

User Guide

AnisEulerSC

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Research paper:

AnisEulerSC: A MATLAB program combined with MTEX for modeling the anisotropic seismic properties of a polycrystalline aggregate with microcracks using self-consistent approximation

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1. Introduction

1.1. AnisEulerSC

AnisEulerSC is a MATLAB-based program developed for calculating the elastic stiffness tensor of polycrystalline materials based on the self-consistent (SC) approximation.

AnisEulerSC requires input data of a polycrystalline aggregate. The AnisEulerSC-Inputs program generates the input data to run the AnisEulerSC program. For the analysis of crystallographic textures of minerals, several MTEX commands are used.

1.1.1. AnisEulerSC-Inputs

AnisEulerSC-Inputs is a MATLAB-based program with graphical user interfaces (GUIs) and developed for generating the input data of the AnisEulerSC program. Using AnisEulerSC-Inputs, the composition of a polycrystalline aggregate, the volume fractions of constituent phases, and the shapes and orientations of grains can be specified. AnisEulerSC-Inputs is designed using MATLAB (R2019a) App Designer in Mac OS X. The AnisEulerSC-Inputs and AnisEulerSC programs run in the MATLAB version after R2016b in Windows or UNIX OS.

1.1.2. MTEX commands

To import, analyze and export crystallographic textures data from experimental measurements (e.g., EBSD; electron backscatter diffraction), several commands of MTEX, which is a free MATLAB toolbox for analyzing crystallographic textures (Hielscher and Schaeben, 2008), are used. For details, visit <http://mTEX-toolbox.github.io/>.

2. Practical usage

2.1. What is your target material?

We consider lherzolite, which is a type of ultramafic igneous rock, to make a polycrystalline aggregate using the SC approximation. A target rock sample is a low-cpx lherzolite, which is one of the spinel peridotite xenoliths from the Tok volcanic field in SE Siberia (Tommasi et al., 2008). Based on EBSD data of a rock sample 9510-16 (Tommasi et al., 2008), the crystallographic textures of constituent minerals are analyzed using MTEX commands. You can find a description of the installation of MTEX toolbox on the homepage (<https://mtex-toolbox.github.io/download>). Download an updated version of MTEX toolbox (e.g., mtex-5.3) and initialize MTEX as follows.

```
>> startup_mtex
initialize MTEX 5.3 .... done!

MTEX 5.3 (show documentation)
Import pole figure data
Import EBSD data
Import ODF data

Uninstall MTEX
```

Visit MTEX homepage (<https://mtex-toolbox.github.io/EBSDImport.html>) for more information on how to import, analyze, and export EBSD data. Create an EBSD variable containing the data using MTEX commands and load the data. This lherzolite sample mainly consists of three indexed phases of forsterite (62%), enstatite (11%), and diopside (3.7%) and not-indexed phases (24%) as follows.

```

>> ebsd
ebsd = EBSD \(show methods, plot\)

Phase Orientations Mineral Color Symmetry Crystal reference frame
 0 58485 (24%) notIndexed
 1 152345 (62%) Forsterite LightSkyBlue mmm
 2 26058 (11%) Enstatite Opx AV77 DarkSeaGreen mmm
 3 9064 (3.7%) Diopside CaMgSi2O6 Goldenrod 12/m1 X||a*, Y||b, Z||c

Properties: bands, bc, bs, error, mad, x, y
Scan unit : um

```

Let us consider only indexed phases of forsterite, enstatite, and diopside to make a polycrystalline material.

```

>> ebsd('indexed')
ans = EBSD \(show methods, plot\)

Phase Orientations Mineral Color Symmetry Crystal reference frame
 1 152345 (81%) Forsterite LightSkyBlue mmm
 2 26058 (14%) Enstatite Opx AV77 DarkSeaGreen mmm
 3 9064 (4.8%) Diopside CaMgSi2O6 Goldenrod 12/m1 X||a*, Y||b, Z||c

Properties: bands, bc, bs, error, mad, x, y
Scan unit : um

```

Once EBSD data is imported into MTEX, the grain properties (e.g., shape and orientation) can be analyzed. A script of ‘Demo_MTEX_Flexible_Data_Export_Lherzolite.m’, provided together with the AnisEulerSC program, is used to extract the grain properties of a lherzolite sample. This script runs several sections that contain loading EBSD variable data, grain modeling protocol, and plotting/exporting grain data. As a result, EBSD variable data is reconstructed from selected grains for only indexed phases. For SC modeling, a polycrystalline aggregate is assumed to be composed of 83% forsterite, 14% enstatite, and 3% diopside as follows.

```

>> ebsd

ebsd = EBSD (show methods, plot)

Phase Orientations Mineral Color Symmetry Crystal reference frame
 1 150658 (83%) Forsterite LightSkyBlue mmm
 2 25078 (14%) Enstatite Opx AV77 DarkSeaGreen mmm
 3 6583 (3.6%) Diopside CaMgSi2O6 Goldenrod 12/m1 X||a*, Y||b, Z||c

Properties: bands, bc, bs, error, mad, x, y, grainId, mis2mean
Scan unit : um

```

As outputs of the script, the data of grain shapes and orientations (Euler angles) are also extracted to text files as follows.

Table 1. Output files of grain analysis for lherzolite EBSD data.

Mineral	Grain analysis data file	Grain Euler angles and volume fraction file
Forsterite	Forsterite_Demo_export.txt	Forsterite_EulerVf.txt
Enstatite	Enstatite_Demo_export.txt	Enstatite_EulerVf.txt
Diopside	Diopside_Demo_export.txt	Diopside_EulerVf.txt

The files named *_Demo_export.txt contain the Euler angles (phi1, PHI, phi2), the area fraction, the angle of long-axis to X-axis (omega), the long- and short-axis lengths (a and b, respectively). The files named *_EulerVf.txt contain only the Euler angles (phi1, PHI, phi2) and the area fraction, which are required to calculate SC approximation. Using these output files, the grain shapes and orientations can be analyzed, visualized, and used as input parameters for SC modeling.

2.2. How to use AnisEulerSC-Inputs

To generate the input data for SC modeling, AnisEulerSC-Inputs program is used. In this section, the construction of a polycrystalline aggregate composed of 83% forsterite, 14% enstatite, and 3% diopside (as described in Section 2.1) and the preparation of input

parameters for SC modeling are described using the AnisEulerSC-Inputs program. To run the program, type AnisEulerSC-Inputs into the MATLAB command window.

```
>> AnisEulerSC_Inputs
```

2.2.1. Setup tab

- Specify the input and output directories as well as the title that is used for the output file name.

AnisEulerSC path	/Users/ekim/Documents/MATLAB/AnisEulerSC/
*Note: e.g., /Users/ekim/	
Title	AnisEulerSC_Example_Lherzolite _Inputs_ModelSC.mat
*Note: Input parameters are stored in a file named 'Title'_Inputs_ModelSC.mat	
<input type="button" value="Load file"/>	

Note: If the file named as 'Title'_Inputs_ModelSC.mat exists in the AnisEulerSC path, you can load data by clicking 'Load file'. If it does not exist, the file is created.

- Select the type of SC scheme.

SC scheme	1 = Mechanical – Willis 1977 (most stable)
	2 = Scattering – Gubernatis & Krumhansl 1975

Note: A mechanical approach given by Willis (1977) for statistically uniform composites with several phases of inclusions is most stable. A scattering approach given by Gubernatis and Krumhansl (1975) is a perturbation method based on quantum mechanical scattering theory (see Mainprice (1997) for details).

- Select the initial value for SC scheme.

Initial value for SC scheme	1 = Voigt (best when fluids present)
	2 = Reuss
	3 = Voigt-Reuss-Hill

- Select the format of Euler file.

Format of Euler file	1 = phi1, PHI, phi2
	2 = no, phi1, PHI, phi2
	3 = phi1, PHI, phi2, volume fraction
	4 = no, phi1, PHI, phi2, volume fraction

- Select the origin of Euler file.

Origin of Euler file	1 = Universal stage (UMII)
	2 = EBSD (Channel+)

- Specify Xs of azimuth (in range 0 to 360 degrees).

Xs of azimuth (in range 0 to 360 degrees)	0
---	---

- Specify maximum values required to calculate SC scheme.

Maximum number of SC iterations (e.g., 40)	40
Maximum error (%) for Green's tensor (e.g., 0.1)	0.1
Maximum error (%) for SC convergence (e.g., 0.1)	0.1

Save

Clear

Note: Click ‘Save’ button to store all properties of a current phase in the data file (e.g., ‘Title’_Inputs_ModelSC.mat). To clean the data for the current phase, click ‘Clear’ button.

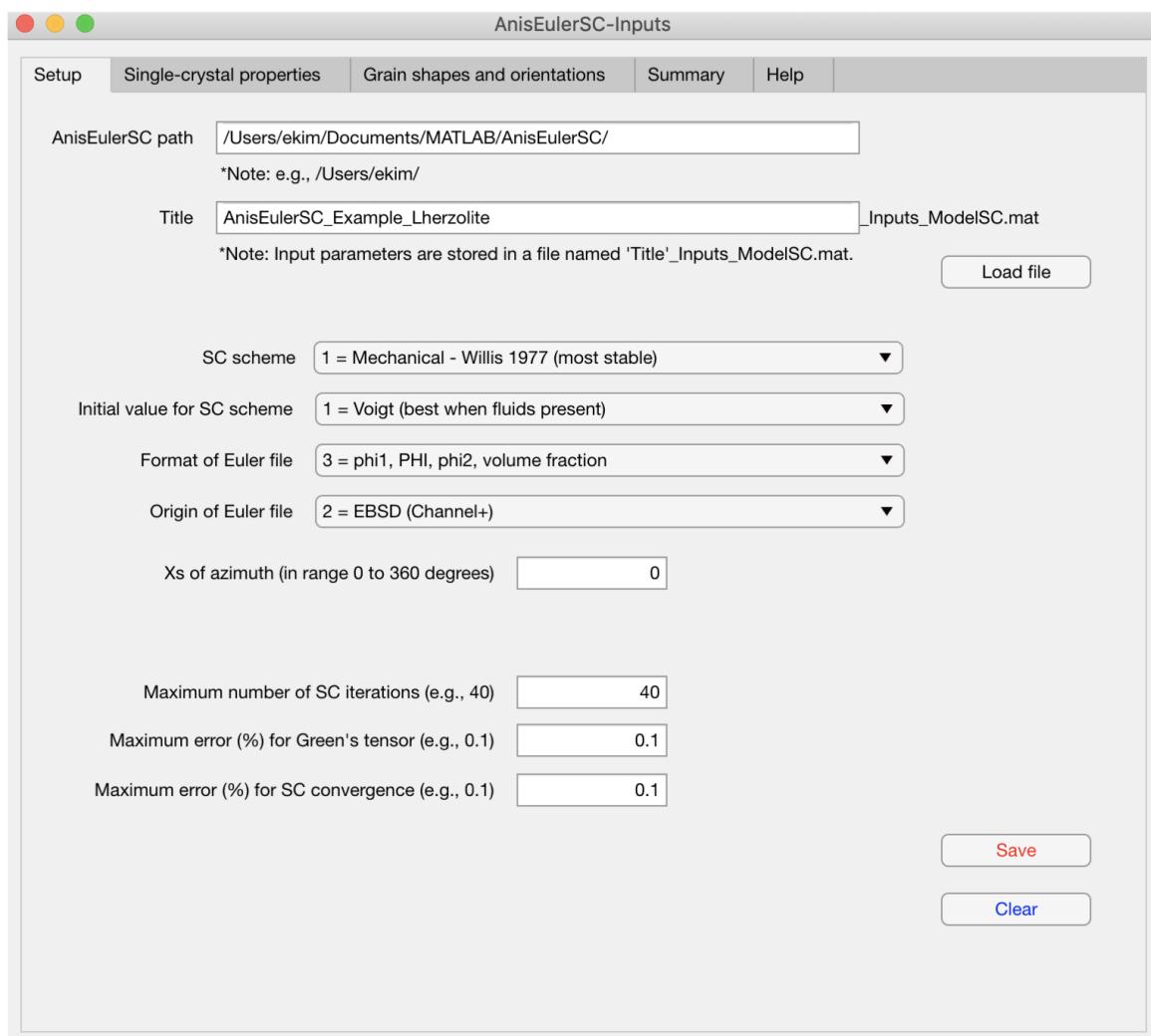


Figure U1. Setup tab of AnisEulerSC-Inputs, a MATLAB-based program composed of graphical user interfaces (GUIs).

