User Guide

AnisEulerSC

January 16, 2020

Contents

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 script. For 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 and runs in MATLAB version after R2016b in Windows or UNIX OS. In Section 2.2, an example is provided as a guideline on how to use AnisEulerSC-Inputs program.

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. Example

2.1. What is your target material?

We consider lherzolite, which is a type of ultramafic igneous rock, to make a polycrystalline aggregate using 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-5.2.7) and initialize MTEX as follows.

```
>> startup_mtex
initialize MTEX 5.2.7  .... done!

MTEX 5.2.7 (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 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

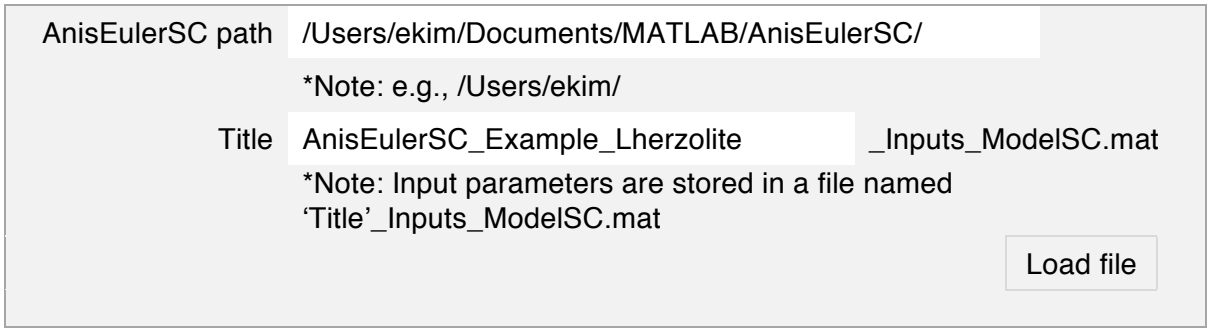
To generate the input data for SC modeling, AnisEulerSC-Inputs program is used. In this section, the construction of a polycrystalline aggregate composed of 83% forsterite, 14% enstatite, and 3% diopside (as described in Section 2.1) and the preparation of input

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
```

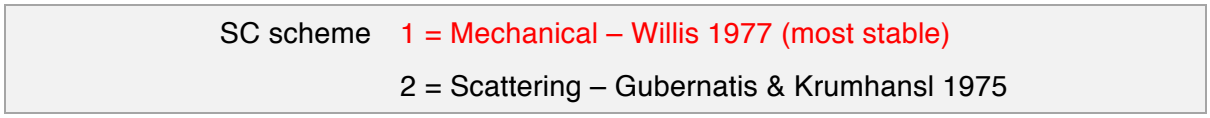
2.2.1. Setup tab

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



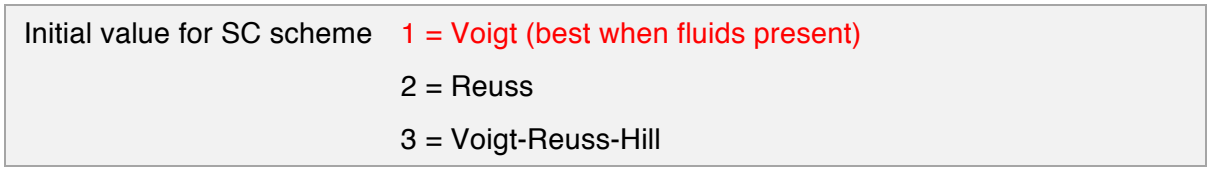
Note: If the file named as 'Title'_Inputs_ModelSC.mat exists in the AnisEulerSC path, you can load data by clicking 'Load file'. If it does not exist, the file is created.

- Select the type of SC scheme.



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.



- 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.

