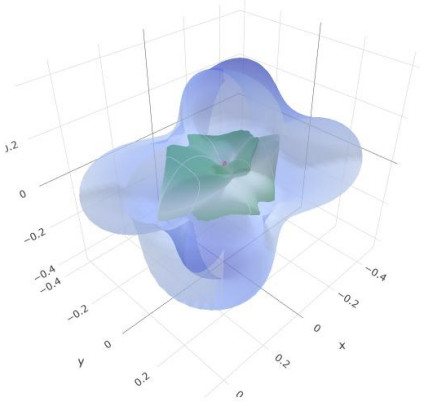
Poisson's ratio in (xy) plane



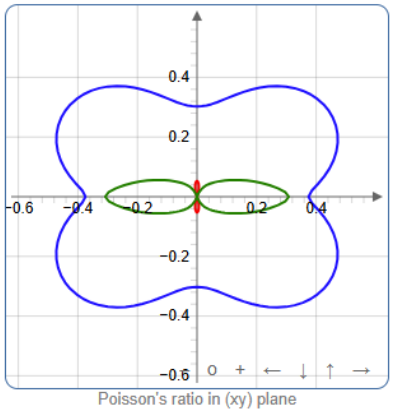
Poisson's ratio in (xz) plane



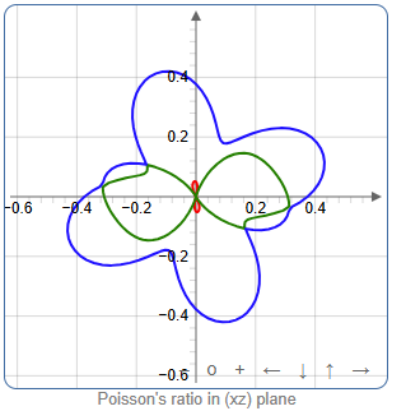
Poisson's ratio in (yz) plane



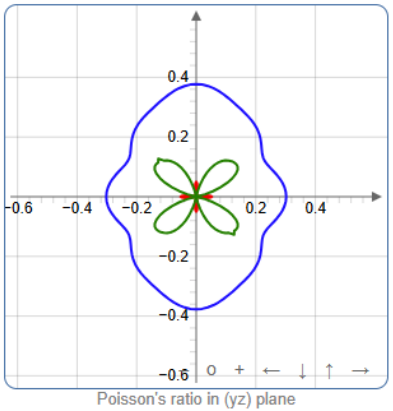
LYSO_2Y



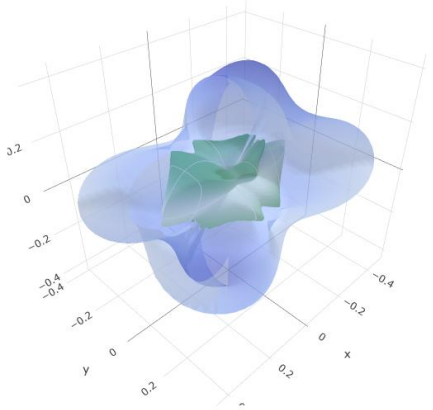
Poisson's ratio in (xy) plane



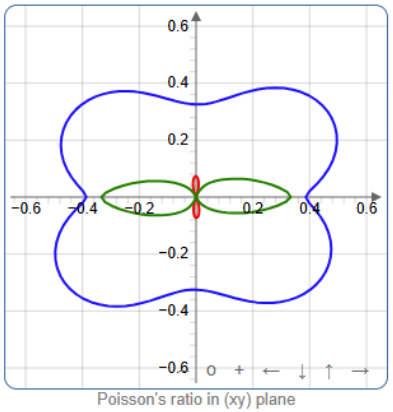
Poisson's ratio in (xz) plane



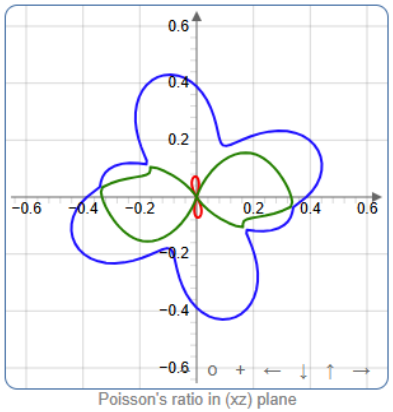
Poisson's ratio in (yz) plane