2.2.2. Single-crystal properties tab

- Specify the total number of phases.

How many phases? 3

- Specify the single-crystal properties for the first phase, **Forsterite** (Isaak et al., 1989; Tommasi et al., 2008), on the ‘Phase’ panel.

No.	Name	Volume fraction		
1	Forsterite	0.83		
Reference	Isaak et al. (1989); Tommasi et al. (2008)			
Density (g/cm ³)	3.221			
Crystal symmetry	mmm			
Crystal reference frame	XIIa, ZIIc			
Crystal coordinate system	a 4.8 alpha 90	b 10 beta 90	c 6 gamma 90	
Single-crystal elastic stiffness tensor in Voigt matrix, C _{ij} (GPa)				
328	69	69	0	0
	200	73	0	0
		235	0	0
			66.7	0
				81.3
				80.9
<input style="background-color: red; color: white; width: 100px; height: 25px; float: right; margin-right: 10px;" type="button" value="Save"/> <input style="background-color: blue; color: white; width: 100px; height: 25px; float: right; margin-right: 10px;" type="button" value="Clear phase"/>				
Name:	Forsterite	Load		

Note: Click ‘Save’ button to store all properties of a phase in the data file (e.g., ‘Title’_Inputs_ModelSC.mat). To specify for the next phase, click ‘Clear phase’ button. To load the saved phase, type the phase name and click ‘Load’ button.

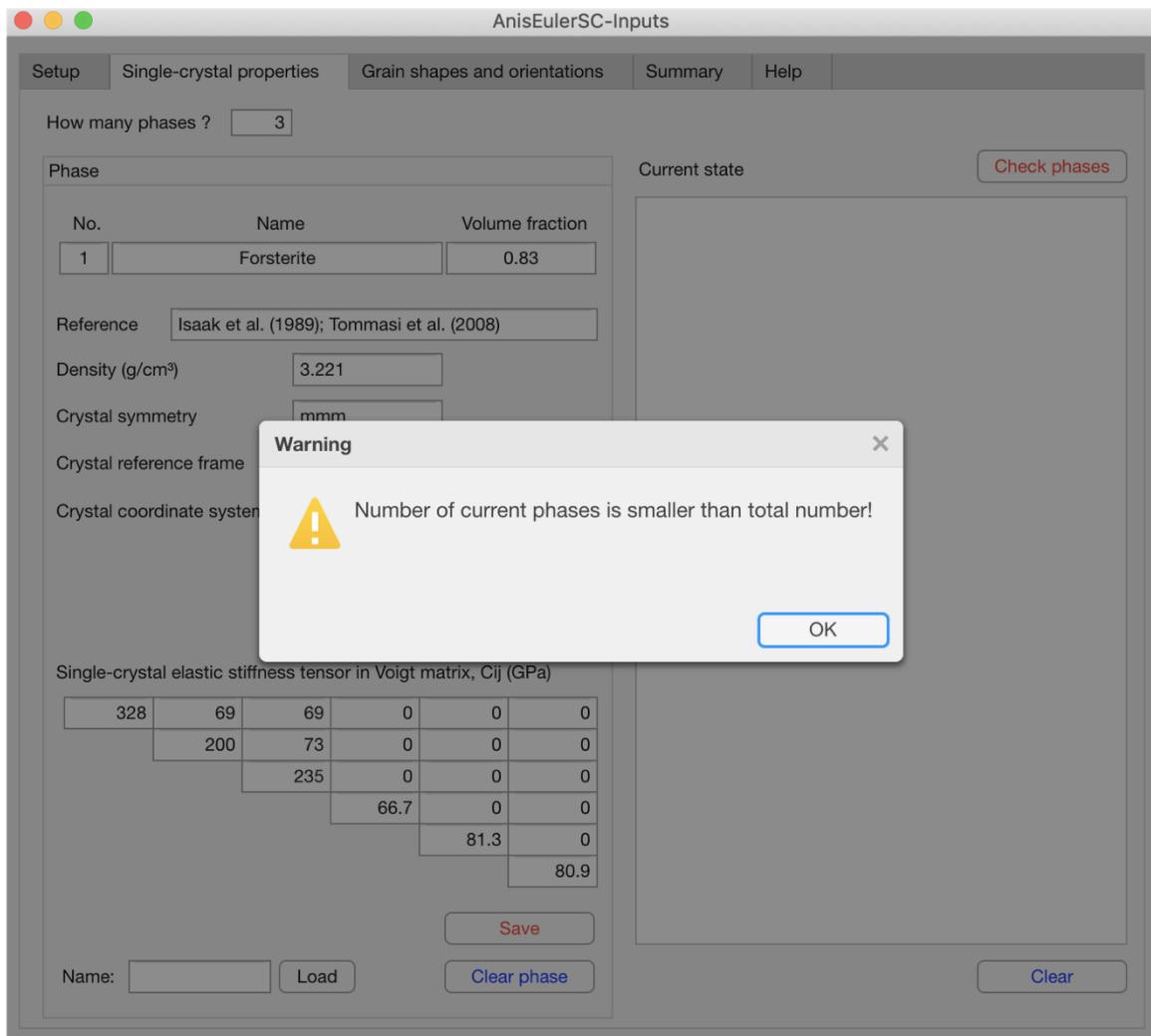


Figure U2. Pop-up message for warning showing that the number of current phases is smaller than the total number specified in advance. Click ‘OK’ to move onto the next phase.

- Check the single-crystal properties of current phases stored in the data file.

Current state	Check phases
No. 1 Forsterite	
Volume fraction: 0.83	
Reference: Isaak et al. (1989); Tommasi et al. (2008)	
Density: 3.2210 (g/cm ³)	
Crystal symmetry: mmm	
Crystal reference frame: Xlla, Zllc	
Crystal coordinate system:	
[a,b,c] = [4.8,10,6]	
[alpha,beta,gamma] = [90,90,90]	
	Clear

Note: Check that all phases are correctly specified. If ‘Check phases’ button is clicked, the single-crystal properties for all phases stored in the data file are printed on ‘Current state’ screen. It is recommended to check each phase just after saving information for each phase before moving onto the next phase. Use ‘Clear’ button to clean ‘Current state’ screen.

AnisEulerSC-Inputs

Setup Single-crystal properties Grain shapes and orientations Summary Help

How many phases ?

Phase			Current state		
No.	Name	Volume fraction			
1	Forsterite	0.83			
Reference Isaak et al. (1989); Tommasi et al. (2008)					
Density (g/cm ³) 3.221					
Crystal symmetry mmm					
Crystal reference frame X a, Z c					
Crystal coordinate system			a 4.8	b 10	c 6
			alpha 90	beta 90	gamma 90
Single-crystal elastic stiffness tensor in Voigt matrix, Cij (GPa)					
328	69	69	0	0	0
200	73		0	0	0
	235		0	0	0
		66.7		0	0
			81.3		0
					80.9
<input type="button" value="Save"/>					
Name: <input type="text"/>	<input type="button" value="Load"/>	<input type="button" value="Clear phase"/>	<input type="button" value="Clear"/>		

Figure U3. Single-crystal properties tab of AnisEulerSC-Inputs. For the first phase (forsterite), all input data are specified, saved and checked on the ‘Current state’ screen.

- Specify the single-crystal properties for the second phase, Enstatite (Chai et al., 1997; Tommasi et al., 2008), on the ‘Phase’ panel.

No.	Name	Volume fraction		
2	Enstatite	0.14		
Reference	Chai et al. (1997); Tommasi et al. (2008)			
Density (g/cm ³)	3.306			
Crystal symmetry	mmm			
Crystal reference frame	XIIa, ZIIc			
Crystal coordinate system	a 18 alpha 90	b 8.8 beta 90	c 5.2 gamma 90	
Single-crystal elastic stiffness tensor in Voigt matrix, C _{ij} (GPa)				
236.9	79.6	63.2	0	0
	180.5	56.8	0	0
		230.4	0	0
			84.3	0
				79.4
				80.1
<input style="background-color: red; color: white; width: 100px; height: 25px; font-weight: bold; margin-bottom: 5px;" type="button" value="Save"/> <input style="width: 100px; height: 25px; font-weight: bold;" type="button" value="Clear phase"/>				
Name:	Enstatite	Load		

Note: Click ‘Save’ button to store all properties of a phase in the data file (e.g., ‘Title’_Inputs_ModelSC.mat). To specify for the next phase, click ‘Clear phase’ button. To load the saved phase, type the phase name and click ‘Load’ button.

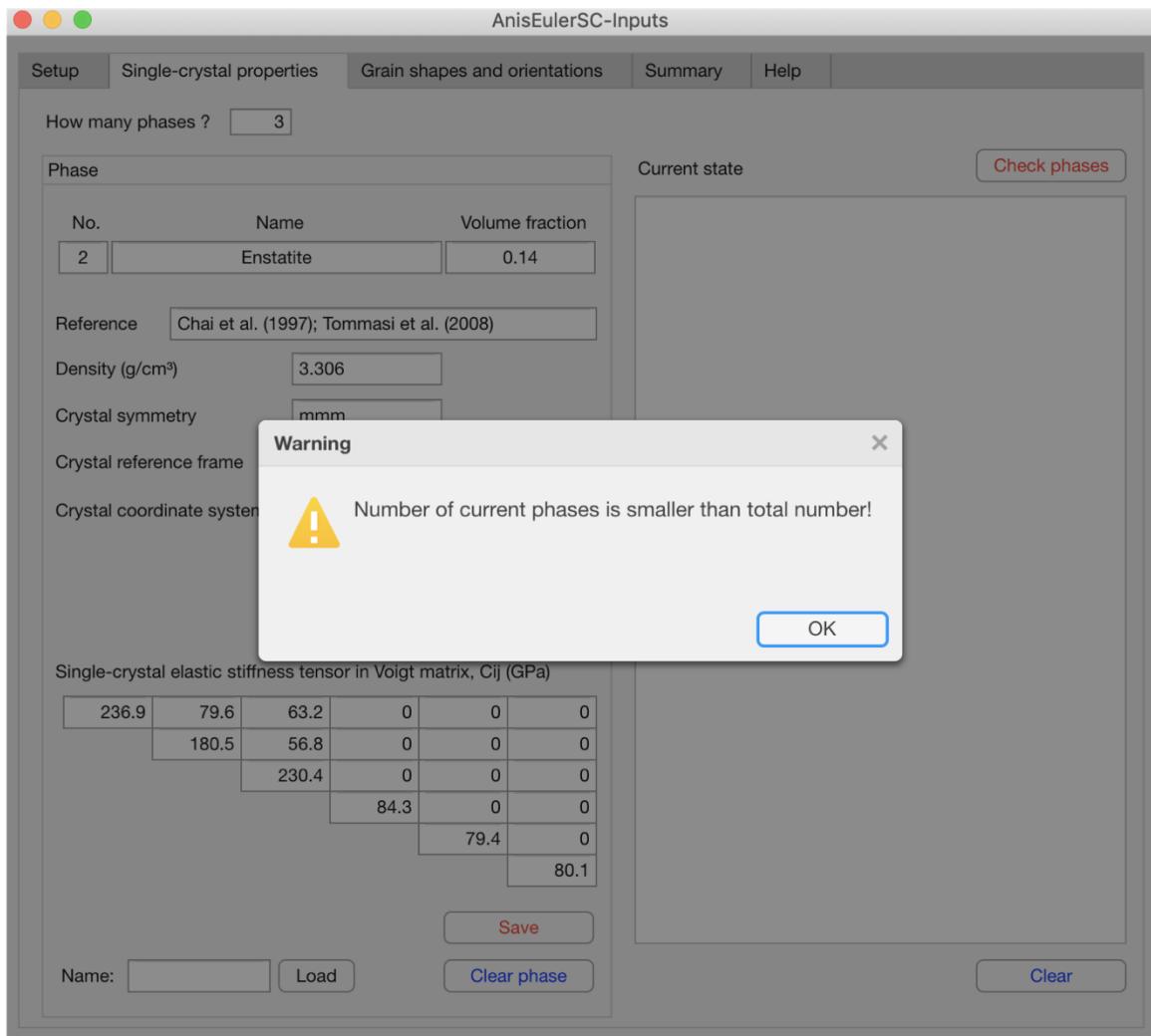


Figure U4. Pop-up message for warning showing that the number of current phases is smaller than the total number specified in advance. Click ‘OK’ to move onto the next phase.