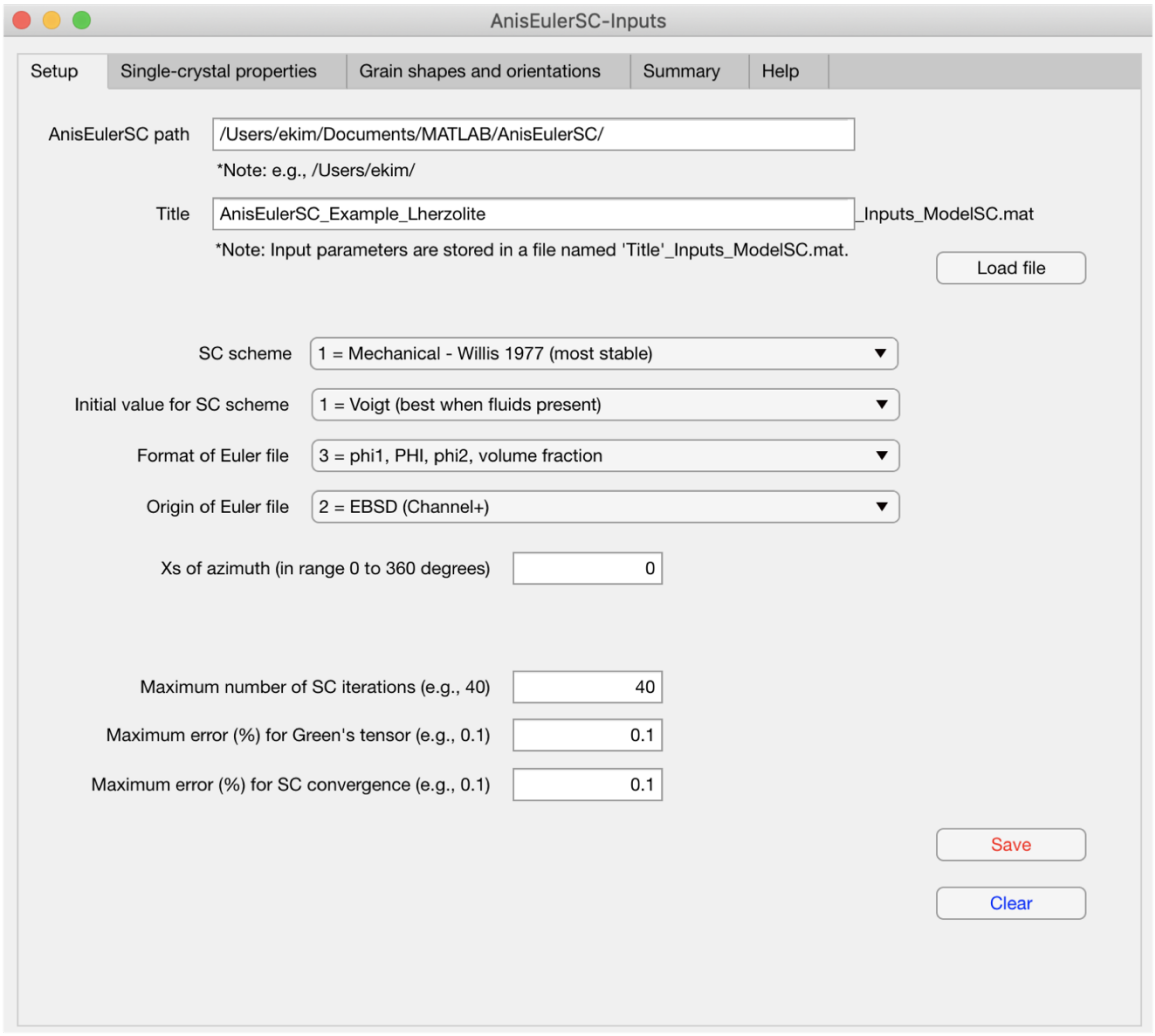


Figure 1. Setup tab of AnisEulerSC-Inputs, a MATLAB-based program composed of graphical user interfaces (GUIs).

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, on the 'Phase' panel.

No.	Name	Volume fraction
1	Forsterite	0.83

Reference	Isaak et al. (1989); Fujino et al. (1981)		
Density (g/cm^3)	3.221		
Crystal symmetry	mmm		
Crystal reference frame	Xlla, Zllc		
Crystal coordinate system	a	b	c
	4.8	10	6
	alpha	beta	gamma
	90	90	90

Single-crystal elastic stiffness tensor in Voigt matrix, C_{ij} (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

Save

Name: Forsterite Load Clear phase

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, click 'Load' button.

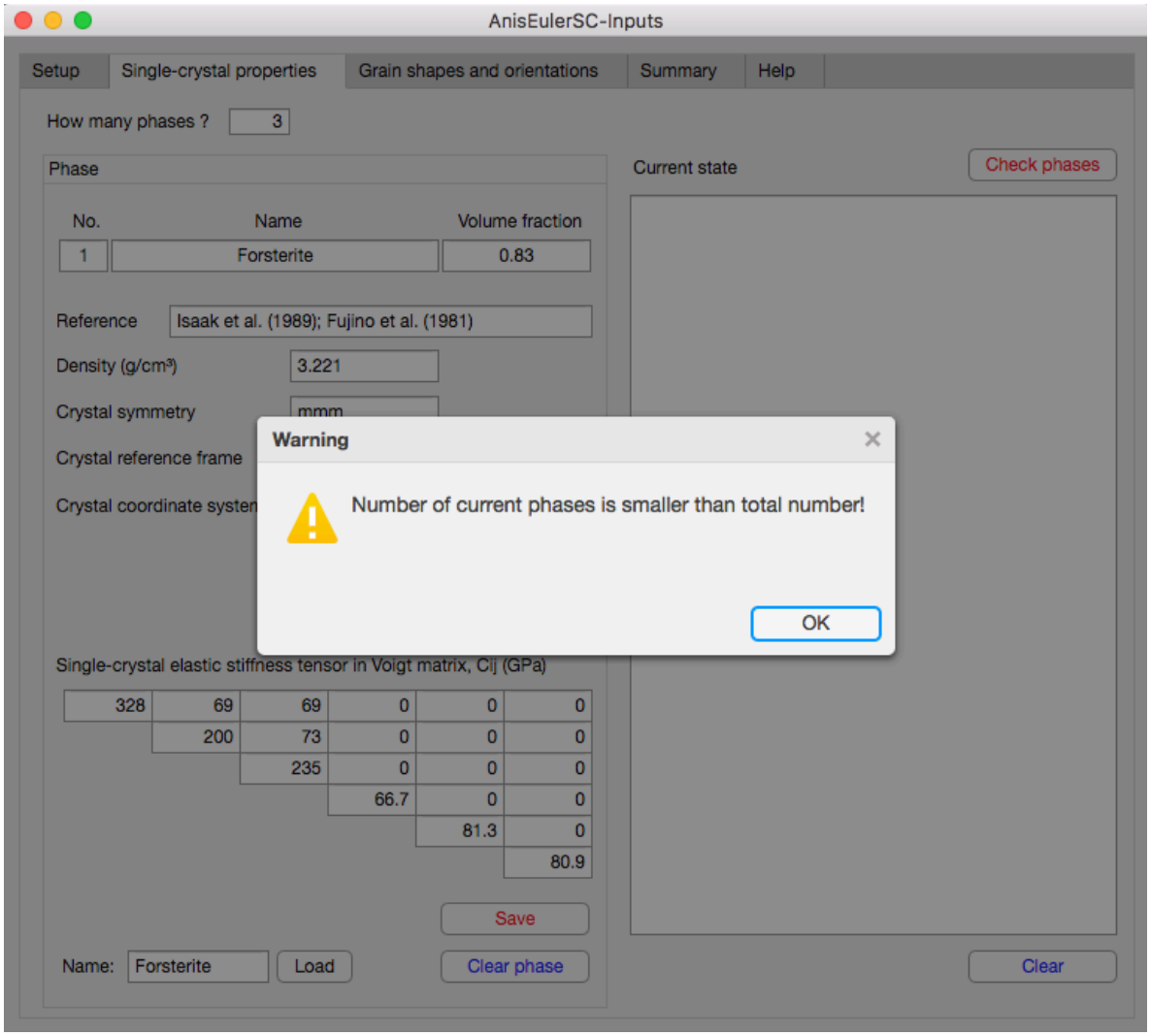
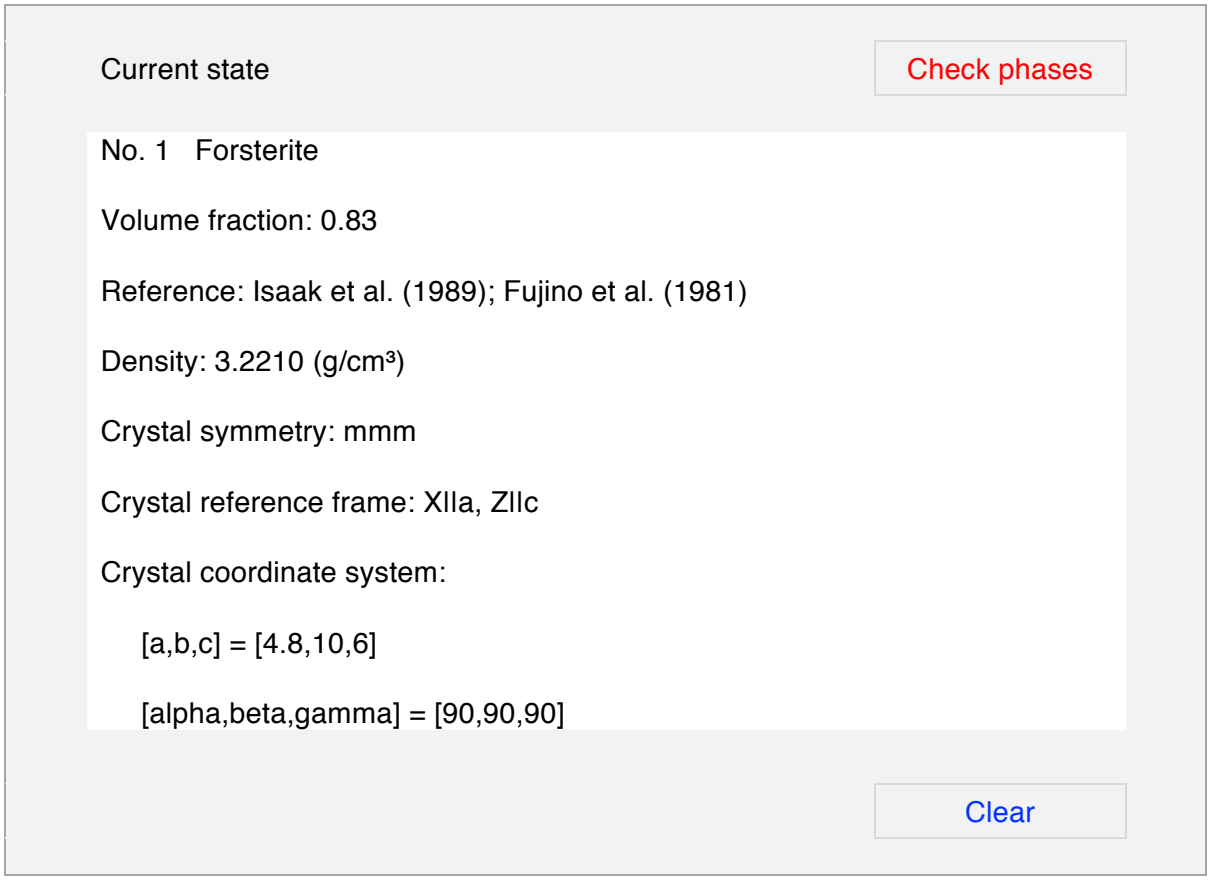