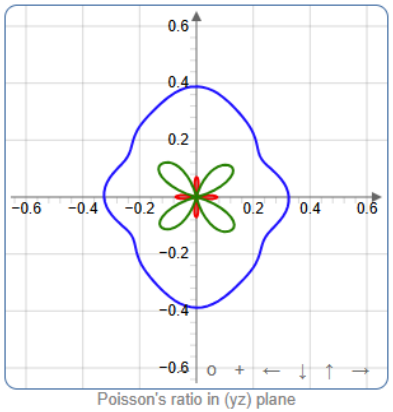
LYSO_3Y



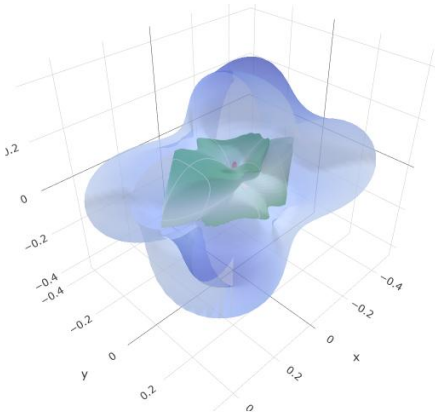
Poisson's ratio in (xy) plane



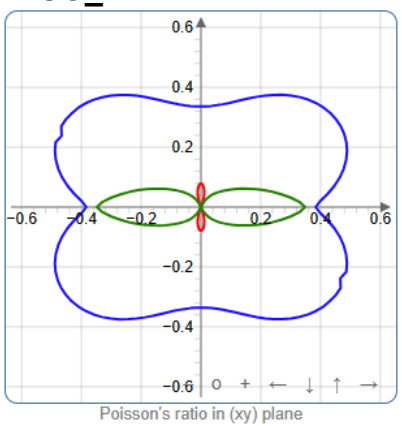
Poisson's ratio in (xz) plane



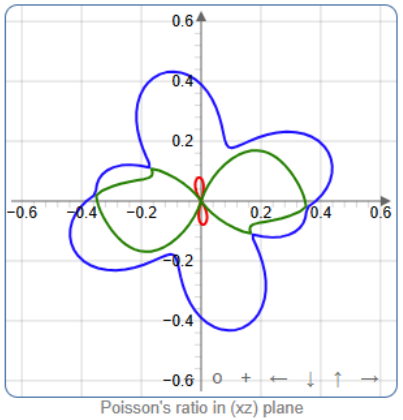
Poisson's ratio in (yz) plane



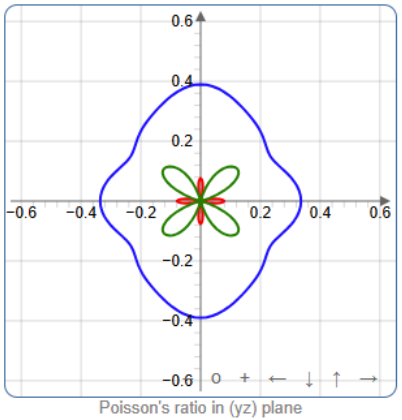
LYSO_4Y



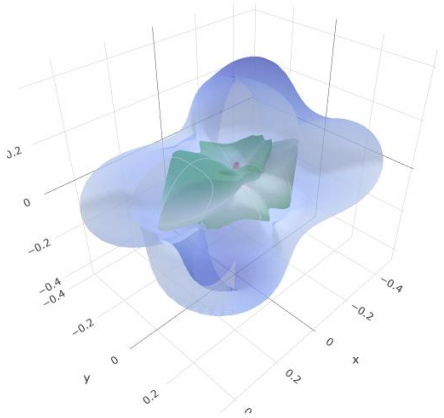
Poisson's ratio in (xy) plane



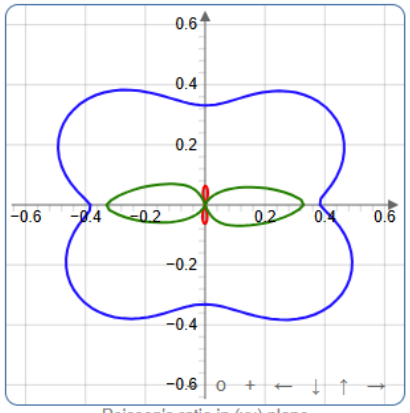
Poisson's ratio in (xz) plane



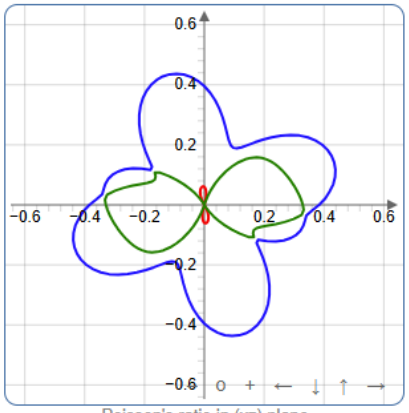