- Check the single-crystal properties of current phases stored in the data file.

Current state
Check phases

No. 1 Forsterite

Volume fraction: 0.83

Reference: Isaak et al. (1989); Tommasi et al. (2008)

Density: 3.2210 (g/cm³)

Crystal symmetry: mmm

Crystal reference frame: XIIa, ZIIc

Crystal coordinate system:

[a,b,c] = [4.8,10,6]

[alpha,beta,gamma] = [90,90,90]

No. 2 Enstatite

Volume fraction: 0.14

Reference: Chai et al. (1997); Tommasi et al. (2008)

Density: 3.3060 (g/cm³)

Crystal symmetry: mmm

Crystal reference frame: XIIa, ZIIc

Crystal coordinate system:

[a,b,c] = [18,8.8,5.2]

[alpha,beta,gamma] = [90,90,90]

Clear

Note: Check that all phases are correctly specified. If ‘Check phases’ button is clicked, the single-crystal properties for all phases stored in the data file are printed on ‘Current state’ screen. It is recommended to check each phase just after saving information for each phase before moving onto the next phase. Use ‘Clear’ button to clean ‘Current state’ screen.

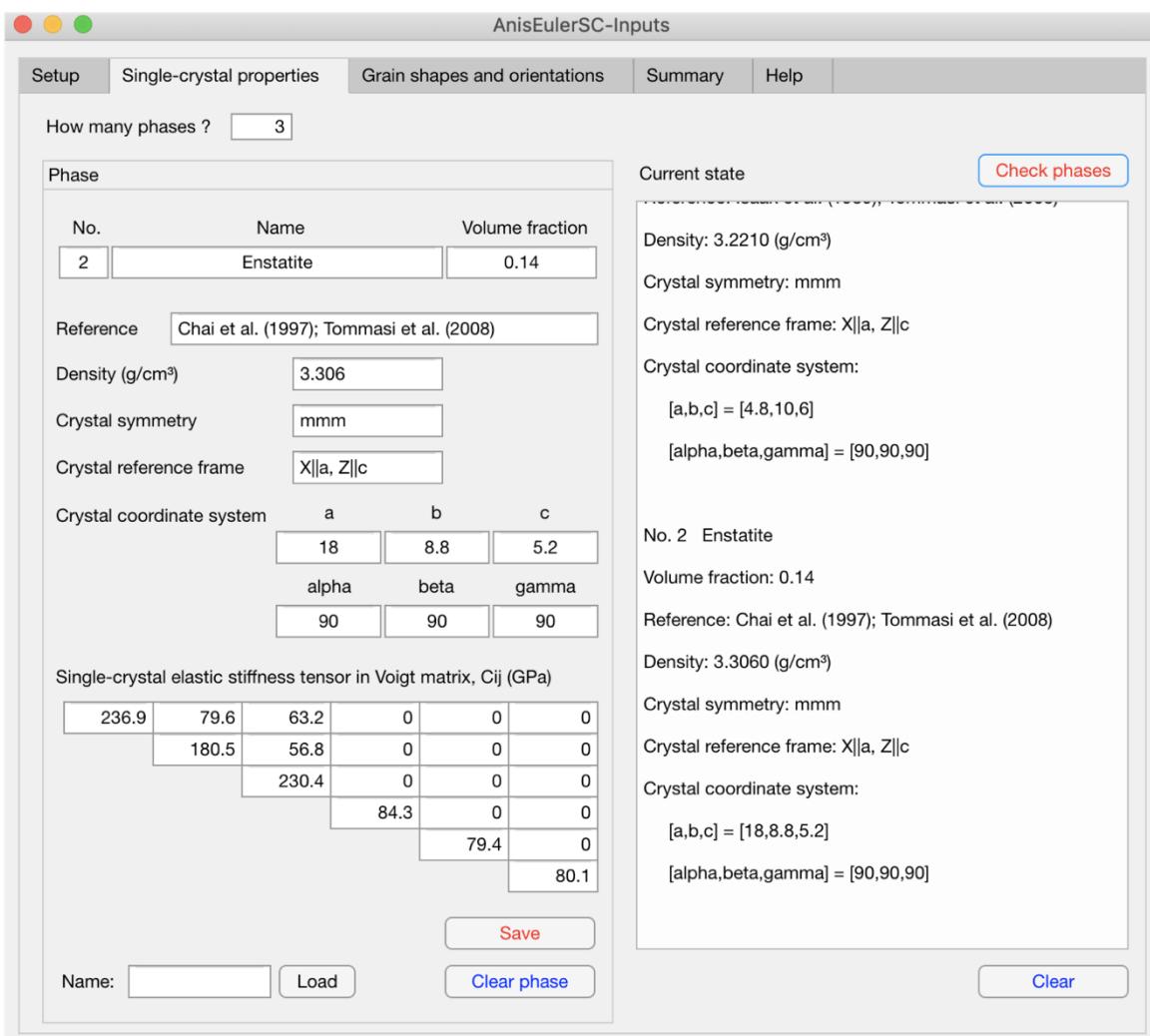


Figure U5. Single-crystal properties tab of AnisEulerSC-Inputs. For the second phase (enstatite), all input data are specified, saved and checked on the ‘Current state’ screen.

- Specify the single-crystal properties for the third phase, Diopside (Isaak et al., 2006; Tommasi et al., 2008), on the ‘Phase’ panel.

No.	Name	Volume fraction		
3	Diopside	0.03		
Reference	Isaak et al. (2006); Tommasi et al. (2008)			
Density (g/cm ³)	3.286			
Crystal symmetry	12/m1			
Crystal reference frame	XIIa*, YIIb*, ZIIc			
Crystal coordinate system	a 9.7 alpha 90	b 9 beta 105.63	c 5.3 gamma 90	
Single-crystal elastic stiffness tensor in Voigt matrix, C _{ij} (GPa)				
228.1	78.8	70.2	0	7.9
	181.1	61.1	0	5.9
		245.4	0	39.7
			78.9	0
				6.4
				68.2
				0
				78.1
<input style="background-color: red; color: white; font-weight: bold; width: 100px; height: 25px; margin-bottom: 5px;" type="button" value="Save"/> <input style="background-color: blue; color: white; font-weight: bold; width: 100px; height: 25px;" type="button" value="Clear phase"/>				
Name:	Diopside	Load		

Note: Click ‘Save’ button to store all properties of a phase in the data file (e.g., ‘Title’_Inputs_ModelSC.mat). To specify for the next phase, click ‘Clear phase’ button. To load the saved phase, type the phase name and click ‘Load’ button.

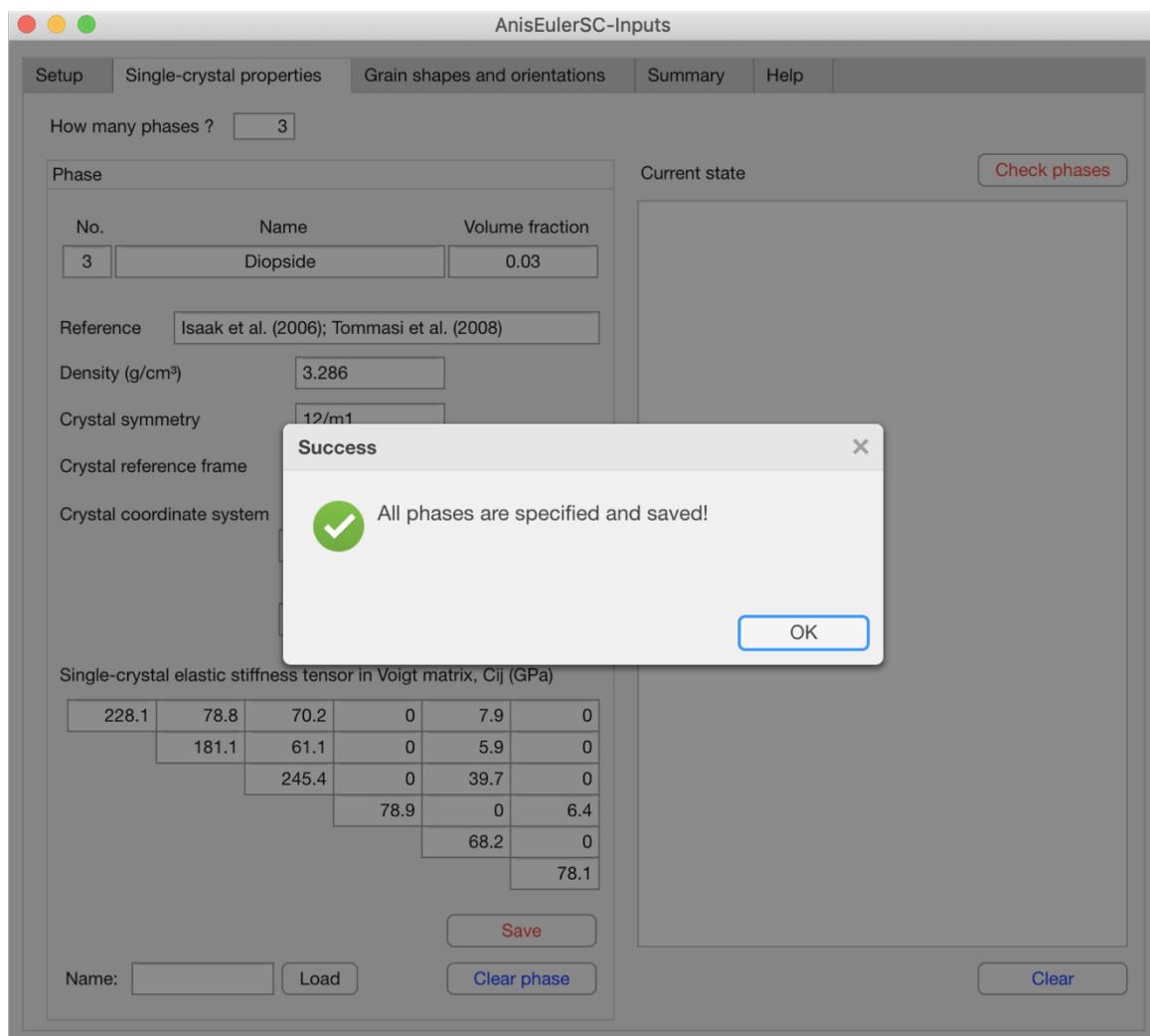


Figure U6. Pop-up message when the number of current phases is same with the total number specified in advance. Click ‘OK’ to move onto the next step.

- Check the single-crystal properties of current phases stored in the data file.

Current state

Check phases

No. 1 Forsterite

Volume fraction: 0.83

Reference: Isaak et al. (1989); Tommasi et al. (2008)

Density: 3.2210 (g/cm³)

Crystal symmetry: mmm

Crystal reference frame: Xlla, Zllc

Crystal coordinate system:

[a,b,c] = [4.8,10,6]

[alpha,beta,gamma] = [90,90,90]

No. 2 Enstatite

Volume fraction: 0.14

Reference: Chai et al. (1997); Tommasi et al. (2008)

Density: 3.3060 (g/cm³)

Crystal symmetry: mmm

Crystal reference frame: Xlla, Zllc

Crystal coordinate system:

[a,b,c] = [18,8.8,5.2]

[alpha,beta,gamma] = [90,90,90]

No. 3 Diopside

Volume fraction: 0.03

Reference: Isaak et al. (2006); Tommasi et al. (2008)

Density: 3.2860 (g/cm³)

Crystal symmetry: 12/m1

Crystal reference frame: X_{II}a*, Y_{II}b*, Z_{II}c

Crystal coordinate system:

[a,b,c] = [9.7,9,5.3]

[alpha,beta,gamma] = [90,105.63,90]

[Clear](#)

Note: Check that all phases are correctly specified. If ‘[Check phases](#)’ button is clicked, the single-crystal properties for all phases stored in the data file are printed on ‘Current state’ screen. It is recommended to check each phase just after saving information for each phase before moving onto the next phase. Use ‘[Clear](#)’ button to clean ‘Current state’ screen.