Figure 2. Pop-up message for warning showing that the number of current phases is smaller than the total number specified in advance. Click 'OK' to move onto the next phase.

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



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.

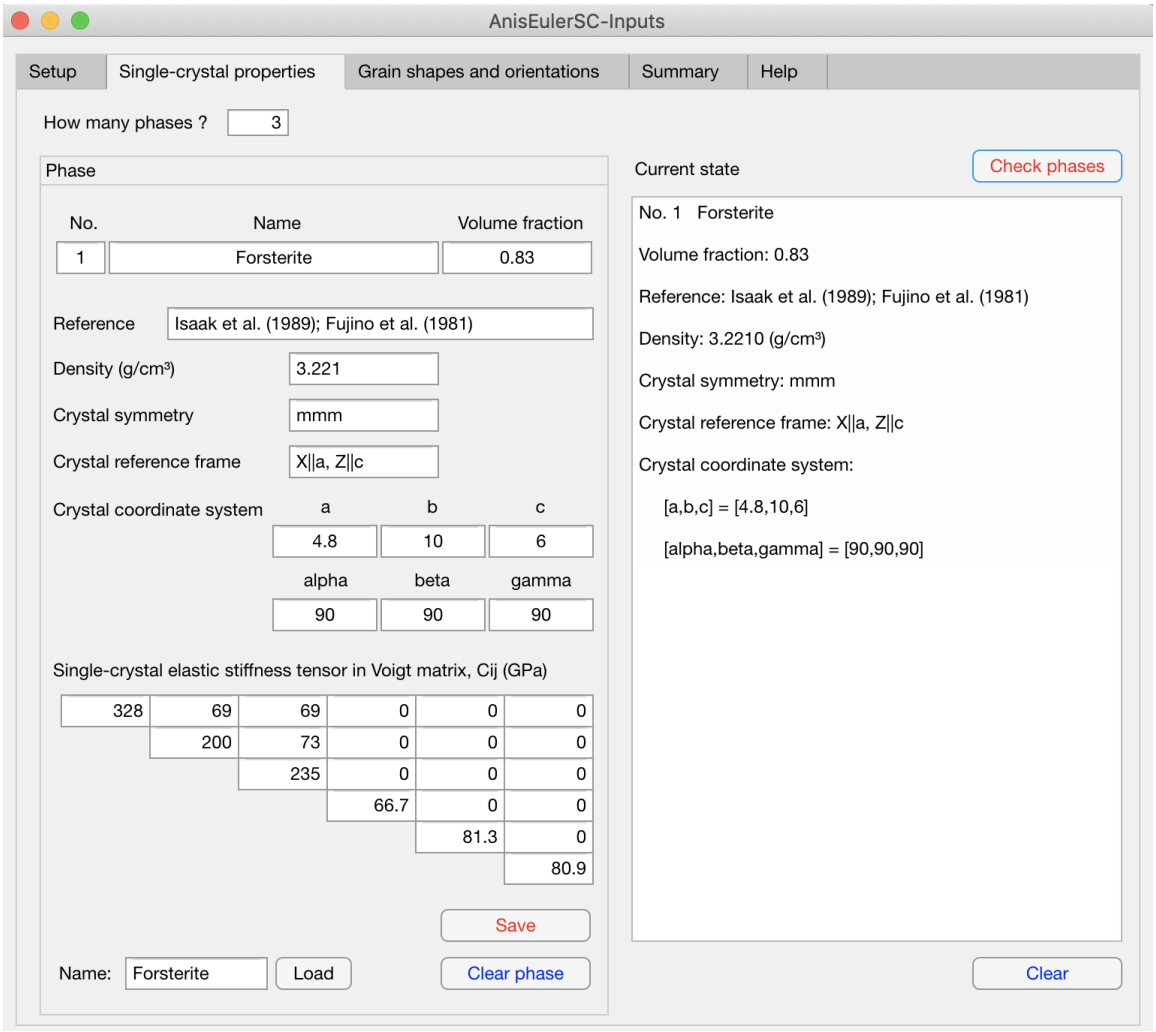


Figure 3. Single-crystal properties tab of AnisEulerSC-Inputs. For the first phase (forsterite), all input data are specified, saved and checked on the 'Current state' screen.

