SPINEL User Documentation

This software is written entirely in Python and has only been tested to run on macOS.

Installation

1. Ensure you have a working Python distribution installed on your machine.
2. Navigate to the following link and download a copy of the entire repository to a suitable location on your machine (a .zip file can be downloaded using the dropdown arrow next to the green "Code" button):
   https://github.com/jdmchardy/SPINEL_XRD
3. Open a terminal window and run (if you have not installed poetry previously on your machine):
   `pip install poetry` (or on windows: `py -m pip install poetry`)
4. Verify the installation with:
   ```
   poetry --version
   ```
5. In the terminal, navigate to the root folder where you saved a copy of the SPINEL Github repository on your machine.
6. Confirm you are in the right directory by running ls (dir on windows). You should see the following contents:
   ```
   logo.png
   pyproject.toml
   requirements.txt
   poetry.lock
   README.md
   SPINEL.py
   SPINEL_user_documentation.pdf
   example_files/
   ```
7. Install the necessary dependencies:
   ```
   poetry install
   ```
8. Start up the program using:
   ```
   poetry run streamlit run SPINEL.py
   ```

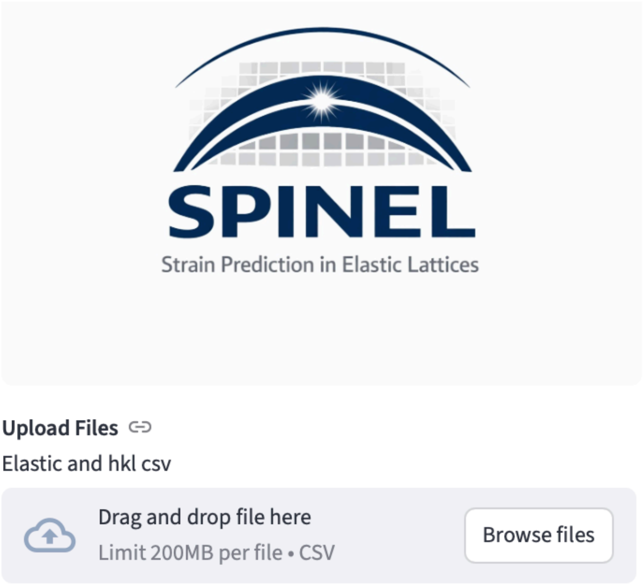
Overview

SPINEL computes the deviatoric strain normal to a set of diffraction planes resulting from a macroscopic uniaxial stress field for cubic, hexagonal and tetragonal crystal systems.

Details of the theoretical models can be found in Uchida *et al*. [https://doi.org/10.1063/1.362920] and Funamori *et al*. [https://doi.org/10.1063/1.365792].

Startup

1. Successful startup will launch the following window in your browser



Upload Files

Elastic and hkl csv

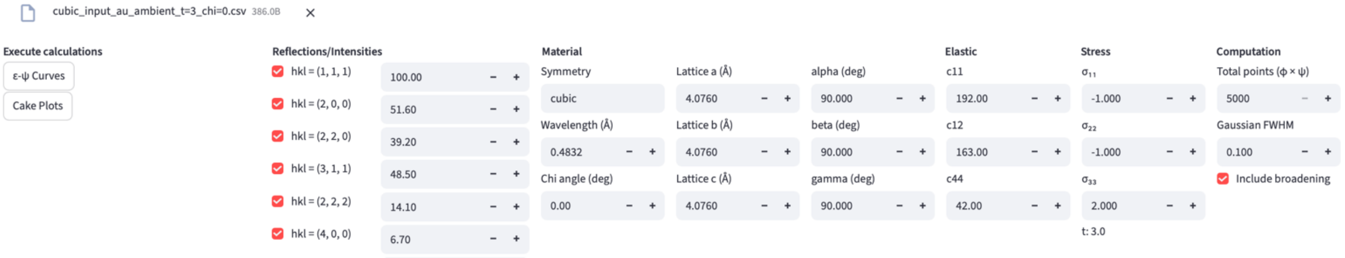
Drag and drop file here

Limit 200MB per file • CSV

Browse files

2. Upload a .csv file from one of the example files or one your have modified for your simulation. The meta data will be imported and displayed on screen.