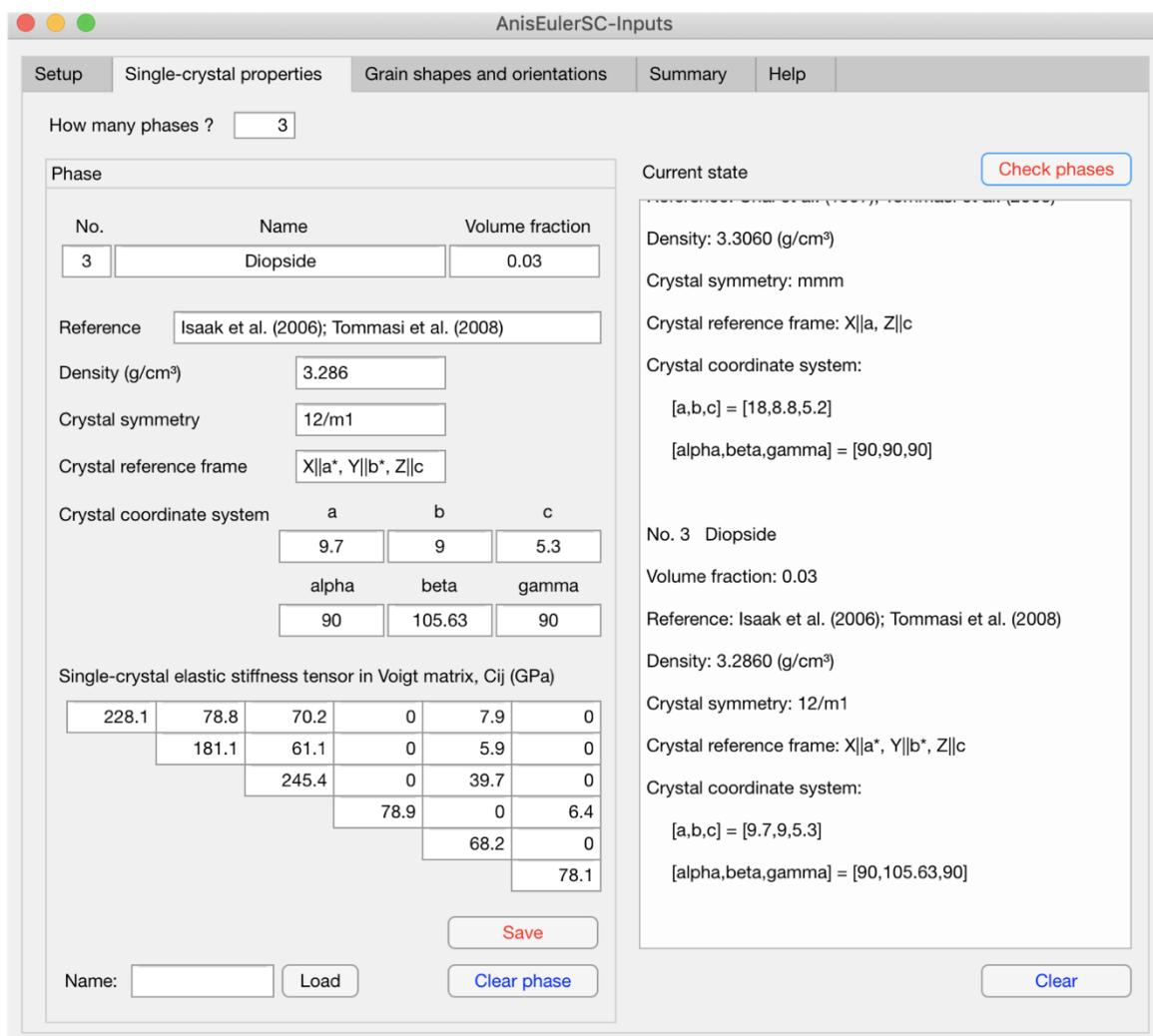


Figure U7. Single-crystal properties tab of AnisEulerSC-Inputs. For the third phase (diopside), all input data are specified, saved and checked on the ‘Current state’ screen.

2.2.3. Grain shapes and orientations tab

For each phase, the grain shapes and orientations can be specified on the ‘Phase’ panel.

- Specify the phase name and the Euler data file.

1. Name	Forsterite	
2. Euler data file	Forsterite_EulerVf.txt	

- Select the Euler space for crystal.

3. Euler space for crystal (e.g., triclinic sample symmetry)

11 Proper point groups (Schoenflies – International) (phi1, PHI, phi2)

Crystal symmetry 0 = Triclinic (C1 – 1) (360, 180, 360)

1 = Monoclinic (C2 – 2) (360, 180, 180)

2 = Orthorhombic (D2 – 222) (180, 180, 180)

3 = Trigonal (D3 – 32) (2-fold//Y) (180, 180, 120)

4 = Trigonal (C3 – 3) (360, 180, 120)

5 = Tetragonal (D4 – 422) (180, 180, 90)

6 = Tetragonal (C4 – 4) (360, 180, 90)

7 = Hexagonal (D6 – 622) (180, 180, 60)

8 = Hexagonal (C6 – 6) (360, 180, 60)

9 = Cubic (0 – 432) (180, 180, 90)

10 = Cubic (T – 23) (360, 180, 90)

Note: 0 = No crystal symmetry operations (e.g., fluids)

- Select the crystal reference directions of X1 and X2 and specify their indices.

4. User defined crystal reference directions (X1, X2, X3)

(As X1, X2 and X3 must be orthogonal, only X1 and X3 need to be specified.)

X1 **1 = direction [UVW]**

1	0	0
---	---	---

2 = pole normal (HKL)

X3 **1 = direction [UVW]**

0	0	1
---	---	---

2 = pole normal (HKL)

- Select the grain shape.

5. Grain shape 1 = Sphere

2 = Ellipsoid

Note: Ellipsoid semi-axes are a1, a2, and a3. Sphere: a1 = a2 = a3. Oblate ellipsoid: a1 = a2 > a3. Prolate ellipsoid: a1 = a2 < a3.

- Select the orientation of ellipsoid semi-axes.

6. Orientation of ellipsoid semi-axes

1 = // tensor axes X1, X2, X3 of each crystal (A1//X1, A2//X2, A3//X3)

2 = // user defined orientation in PF (pole figure) coordinate (e.g., fluids)

- Specify the ellipsoid semi-axes lengths (A1, A2, A3).

7. Ellipsoid semi-axes lengths (A1, A2, A3)

3 3 1

- If you select 2 for ‘6. Orientation of ellipsoid semi-axes’, specify the azimuth and inclination of ellipsoid semi-axes A1 and A3.

8. Foliation with pole given by AZ (0 – 360) and INC (0 – 90)

AZ: Azimuth of ellipsoid semi-axis

	AZ	INC
A1		
A3		

INC: Inclination of ellipsoid semi-axis

Name: Forsterite

Load

Save

Clear phase

Note: Click ‘Save’ button to store all properties of each phase in the data file (e.g., ‘Title’_Inputs_ModelSC.mat). To specify for the next phase, click ‘Clear phase’ button. To load the saved phase, click ‘Load’ button.

- Check the grain shapes and orientations of current phases stored in the data file.

Current state	Check phases
No. 1	
1. Name: Forsterite	
2. Euler data file: Forsterite_EulerVf.txt	
3. Crystal symmetry: 2 = Orthorhombic (D2 - 222) (180, 180, 180)	
4. Crystal reference direction:	
X1: 1 = direction [UVW] [1,0,0]	
X3: 1 = direction [UVW] [0,0,1]	
5. Grain shape: 2 = Ellipsoid	
6. Orientation of ellipsoid semi-axes:	
1 = // tensor axes X1, X2, X3 of each crystal (A1//X1, A2//X2, A3//X3)	
7. Ellipsoid [A1,A2,A3] = [3,3,1]	
Clear	

Note: Check that all phases are correctly specified. If ‘[Check phases](#)’ button is clicked, the grain shapes and orientations for all phases stored in the data file are printed on ‘Current state’ screen. It is recommended to check each phase just after saving information for each phase before moving onto the next phase. Use ‘[Clear](#)’ button to clean the ‘Current state’ screen.

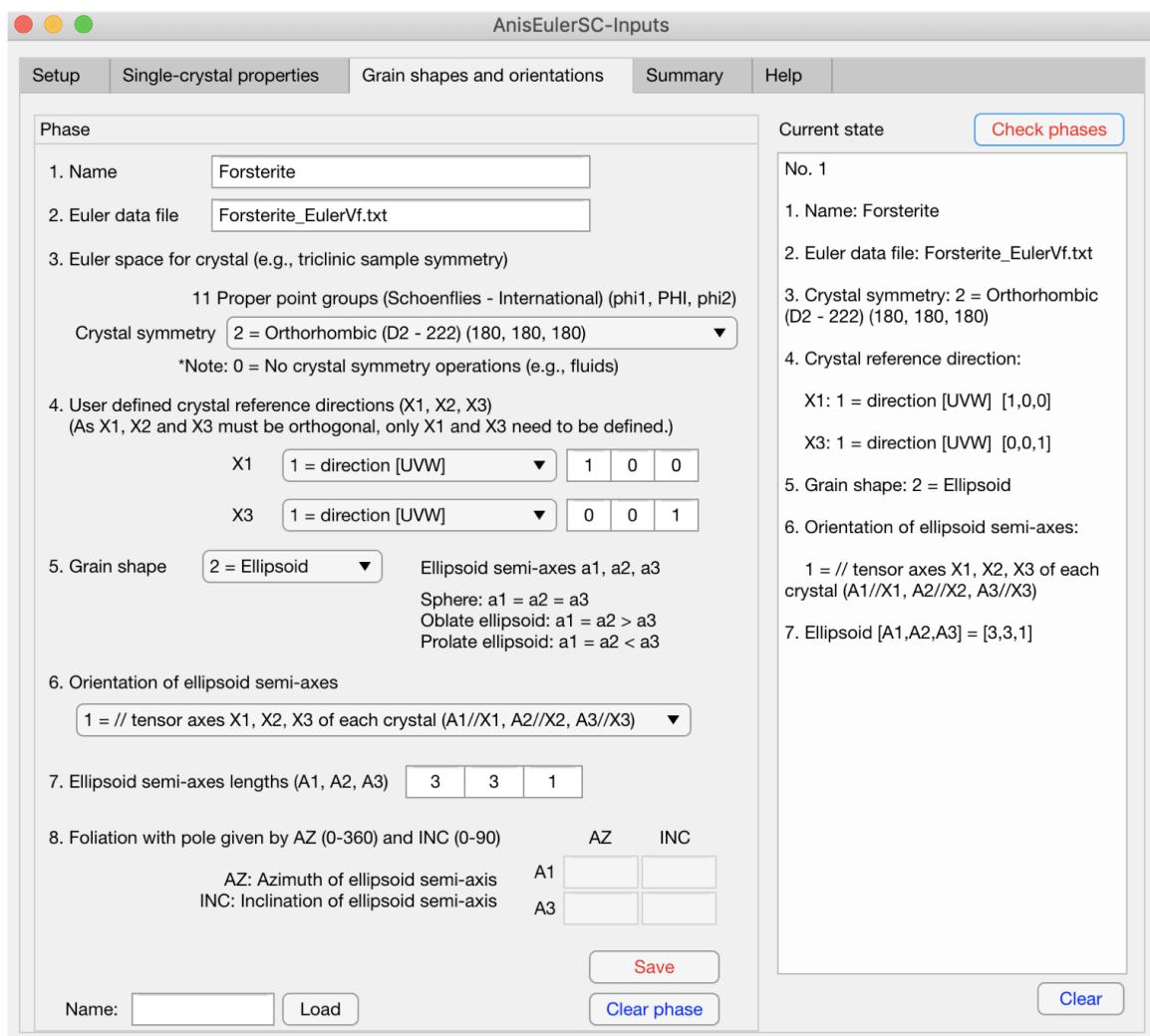


Figure U8. Grain shapes and orientations tab of AnisEulerSC-Inputs. For the first phase (forsterite), all input data are specified, saved and checked on the ‘Current state’ screen.