- Specify the single-crystal properties for the second phase, Enstatite, on the 'Phase' panel.

No.	Name	Volume fraction
2	Enstatite	0.14

Reference	Chai et al. (1997)		
Density (g/cm^3)	3.306		
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

Single-crystal elastic stiffness tensor in Voigt matrix, C_{ij} (GPa)

236.9	79.6	63.2	0	0	0
	180.5	56.8	0	0	0
		230.4	0	0	0
			84.3	0	0
				79.4	0
					80.1

Save

Name: Enstatite Load Clear phase

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, click 'Load' button.

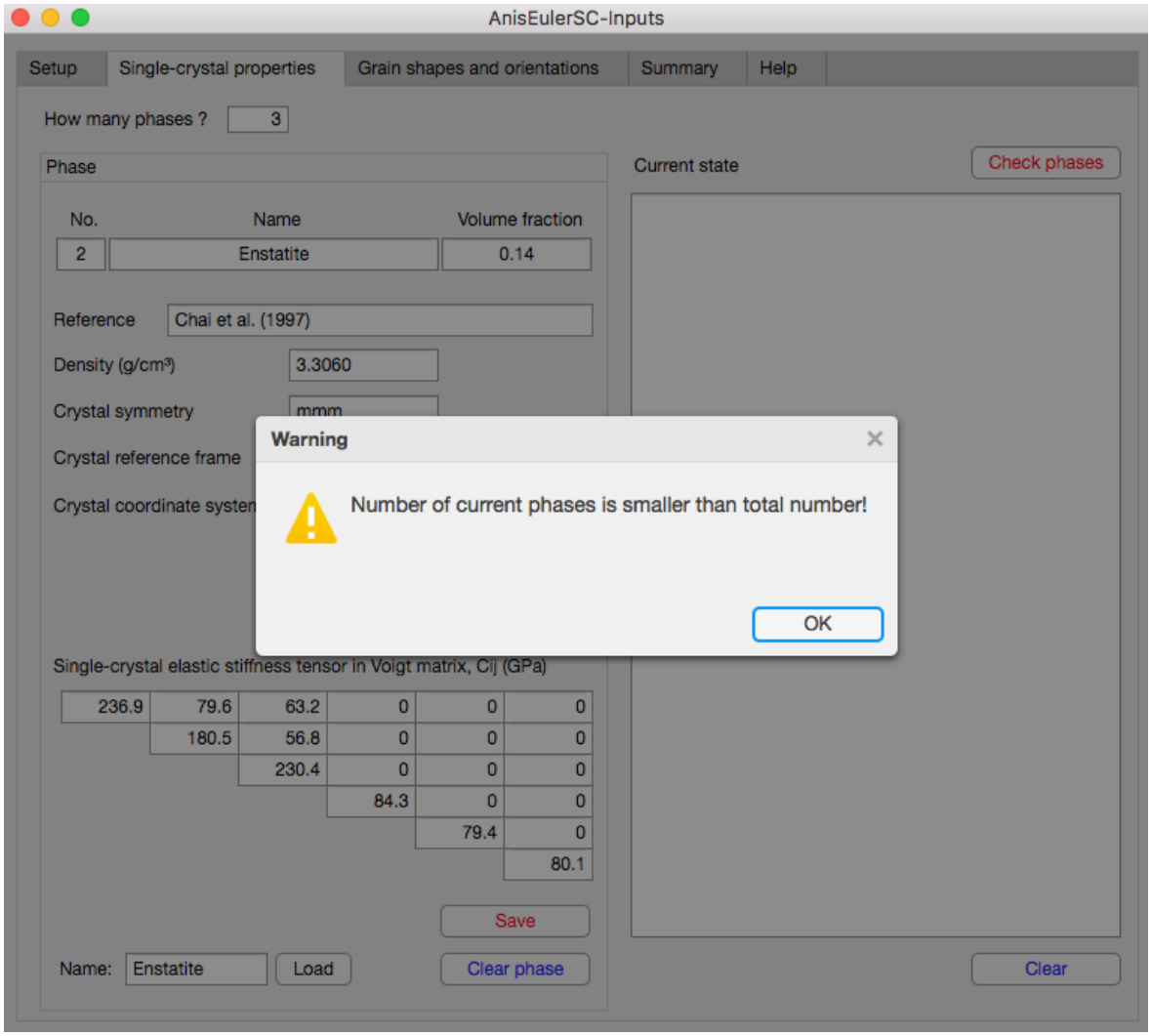
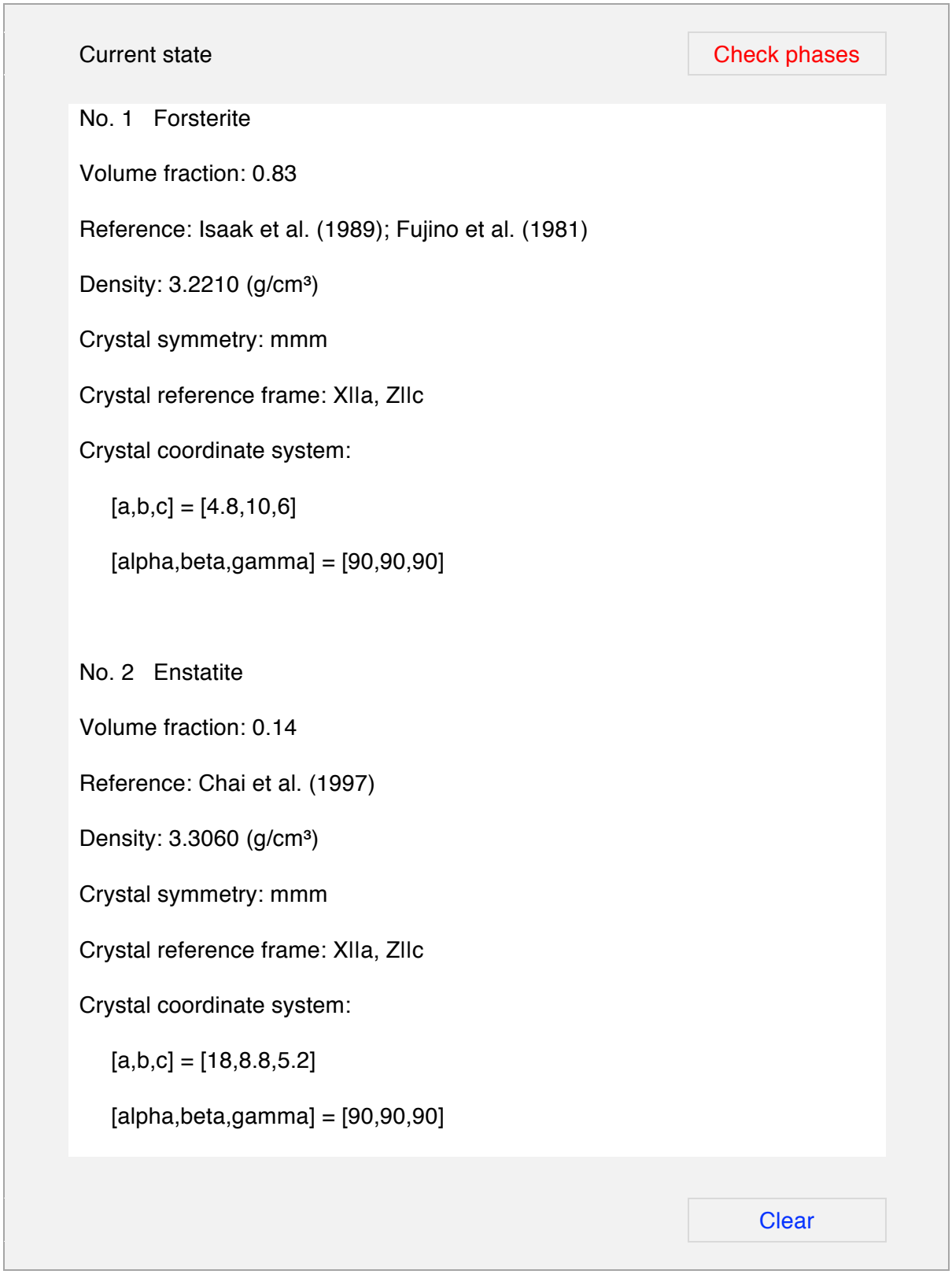