The imported values can be adjusted and the hkl reflections included can be toggled on and off.



cubic_input_au_ambient_t=3_chi=0.csv 386.0B ×

Execute calculations

ε-ψ Curves

Cake Plots

Reflections/Intensities

☑ hkl = (1, 1, 1) 100.00 − +

☑ hkl = (2, 0, 0) 51.60 − +

☑ hkl = (2, 2, 0) 39.20 − +

☑ hkl = (3, 1, 1) 48.50 − +

☑ hkl = (2, 2, 2) 14.10 − +

☑ hkl = (4, 0, 0) 6.70 − +

Material

Symmetry: cubic

Wavelength (Å): 0.4832

Chi angle (deg): 0.00

Lattice a (Å): 4.0760

Lattice b (Å): 4.0760

Lattice c (Å): 4.0760

alpha (deg): 90.000

beta (deg): 90.000

gamma (deg): 90.000

Elastic

c11: 192.00

c12: 163.00

c44: 42.00

Stress

σ_{11}: -1.000

σ_{22}: -1.000

σ_{33}: 2.000

t: 3.0

Computation

Total points (ϕ × ψ): 5000

Gaussian FWHM: 0.100

☑ Include broadening

Simulation Options

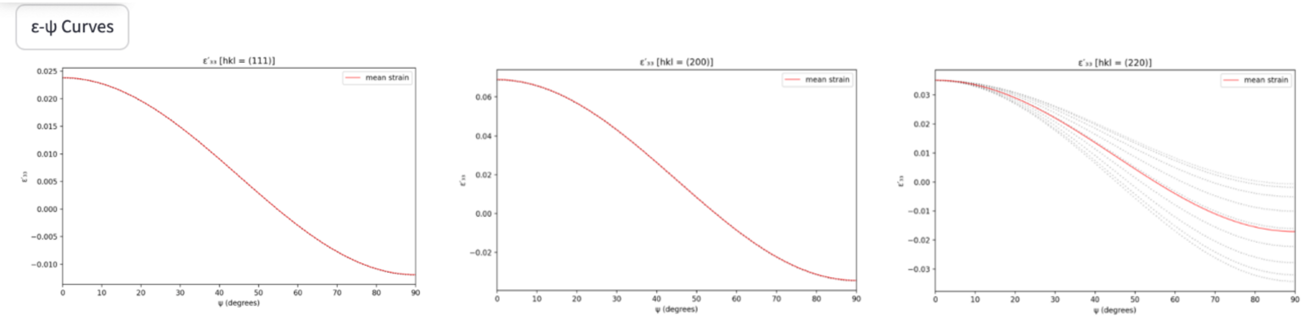
1. Current permissible crystal symmetry options are:
   - cubic (space group #195-230),
   - hexagonal (space group #195-230),
   - tetragonal_A (space group #89-142),
   - tetragonal_B (space group #75-88)
2. chi angle (deg): the angle between compression axis and x-ray axis (0° = axial, 90° = radial)
3. elastic constants and stress component units - (GPa)
4. The uniaxial stress component ($t = \sigma_{33}-\sigma_{11}$) is displayed below the stress parameters
5. Total points (φ x ψ): the number of points at which to evaluate the stress at (φ ranges from 0 to 360° and ψ between 0 to 90°)
6. Gaussian FWHM: the width of the peak shape used for each crystallite orientation contribution in 2th degrees
7. Include broadening: toggles the effects of broadening on the XRD and cake plots. With broadening off, all peaks have equal FWHM but are displaced from the ideal lattice sites based on the magnitude of t. The peak positions are computed from the mean strain across contributing orientations. In axial geometry (chi = 0), broadening off yields results equivalent to the Singh formalism.

Output

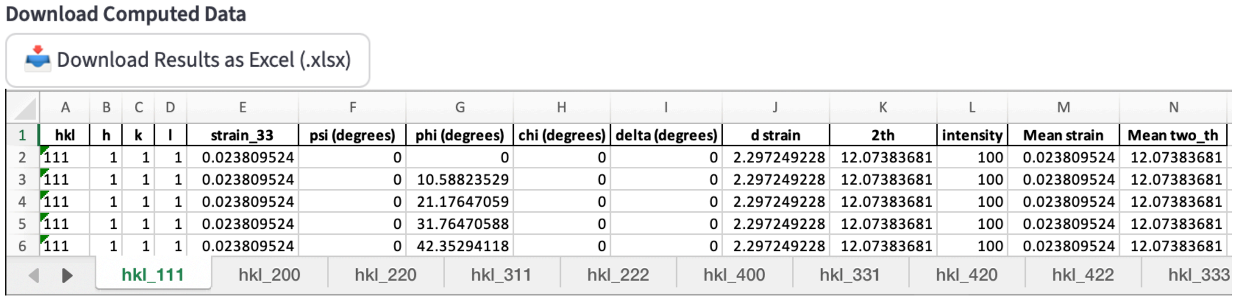
Once the simulations parameters are set, several calculations are possible:

1. ε-ψ Curves

Generates a series of plots (one per hkl reflection) showing the deviatoric strain distribution over all crystal orientations. The point density for these simulations is controlled by Total points (φ x ψ).



All calculated values are downloadable beneath the plots as an excel file.