- Repeat for the next phase of Enstatite.

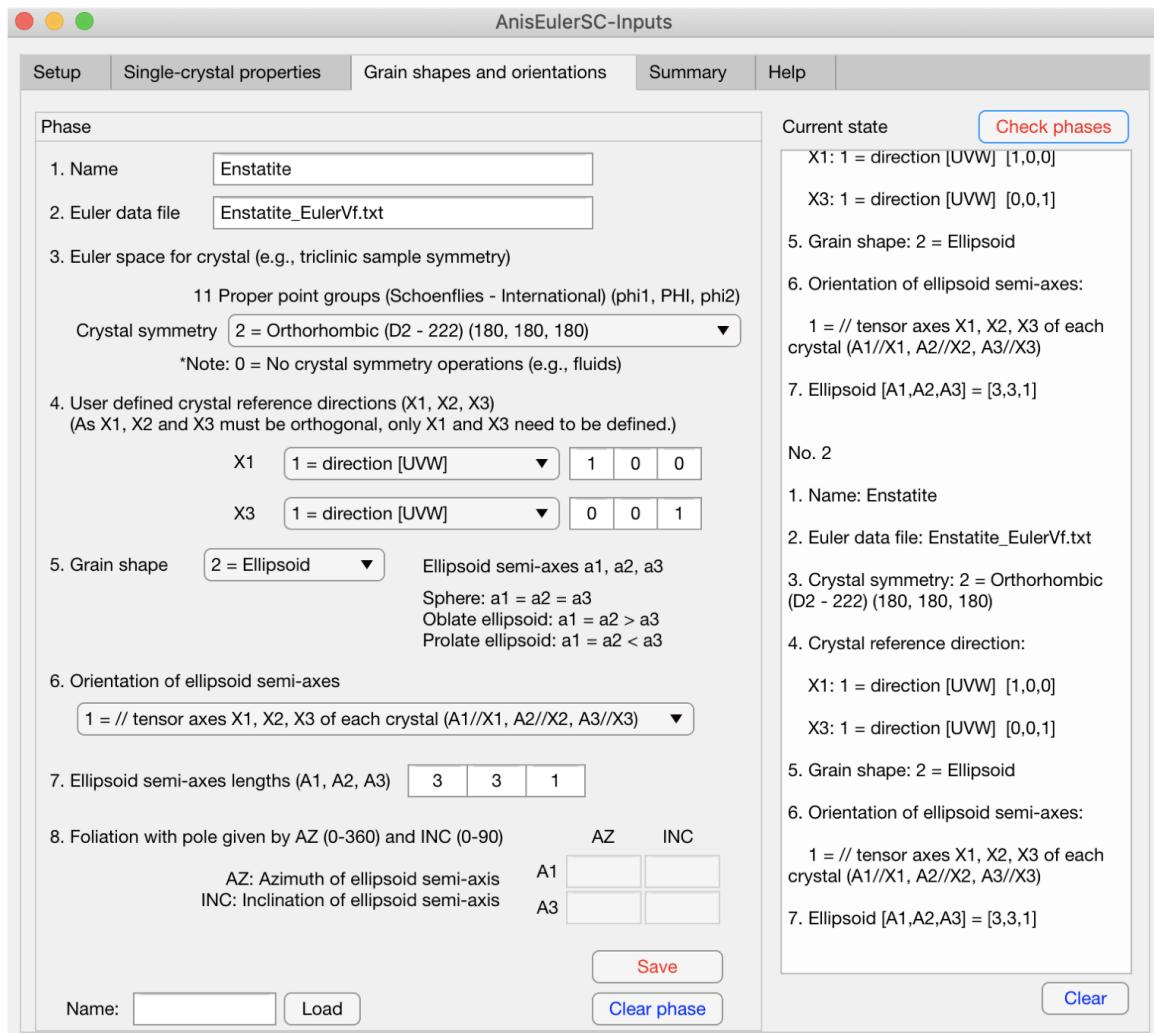


Figure U9. Grain shapes and orientations tab of AnisEulerSC-Inputs. For the second phase (enstatite), all input data are specified, saved and checked on the ‘Current state’ screen.

- Repeat for the next phase of Diopside.

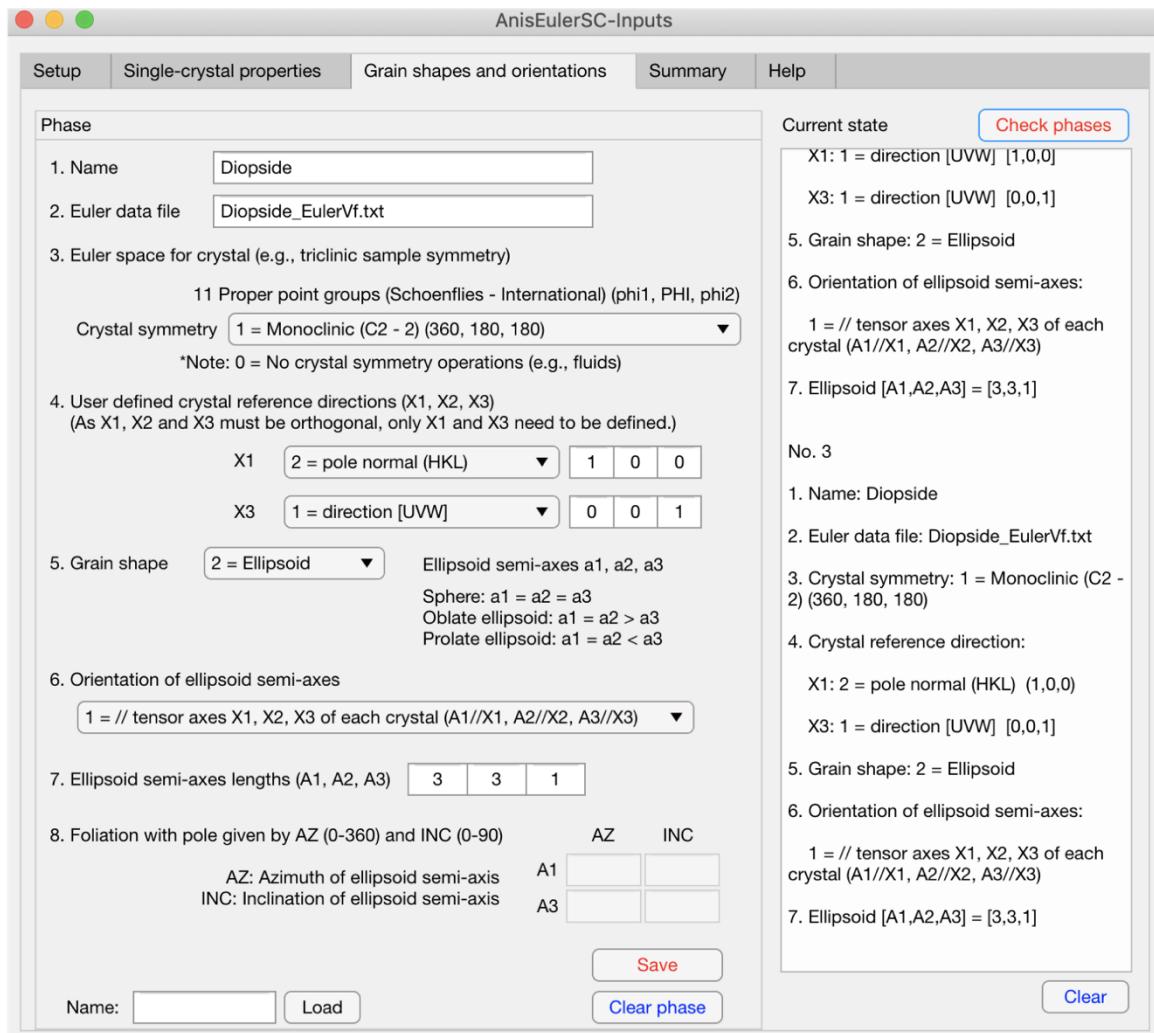


Figure U10. Grain shapes and orientations tab of AnisEulerSC-Inputs. For the third phase (diopside), all input data are specified, saved and checked on the ‘Current state’ screen.

2.2.4. Summary tab

- Click ‘Show’ button to print a brief summary on the screen.

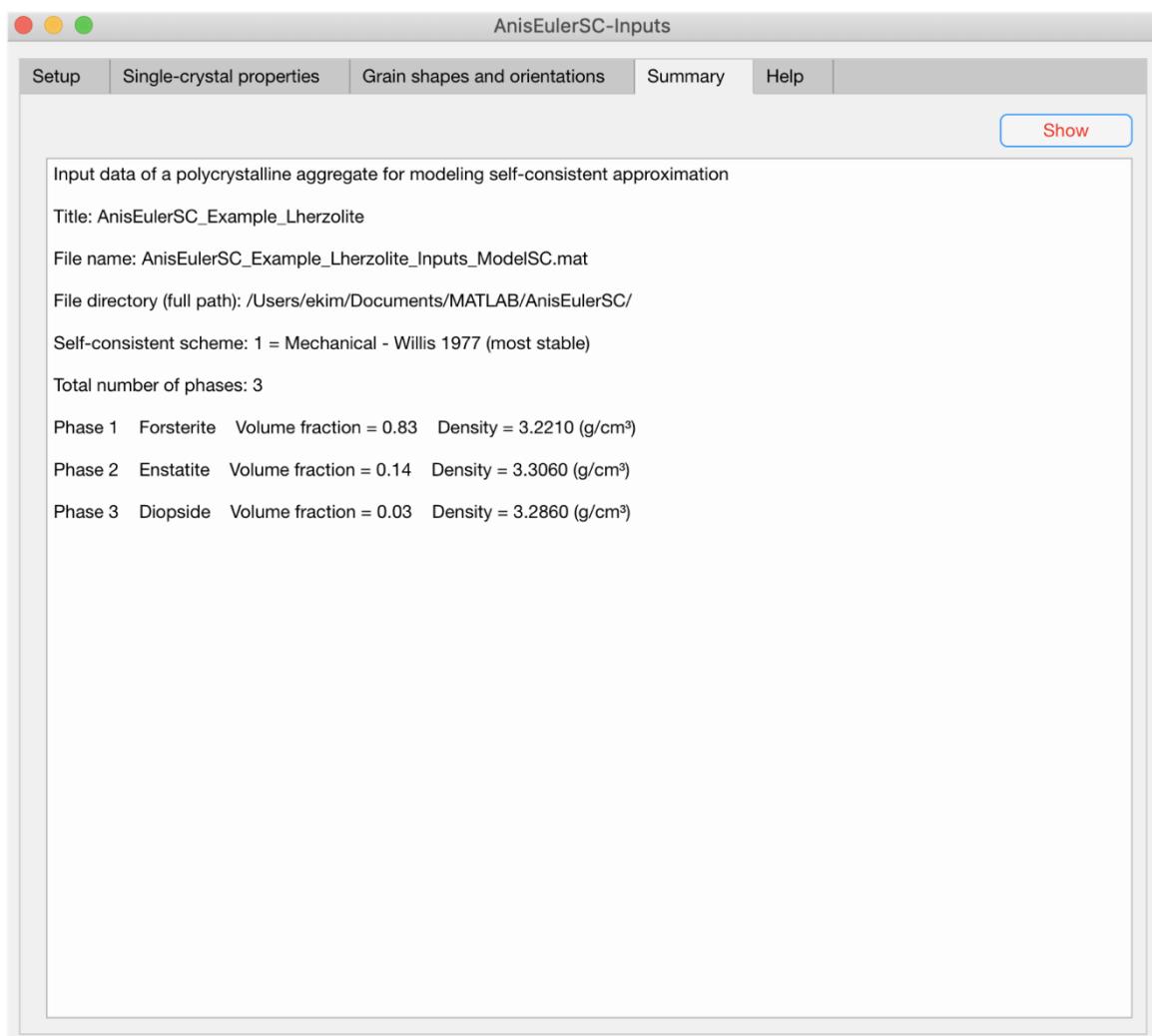


Figure U11. Summary tab of AnisEulerSC-Inputs.