Figure 4. Pop-up message for warning showing that the number of current phases is smaller than the total number specified in advance. Click 'OK' to move onto the next phase.

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



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.

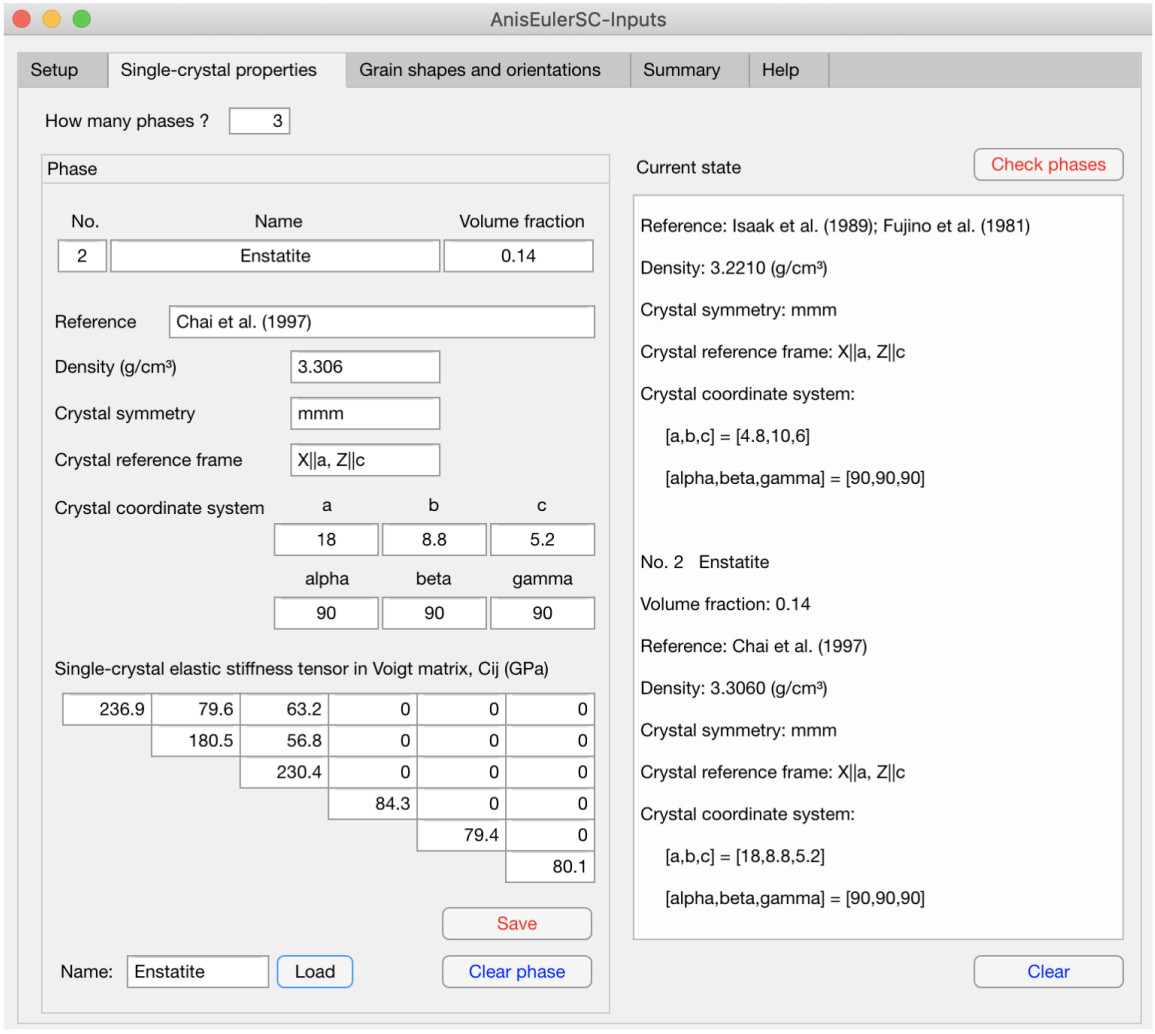


Figure 5. Single-crystal properties tab of AnisEulerSC-Inputs. For the second phase (enstatite), all input data are specified, saved and checked on the 'Current state' screen.

- Specify the single-crystal properties for the third phase, Diopside, on the 'Phase' panel.