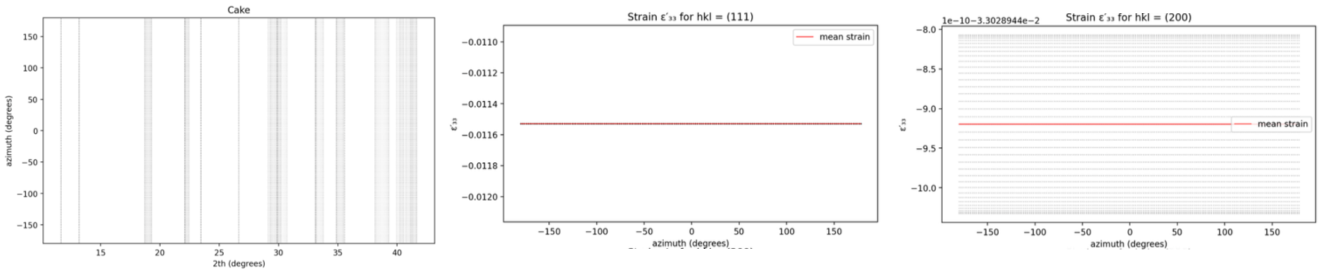
Download Computed Data

	A	B	C	D	E	F	G	H	I	J	K	L	M	N
1	hkl	h	k	l	strain_33	psi (degrees)	phi (degrees)	chi (degrees)	delta (degrees)	d strain	2th	intensity	Mean strain	Mean two_th
2	111	1	1	1	0.023809524	0	0	0	0	2.297249228	12.07383681	100	0.023809524	12.07383681
3	111	1	1	1	0.023809524	0	10.58823529	0	0	2.297249228	12.07383681	100	0.023809524	12.07383681
4	111	1	1	1	0.023809524	0	21.17647059	0	0	2.297249228	12.07383681	100	0.023809524	12.07383681
5	111	1	1	1	0.023809524	0	31.76470588	0	0	2.297249228	12.07383681	100	0.023809524	12.07383681
6	111	1	1	1	0.023809524	0	42.35294118	0	0	2.297249228	12.07383681	100	0.023809524	12.07383681

Results are separated on different tabs by hkl and one row is given per (φ , ψ) pairing. Mean strain and mean 2th are evaluated for each unique ψ-value.

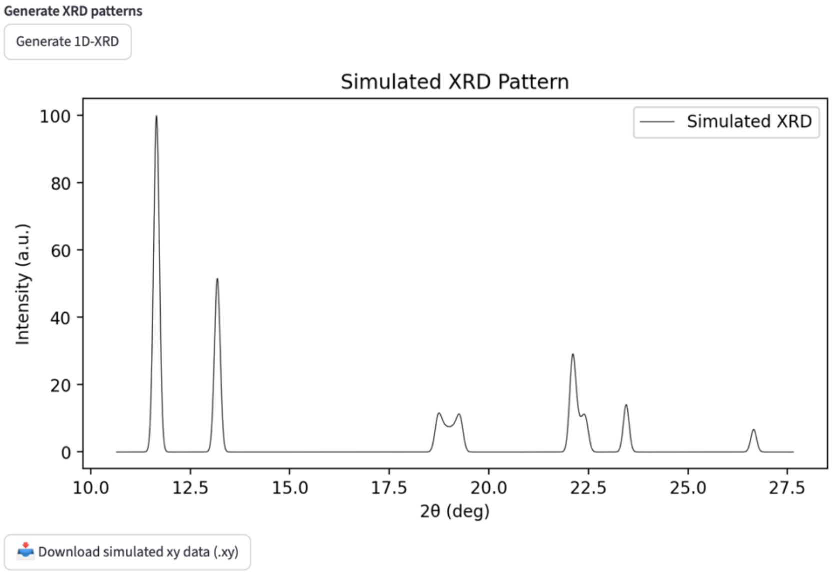
2. Cake plots

Iterates over azimuth (delta) and phi to evaluate only the (φ , ψ) pairings contributing to the x-ray diffraction (XRD) pattern. For each hkl, ψ is evaluated using the list of azimuth values, chi input, and theta (Bragg angle for each hkl). A 'cake' plot of azimuth vs. 2th is generated as well as individual strain vs 2th curves for each reflection. Again, calculation results may be downloaded as .xlsx files.



3. Generate 1D-XRD

Contributions from all incorporated orientations are combined to simulate an XRD pattern. The pattern is constructed by convoluting a Gaussian kernal with a histogram of weighted contributions in 2th. The contributions are weighted by the specified peak intensity. Simulated patterns can be downloaded as .xy files of 2th coordinate vs intensity.


Generate XRD patterns
Generate 1D-XRD
Simulated XRD Pattern
Simulated XRD
Intensity (a.u.)
0
20
40
60
80
100
10.0
12.5
15.0
17.5
20.0
22.5
25.0
27.5
2θ (deg)
Download simulated xy data (.xy)