2.2.5. Help tab

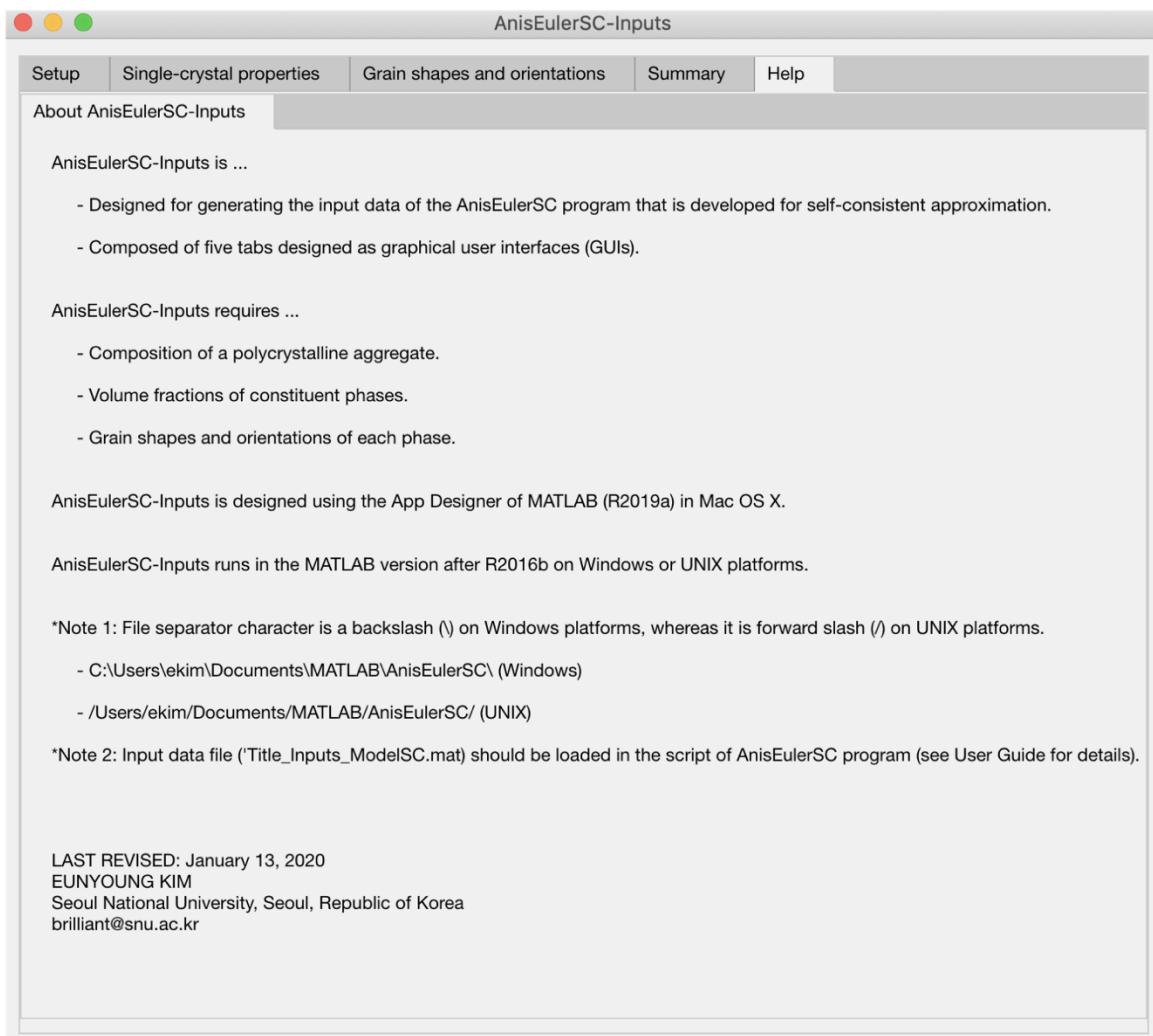


Figure U12. Help tab of AnisEulerSC-Inputs. The information of AnisEulerSC-Inputs is described in the About AnisEulerSC-Inputs tab.

2.3. Run AnisEulerSC script

A MAT-file ('Title'_Inputs_ModelSC.mat) generated using AnisEulerSC-Inputs program is required to run the AnisEulerSC script (AnisEulerSC.m). To run the script, specify the MAT-file name to load input data as follows.

```
% Load input data file ('Title'_Inputs_ModelSC.mat)
load('AnisEulerSC_Example_Lherzolite_Inputs_ModelSC.mat');
```

2.4. Example: A polycrystalline aggregate with cracks

We apply the SC approximation to a cracked material. We assume that a solid-crack composite is composed of a polycrystalline aggregate (98%) and ellipsoidal cracks (2%). The solid phase (LherzoliteSC; Figure U13) is an SC aggregate composed of 83% forsterite, 14% enstatite, and 3% diopside with ellipsoidal grains (semi-axes $a_1:a_2:a_3 = 3:3:1$), which is described in Sections 2.1–2.3. Using the elastic properties of LherzoliteSC, the solid phase is specified in the AnisEulerSC-Inputs program (Figure U13). The crack phase (CrackAir; Figure U14) is assumed to be air-filled cracks with ellipsoidal shape (semi-axes $a_1:a_2:a_3 = 5:5:1$) and to be aligned with the user-defined orientation.

In the Single-crystal properties tab, the volume fraction and density are specified for LherzoliteSC (Figure U13) and CrackAir (Figure U14). The crystal symmetries of LherzoliteSC and CrackAir are specified as triclinic crystal structure. Because there is no crystal symmetry operation for triclinic crystal structure in the AnisEulerSC program, the crystal reference frame and crystal coordinate system are specified as cubic crystal structure (Figures U13 and U14). The single-crystal elastic stiffness tensors of LherzoliteSC and CrackAir are also specified (Figures U13 and U14).

In the Grain shapes and orientations tab, Euler data file is specified as ‘Single_orientation.txt’, because both LherzoliteSC and CrackAir have no crystal distribution functions. In this case, Euler angles are zero (Figures U15 and U16). The crystal symmetries of LherzoliteSC and CrackAir are triclinic and there are no crystal symmetry operations for triclinic structure (e.g., fluids) (Figures U15 and U16). The user-defined crystal reference directions are $X1 = [1,0,0]$ and $X3 = [0,0,1]$ (Figures U15 and U16). Because the grain shape of LherzoliteSC is a sphere (semi-axes $a_1=a_2=a_3$), the orientation of grains are not

meaningful (Figure U15). The grain shape of CrackAir is an ellipsoid and the ellipsoid semi-axes are $a_1:a_2:a_3 = 5:5:1$ (Figure U16). Because the elastic stiffness tensor of CrackAir is isotropic, the user-defined orientation of ellipsoidal grains in Pole Figure coordinate are specified using the azimuth and inclination of ellipsoid semi-axes A1 and A3 (Figure U16).

AnisEulerSC-Inputs

Setup Single-crystal properties Grain shapes and orientations Summary Help

How many phases ?

Phase			Current state																																						
No.	Name	Volume fraction																																							
1	LherzoliteSC	0.98	No. 1 LherzoliteSC Volume fraction: 0.98 Reference: Tommasi et al. (2008); Isaak et al. (1989); Chai et al. (1997); Isaak et al. (2006) Density: 3.2348 (g/cm ³) Crystal symmetry: triclinic Crystal reference frame: X a, Z c Crystal coordinate system: [a,b,c] = [1,1,1] [alpha,beta,gamma] = [90,90,90]																																						
Reference: Tommasi et al. (2008); Isaak et al. (1989); Chai et al. (1997); Isaak et al. (2006)			Check phases																																						
Density (g/cm ³) <input type="text" value="3.2348"/> Crystal symmetry <input type="text" value="triclinic"/> Crystal reference frame <input type="text" value="X a, Z c"/> Crystal coordinate system <table border="1"> <tr><td>a</td><td>b</td><td>c</td></tr> <tr><td>1</td><td>1</td><td>1</td></tr> <tr><td>alpha</td><td>beta</td><td>gamma</td></tr> <tr><td>90</td><td>90</td><td>90</td></tr> </table>			a	b	c	1	1	1	alpha	beta	gamma	90	90	90	No. 2 CrackAir Volume fraction: 0.02 Reference: Blevins (1984); Dengler & Lehre (1987) Density: 0.0012 (g/cm ³) Crystal symmetry: triclinic Crystal reference frame: X a, Z c Crystal coordinate system: [a,b,c] = [1,1,1] [alpha,beta,gamma] = [90,90,90]																										
a	b	c																																							
1	1	1																																							
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Single-crystal elastic stiffness tensor in Voigt matrix, C _{ij} (GPa)			Save																																						
<table border="1"> <tr><td>210.0231</td><td>71.9622</td><td>71.8582</td><td>-0.4627</td><td>3.3971</td><td>-1.7974</td></tr> <tr><td></td><td>245.3279</td><td>75.6352</td><td>4.6733</td><td>0.5366</td><td>-3.4292</td></tr> <tr><td></td><td></td><td>252.6175</td><td>4.6083</td><td>6.4734</td><td>-0.0042</td></tr> <tr><td></td><td></td><td></td><td>86.8874</td><td>-0.5538</td><td>2.2239</td></tr> <tr><td></td><td></td><td></td><td></td><td>77.2407</td><td>1.5971</td></tr> <tr><td></td><td></td><td></td><td></td><td></td><td>75.808</td></tr> </table>			210.0231	71.9622	71.8582	-0.4627	3.3971	-1.7974		245.3279	75.6352	4.6733	0.5366	-3.4292			252.6175	4.6083	6.4734	-0.0042				86.8874	-0.5538	2.2239					77.2407	1.5971						75.808	Clear		
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Figure U13. Single-crystal properties tab of AnisEulerSC-Inputs. The solid phase (LherzoliteSC) is an SC aggregate, which is composed of 83% forsterite, 14% enstatite, and 3% diopside with ellipsoidal grains, described in Sections 2.1–2.3. LherzoliteSC has the crystal symmetry of triclinic structure for which no crystal symmetry operations work

in the AnisEulerSC program. The crystal reference frame and crystal coordinate system are assumed to be the same as those of cubic structure.