No.	Name	Volume fraction
3	Diopside	0.03

Reference	Isaak et al. (2005)		
Density (g/cm^3)	3.286		
Crystal symmetry	12/m1		
Crystal reference frame	Xlla*, Ylb*, Zllc		
Crystal coordinate system	a	b	c
	9.7	9	5.3
	alpha	beta	gamma
	90	105.63	90

Single-crystal elastic stiffness tensor in Voigt matrix, C_{ij} (GPa)

228.1	78.8	70.2	0	7.9	0
	181.1	61.1	0	5.9	0
		245.4	0	39.7	0
			78.9	0	6.4
				68.2	0
					78.1

Save

Name: Diopside Load Clear phase

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, click 'Load' button.

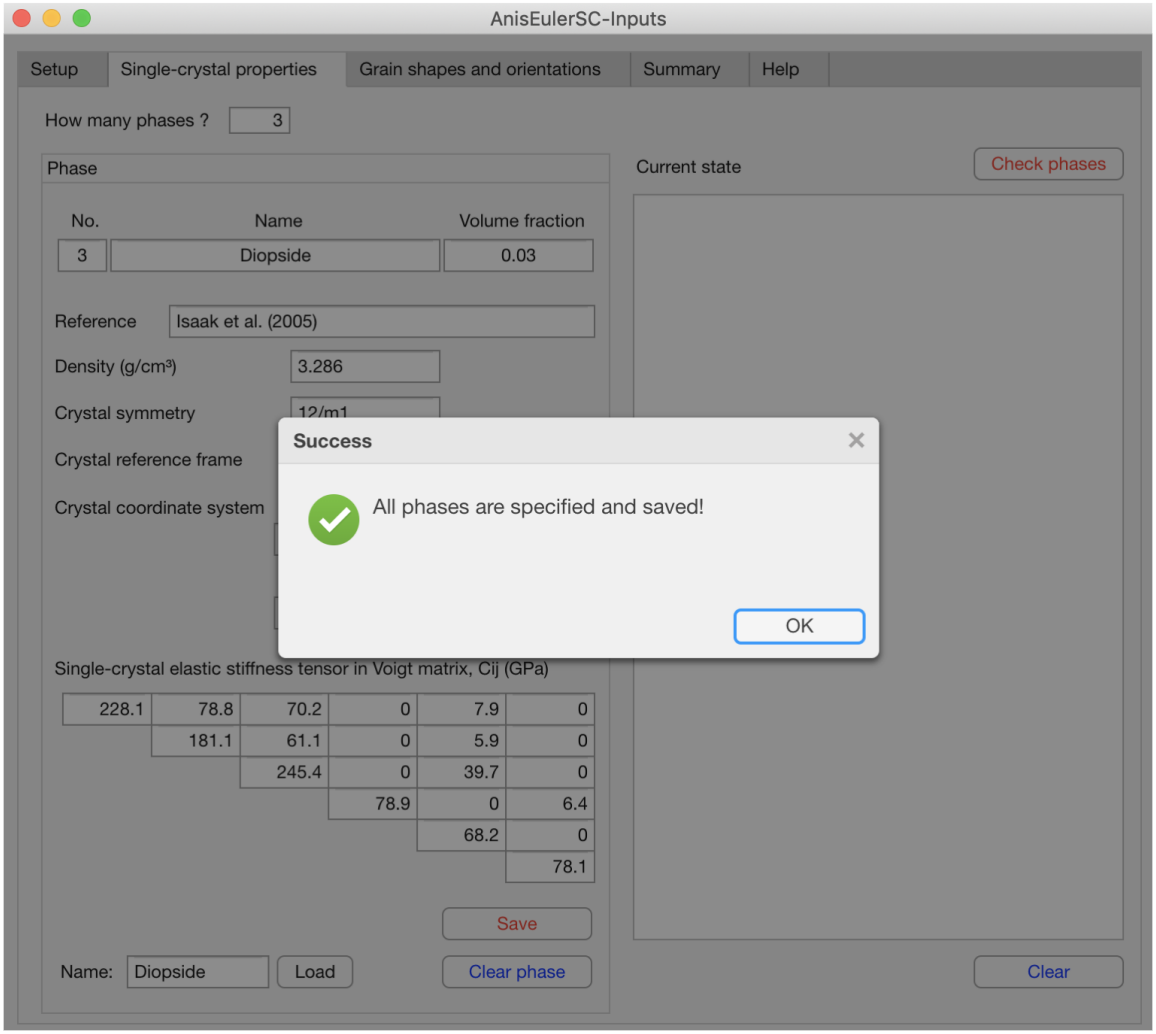


Figure 6. Pop-up message when the number of current phases is same with the total number specified in advance. Click 'OK' to move onto the next step.

- 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); Fujino et al. (1981)

Density: 3.2210 (g/cm³)

Crystal symmetry: mmm

Crystal reference frame: X||a, Z||c

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)

Density: 3.3060 (g/cm³)

Crystal symmetry: mmm

Crystal reference frame: X||a, Z||c

Crystal coordinate system:

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

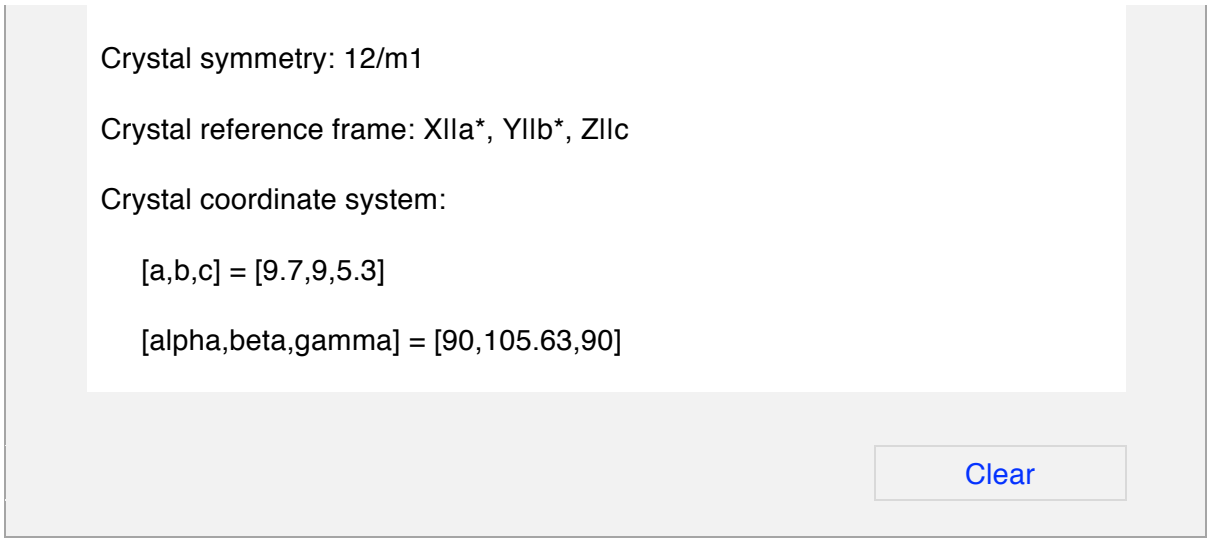
[alpha,beta,gamma] = [90,90,90]

No. 3 Diopside

Volume fraction: 0.03

Reference: Isaak et al. (2005)

Density: 3.2860 (g/cm³)



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.