Poisson's ratio in (yz) plane



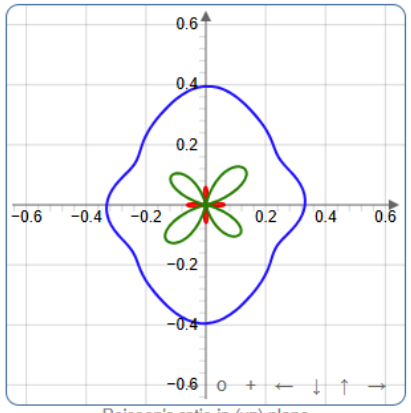
LYSO_5Y



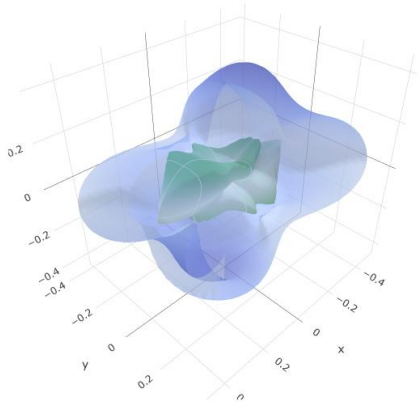
Poisson's ratio in (xy) plane



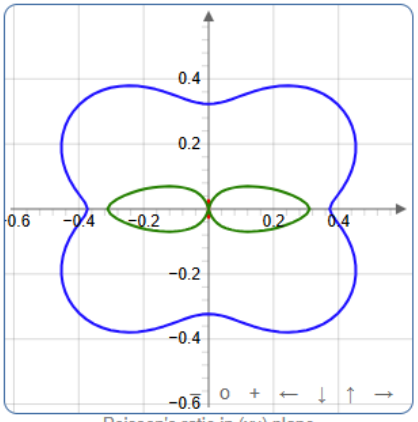
Poisson's ratio in (xz) plane



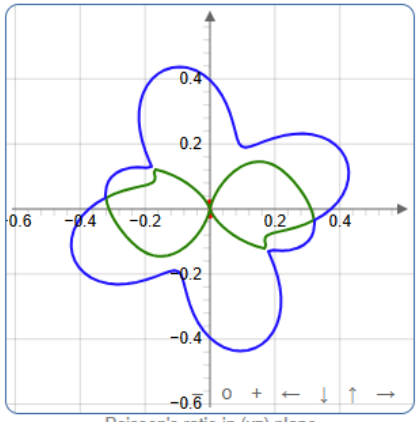
Poisson's ratio in (yz) plane



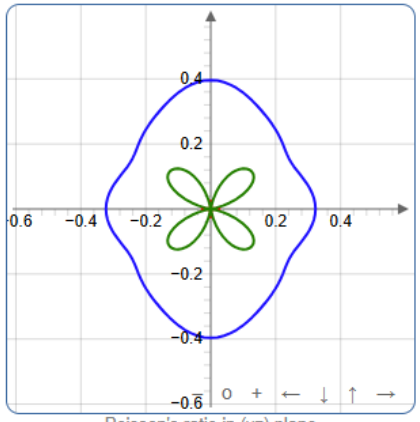
LYSO_6Y



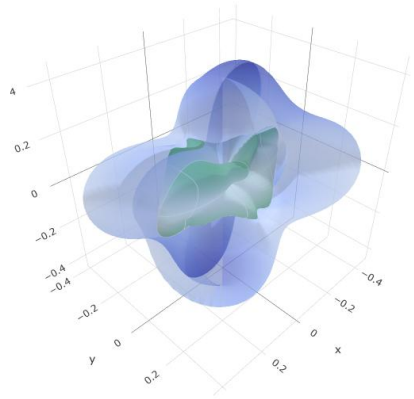
Poisson's ratio in (xy) plane



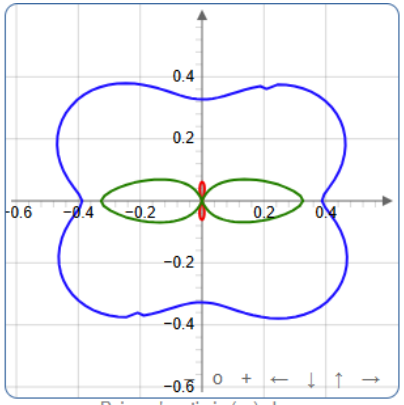
Poisson's ratio in (xz) plane