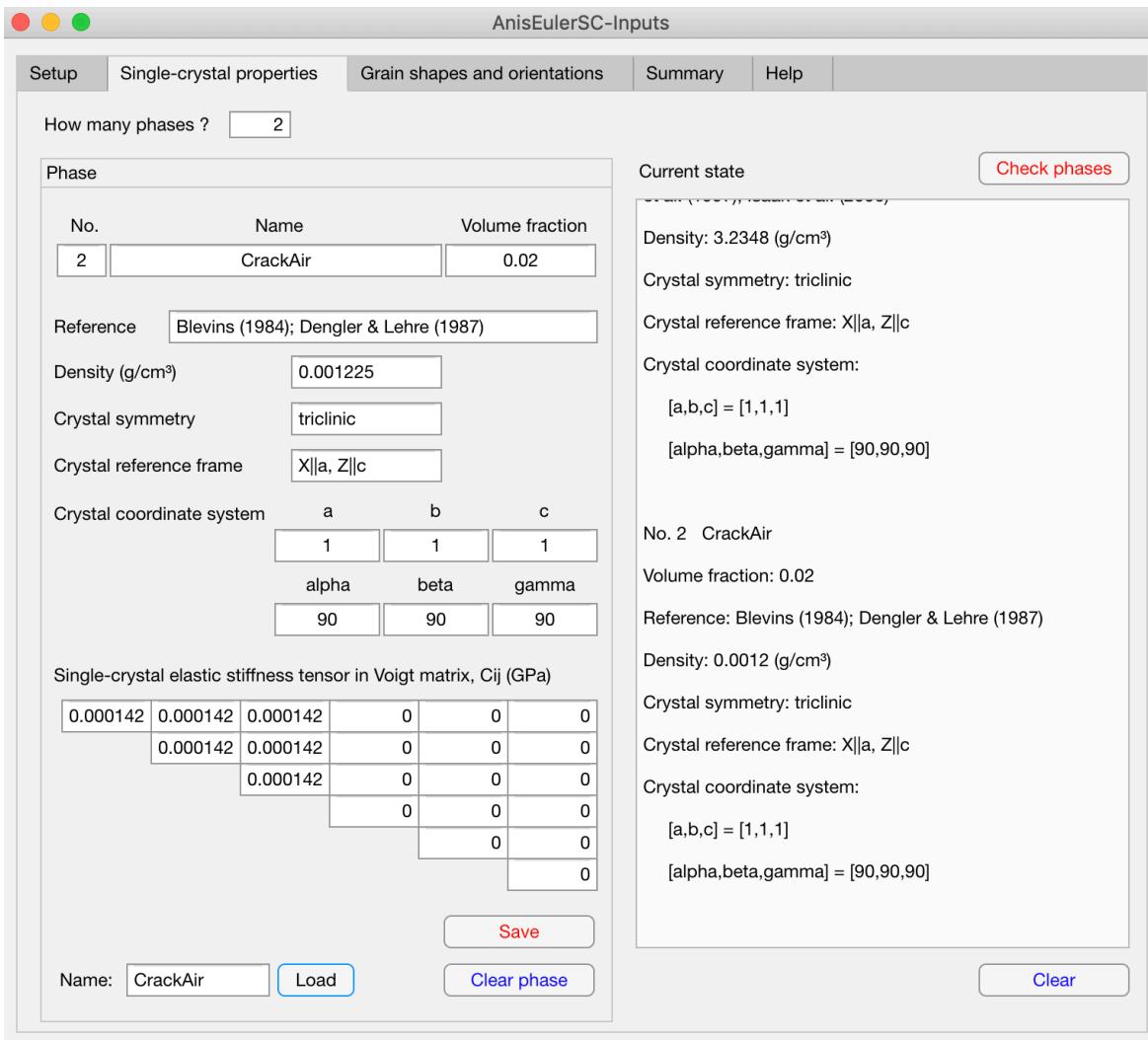


Figure U14. Single-crystal properties tab of AnisEulerSC-Inputs. The crack phase (CrackAir) is assumed to be air-filled cracks with ellipsoidal grains. The crystal symmetry of CrackAir is specified as triclinic because no crystal symmetry operations work for triclinic crystal structure in the AnisEulerSC program. The crystal reference frame and crystal coordinate system are assumed to be the same as those of cubic structure.

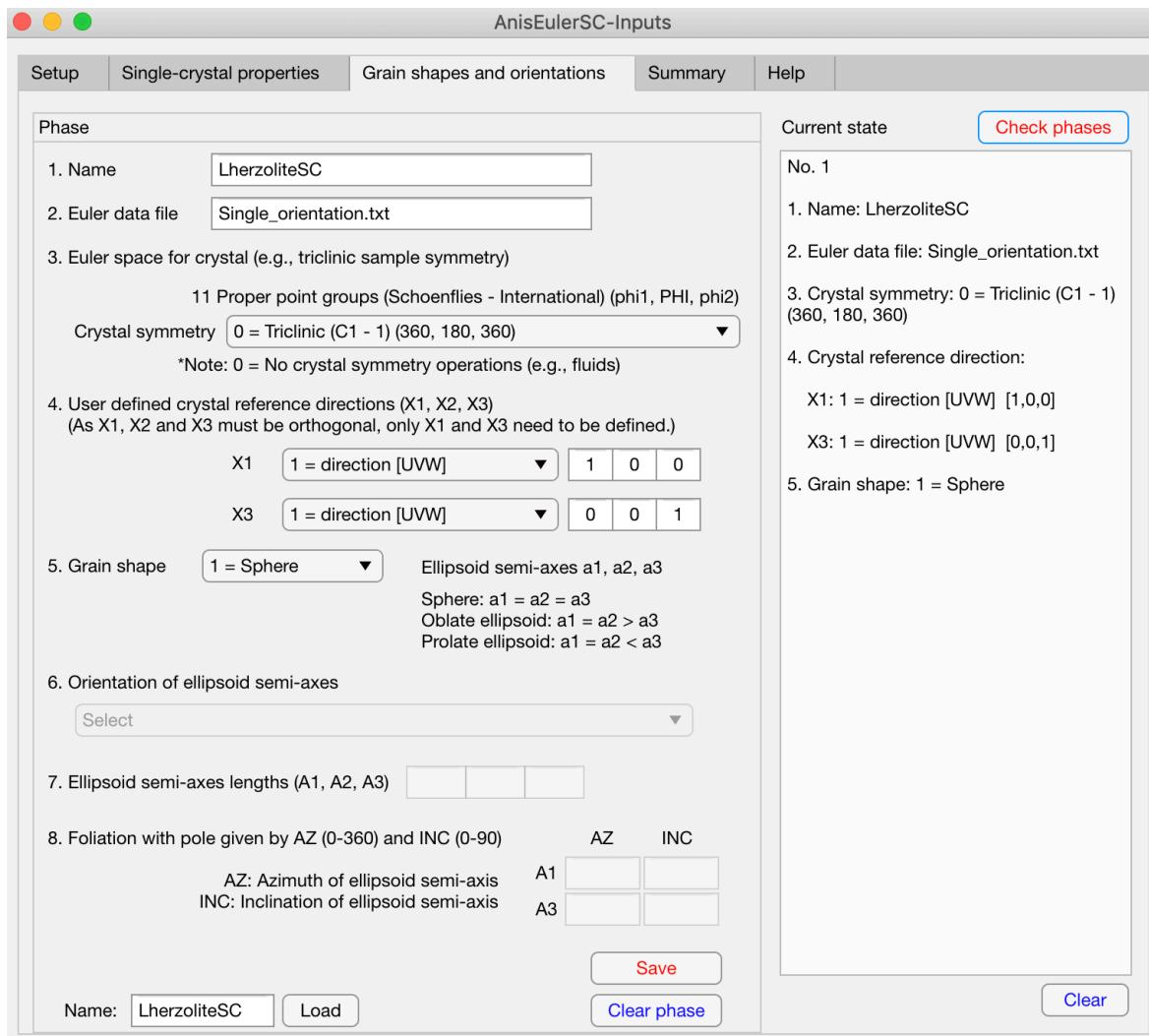


Figure U15. Grain shapes and orientations tab of AnisEulerSC-Inputs. The solid phase (LherzoliteSC) has triclinic crystal structure. Because no crystal symmetry operations work for triclinic crystal structure in the AnisEulerSC program, user-defined crystal reference directions are specified as $X1 = [1,0,0]$ and $X3 = [0,0,1]$. The grain shape is a sphere (semi-axes $a_1=a_2=a_3$). In this case, the orientation of grains are not meaningful.

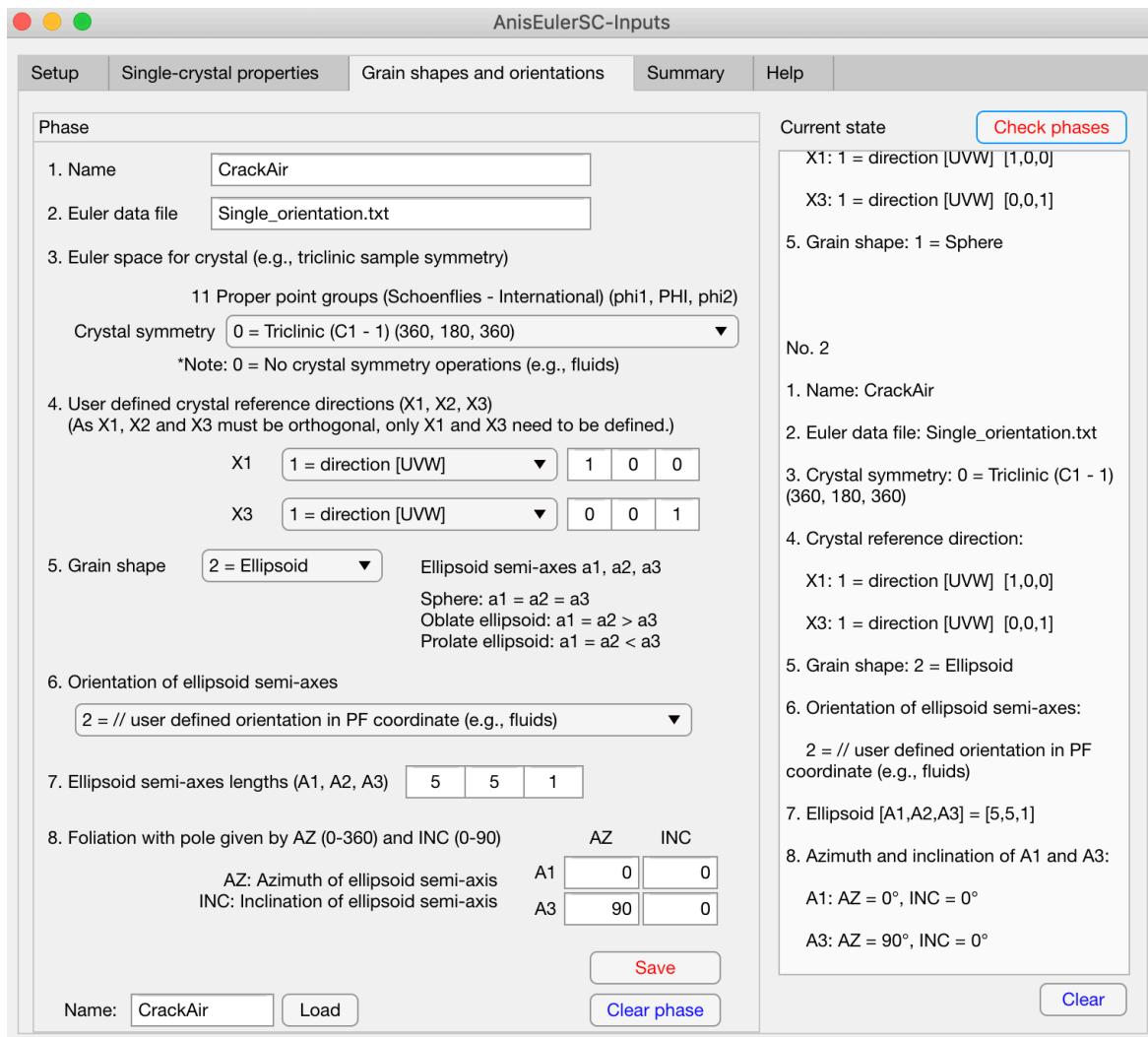


Figure U16. Grain shapes and orientations tab of AnisEulerSC-Inputs. The crack phase (CrackAir) has triclinic crystal structure. Because no crystal symmetry operations work for triclinic crystal structure in the AnisEulerSC program, user-defined crystal reference directions are specified as X1 = [1,0,0] and X3 = [0,0,1]. The grain shape is an ellipsoid (semi-axes a1:a2:a3 = 5:5:1). The orientation of ellipsoid semi-axes is the user-defined orientation in Pole Figure coordinate (e.g., fluids), which is specified using the azimuth and inclination of semi-axes A1 and A3.

Appendix A. Single-crystal elastic stiffness tensor

The reference frame for tensors describing macroscopic properties of a polycrystalline specimen is the specimen coordinate system, whereas the reference frame for single-crystal tensors describing crystal properties is associated with the crystal coordinate system (Mainprice et al., 2011). We describe the single-crystal tensor reference frame and the crystal orientations in the specimen reference frame required to understand prior to calculating of the overall elastic properties of a polycrystalline aggregate.

A1. Crystal reference frame

We describe the elastic stiffness tensors defined in a Cartesian reference frame with unit vectors \vec{X} , \vec{Y} , and \vec{Z} . The crystal reference frame, in the general case (e.g., triclinic crystal symmetry in Figure A1), for the single-crystal elastic stiffness tensor is defined using the crystal coordinate system that is specified by its axis lengths a , b , and c and inter-axial angles α , β , and γ indicating a non-Euclidean coordinate system \vec{a} , \vec{b} , \vec{c} (Mainprice et al., 2011).

The alignment of the Euclidean tensor reference frame \vec{X} , \vec{Y} , \vec{Z} in the crystal coordinate system can be expressed using several conventions (Table A1).