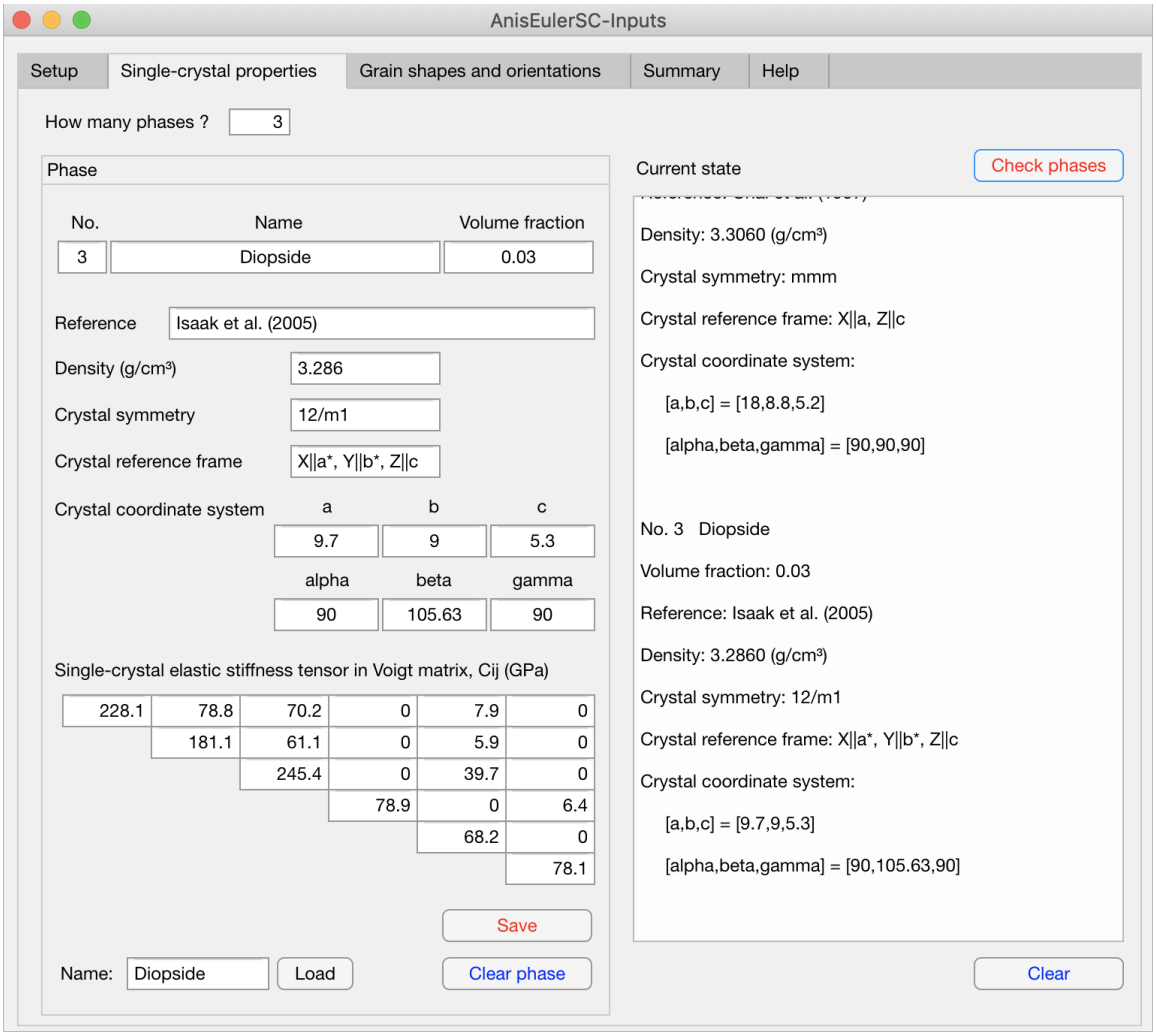


Figure 7. Single-crystal properties tab of AnisEulerSC-Inputs. For the third phase (diopside), all input data are specified, saved and checked on the 'Current state' screen.

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)