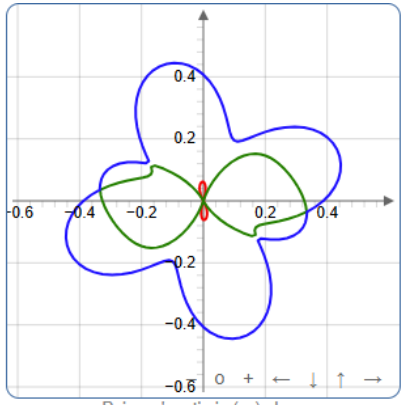
Poisson's ratio in (yz) plane



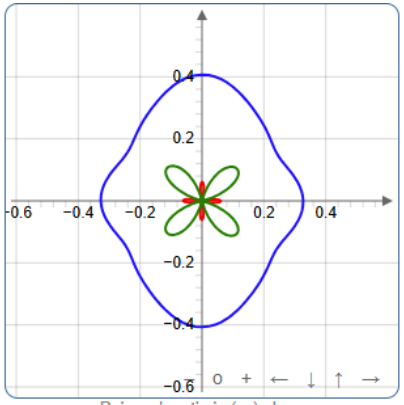
LYSO_7Y



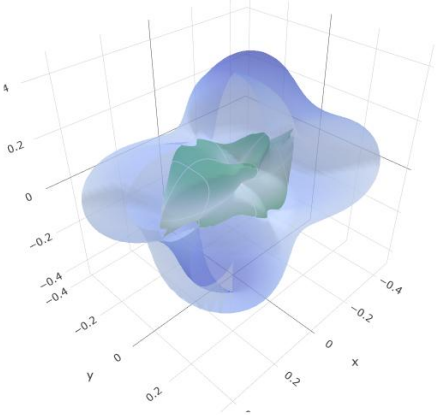
Poisson's ratio in (xy) plane



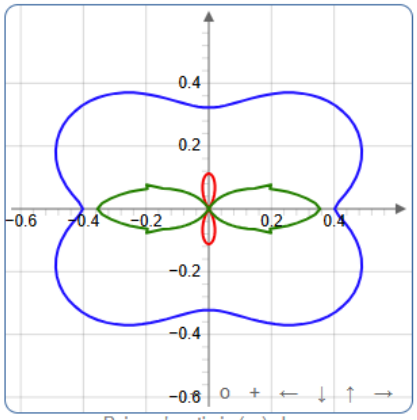
Poisson's ratio in (xz) plane



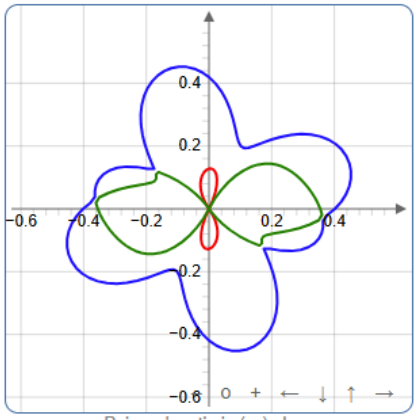
Poisson's ratio in (yz) plane



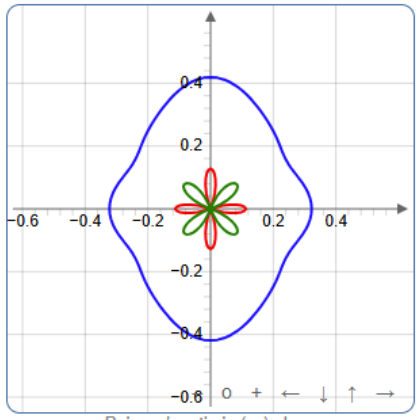
YSO



Poisson's ratio in (xy) plane



Poisson's ratio in (xz) plane



Poisson's ratio in (yz) plane