A2. Crystal orientations

For a polycrystalline specimen, a crystal reference frame \vec{X}^c , \vec{Y}^c , \vec{Z}^c generally does not coincide with the specimen reference frame \vec{X}^s , \vec{Y}^s , \vec{Z}^s (Figure A2a). The crystal orientation within the specimen is defined by Euler angles that are described by various conventions, for example Bunge Euler angles ϕ_1 , Φ , ϕ_2 (Bunge, 1982) (Figure A2b) or Matthies Euler angles (Matthies and Wenk, 2009). If the Bunge Euler angles are given, the r-rank tensor T_{j_1, \dots, j_r}^T has to be rotated according to the crystal orientation $g = (\phi_1, \Phi, \phi_2)$. The rotated tensor T_{i_1, \dots, i_r} is

calculated using the rotation matrix $R_{i_r j_r}(g)$ which is defined by the orientation g (Mainprice et al., 2011) as follows:

$$\begin{aligned} T_{i_1, \dots, i_r} &= T_{j_1, \dots, j_r}^T(g) \\ &= T_{j_1, \dots, j_r}^T R_{i_1 j_1}(g) \cdots R_{i_r j_r}(g). \end{aligned} \quad (\text{A1})$$

Note that, in this equation, the tensor reference frame should coincide with the crystal reference frame used for describing the orientation to make sense physically (Mainprice et al., 2011). To express the elastic stiffness tensor C_{ijkl} , defined in the crystal reference frame $\vec{X}^C, \vec{Y}^C, \vec{Z}^C$, with respect to a specimen reference frame $\vec{X}^S, \vec{Y}^S, \vec{Z}^S$, it is required to transform the coordinate from the crystal coordinate system to the specimen coordinate system. A vector \vec{h} given as the coordinates h_1^C, h_2^C, h_3^C with respect to the crystal reference frame $\vec{X}^C, \vec{Y}^C, \vec{Z}^C$ is expressed as follows:

$$\vec{h} = h_1^C \vec{X}^C + h_2^C \vec{Y}^C + h_3^C \vec{Z}^C. \quad (\text{A2})$$

The vector \vec{h} also given as the coordinates h_1, h_2, h_3 with respect to the specimen reference frame $\vec{X}^S, \vec{Y}^S, \vec{Z}^S$ is expressed as follows:

$$\vec{h} = h_1 \vec{X}^S + h_2 \vec{Y}^S + h_3 \vec{Z}^S. \quad (\text{A3})$$

The transformation rule is represented as

$$\begin{aligned} \begin{pmatrix} h_1 \\ h_2 \\ h_3 \end{pmatrix} &= \begin{pmatrix} \vec{X}^S \cdot \vec{X}^C & \vec{X}^S \cdot \vec{Y}^C & \vec{X}^S \cdot \vec{Z}^C \\ \vec{Y}^S \cdot \vec{X}^C & \vec{Y}^S \cdot \vec{Y}^C & \vec{Y}^S \cdot \vec{Z}^C \\ \vec{Z}^S \cdot \vec{X}^C & \vec{Z}^S \cdot \vec{Y}^C & \vec{Z}^S \cdot \vec{Z}^C \end{pmatrix} \begin{pmatrix} h_1^C \\ h_2^C \\ h_3^C \end{pmatrix} \\ &= R \begin{pmatrix} h_1^C \\ h_2^C \\ h_3^C \end{pmatrix}, \end{aligned} \quad (\text{A4})$$

where the matrix R rotates the specimen reference frame into coincidence with the crystal reference frame (Mainprice et al., 2011). For the coefficients of a 4-rank elastic stiffness tensor C_{pqrs}^C with respect to the crystal reference frame, the coefficients of C_{ijkl} with respect

to the specimen reference frame is represented by the linear orthogonal transformation law for Cartesian tensors as follows:

$$C_{ijkl} = C_{pqrs}^C R_{ip} R_{jq} R_{kr} R_{ls}. \quad (\text{A5})$$

Then, the single-crystal elastic tensor with respect to the specimen reference frame can be used to calculate the overall properties of a polycrystalline specimen.

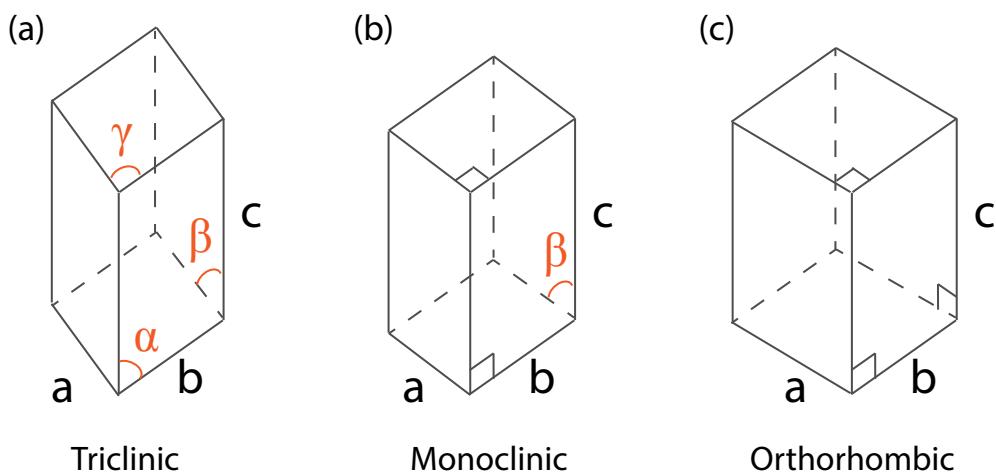


Figure A1. Crystal coordinate system defined as the axis lengths a , b , c and inter-axial angles α , β , γ for (a) triclinic ($a \neq b \neq c$ and $\alpha \neq \beta \neq \gamma \neq 90^\circ$), (b) monoclinic ($a \neq b \neq c$ and $\beta \neq 90^\circ$), and (c) orthorhombic ($a \neq b \neq c$) crystal symmetry.

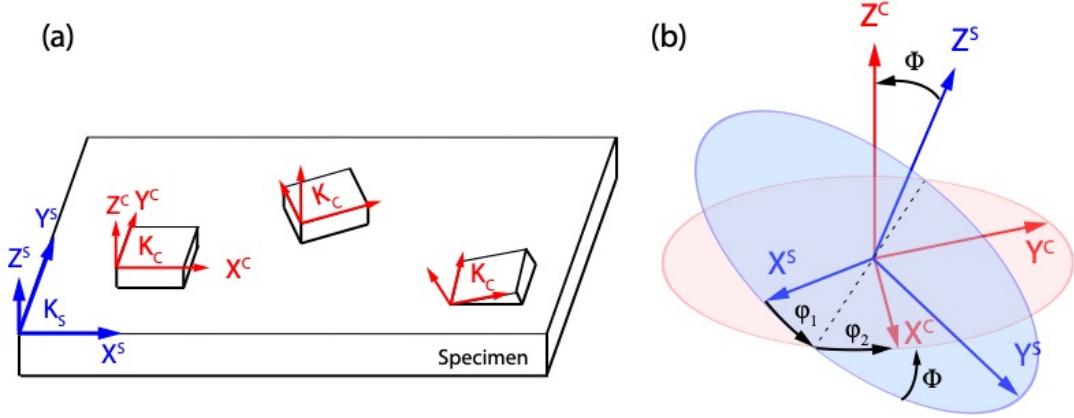


Figure A2. (a) Specimen reference frame K_S (\vec{X}^S , \vec{Y}^S , \vec{Z}^S) and crystal reference frame K_C (\vec{X}^C , \vec{Y}^C , \vec{Z}^C) in the specimen. (b) Definition of Bunge Euler angles ϕ_1 , Φ , ϕ_2 (after Bunge, 1982).

Table A1. Crystal reference frame defined as \vec{a} , \vec{b} , \vec{c} , \vec{m} which are crystallographic directions in the direct lattice space and as \vec{a}^* , \vec{b}^* , \vec{c}^* which are the corresponding directions in the reciprocal lattice space (e.g., $\vec{a}^* \parallel (\perp a)$; after Mainprice et al., 2011).

Crystal symmetry	Crystal reference frame		
	\vec{X}	\vec{Y}	\vec{Z}
Orthorhombic, tetragonal, cubic	\vec{a}	\vec{b}	\vec{c}
Trigonal, hexagonal	\vec{a}	\vec{m}	\vec{c}
	\vec{m}	$-\vec{a}$	\vec{c}
Monoclinic	\vec{a}^*	\vec{b}	\vec{c}
	\vec{a}	\vec{b}	\vec{c}^*
Triclinic	\vec{a}^*	$\vec{Z} \times \vec{X}$	\vec{c}
	\vec{a}	$\vec{Z} \times \vec{X}$	\vec{c}^*
	$\vec{Y} \times \vec{Z}$	\vec{b}^*	\vec{c}
	$\vec{Y} \times \vec{Z}$	\vec{b}	\vec{c}^*

Appendix B. Theories

B1. Simple averages for effective elastic properties of polycrystals

Voigt (1928) and Reuss (1929) averages are upper and lower bounds, respectively, of the effective elastic properties of polycrystals. The Voigt average simply assumes a constant strain field, which means that the strain at every position equals the macroscopic strain of the specimen (e.g., Mainprice, 2007). The Voigt average C^{Voigt} is defined by the volume average of local stiffnesses $C(g_i)$ with orientation g_i and volume fraction V_i :

$$C^{\text{Voigt}} = \sum_i V_i C(g_i). \quad (\text{B1})$$

The Reuss average assumes a constant stress field, which means that the stress at every position equals the macroscopic stress of the specimen. The Reuss average C^{Reuss} is defined by a volume average of the local compliances $S(g_i)$:

$$C^{\text{Reuss}} = \left[\sum_i V_i S(g_i) \right]^{-1}. \quad (\text{B2})$$

The experimentally measured elastic properties of the specimen are generally between the Voigt and Reuss bounds because the stress and strain distributions are expected to be between uniform strain (Voigt bound) and uniform stress (Reuss bound) field limits. The arithmetic mean of the Voigt and Reuss bounds (Hill, 1952), called Hill or Voigt-Reuss-Hill (VRH) average C^{VRH} , given by

$$C^{\text{VRH}} = \frac{1}{2} (C^{\text{Voigt}} + C^{\text{Reuss}}), \quad (\text{B3})$$

is often close to an experimental value and widely used in earth and materials sciences, although the VRH average has no theoretical justification (Mainprice and Humbert, 1994). In contrast to VRH, the geometric mean is based on a physical importance that the ensemble average elastic stiffness $\langle C \rangle$ should equal the inverse of the ensemble average elastic

compliance $\langle S \rangle^{-1}$ (Aleksandrov and Aizenberg, 1966). A geometric mean of oriented polycrystals C^G (Morawiec, 1989; Matthies and Humbert, 1993; Mainprice and Humbert, 1994; Matthies and Humbert, 1995) is described as follows:

$$C^G = \exp \left[\frac{1}{V} \int \ln C(g) dV \right], \quad (\text{B4})$$

Where V is the total volume of an aggregate, dV is the volume element, and $C(g)$ is the local elastic stiffness tensor with a grain orientation g (e.g., Bunge Euler angles $g = (\phi_1, \Phi, \phi_2)$; see Appendix A for further details).

B2. Christoffel equation

Elastic wave velocities and polarizations (or displacement vectors) in an anisotropic elastic medium can be calculated using the Christoffel (1877) equation (e.g., Mainprice et al., 2011). The Christoffel tensor T_{ik} for a unit propagation direction \vec{n} in an anisotropic elastic medium with the elastic stiffness tensor C_{ijkl} is defined as follows:

$$T_{ik}(\vec{n}) = C_{ijkl} \vec{n}_j \vec{n}_l. \quad (\text{B5})$$

The eigenvalues λ_1 , λ_2 , and λ_3 of the Christoffel tensor $T_{ik}(\vec{n})$ are related to the compressional (P) wave and fast (S1) and slow (S2) shear wave, respectively. The plane wave velocities V_P , V_{S1} , and V_{S2} propagating in the direction \vec{n} are described with the material density ρ as follows:

$$V_P = \sqrt{\frac{\lambda_1}{\rho}}, \quad (\text{B6})$$

$$V_{S1} = \sqrt{\frac{\lambda_2}{\rho}}, \quad (\text{B7})$$

$$V_{S2} = \sqrt{\frac{\lambda_3}{\rho}}, \quad (V_{S1} > V_{S2}). \quad (\text{B8})$$

The three eigenvectors of the Christoffel tensor represent the polarization directions of P-, S1-, and S2-waves.

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