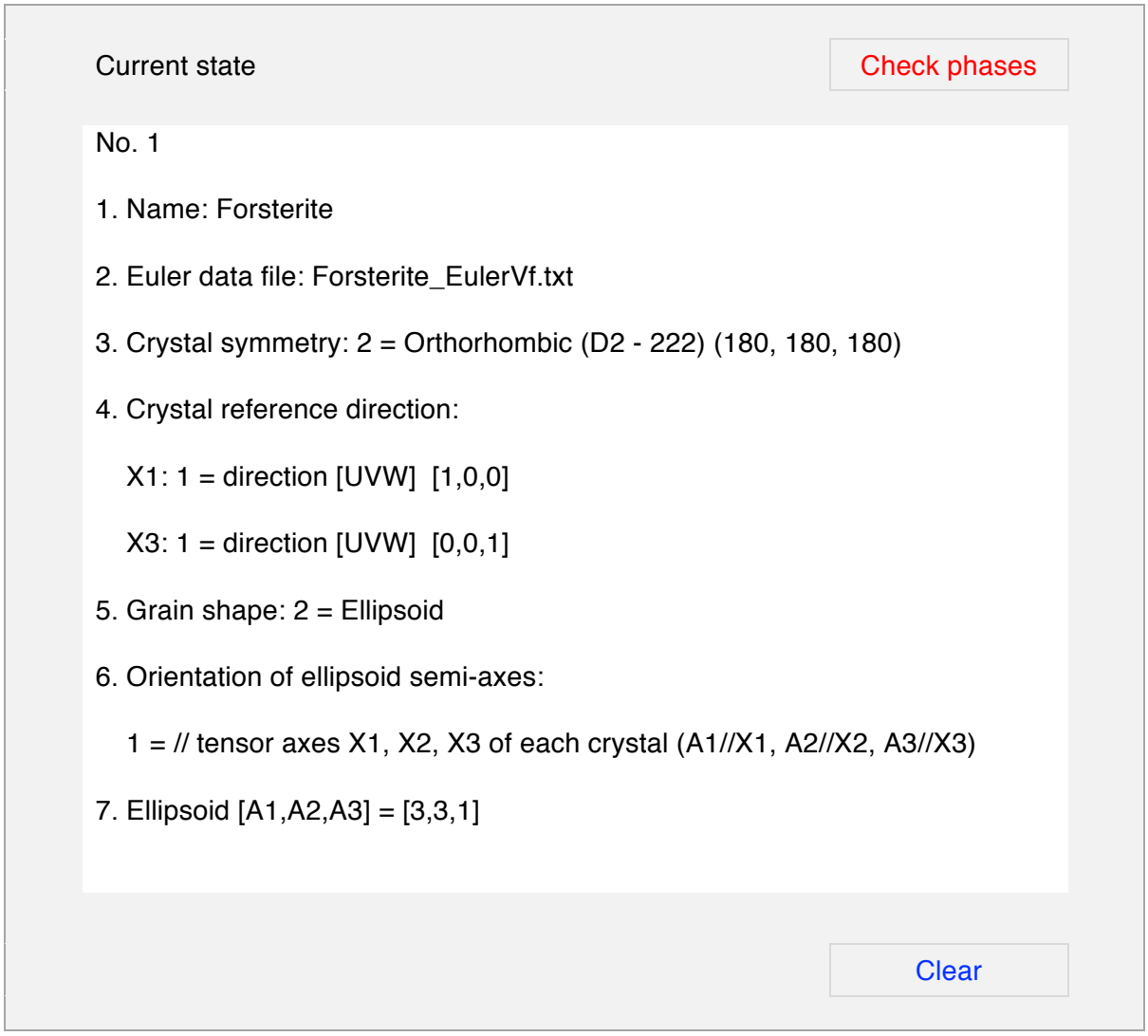
		AZ	INC
AZ: Azimuth of ellipsoid semi-axis	A1		
INC: Inclination of ellipsoid semi-axis	A3		

Save

Name: Forsterite Load 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.



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.

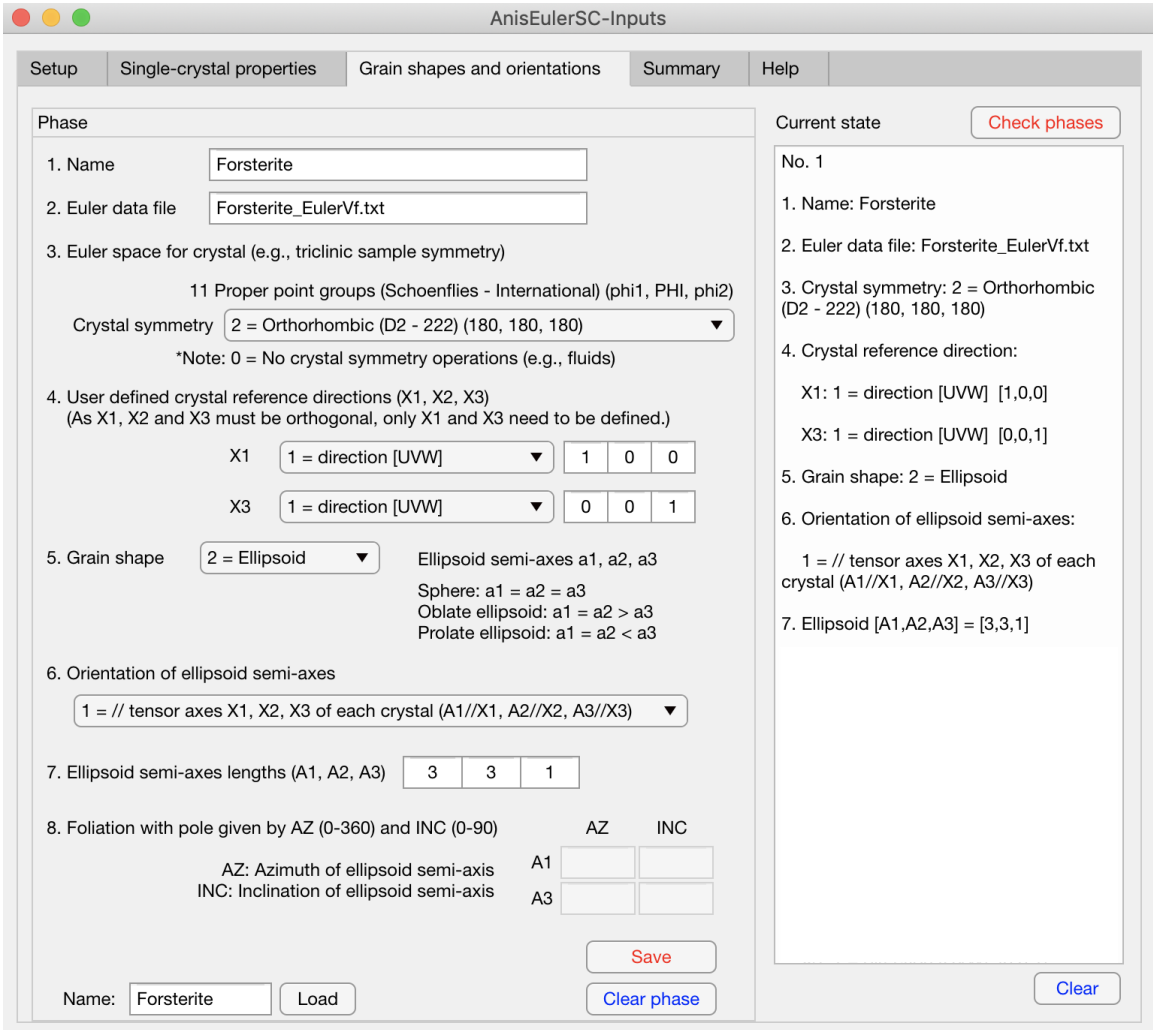


Figure 8. Grain shapes and orientations tab of AnisEulerSC-Inputs. For the first phase (forsterite), all input data are specified, saved and checked on the 'Current state' screen.

- Repeat for the next phase of Enstatite.

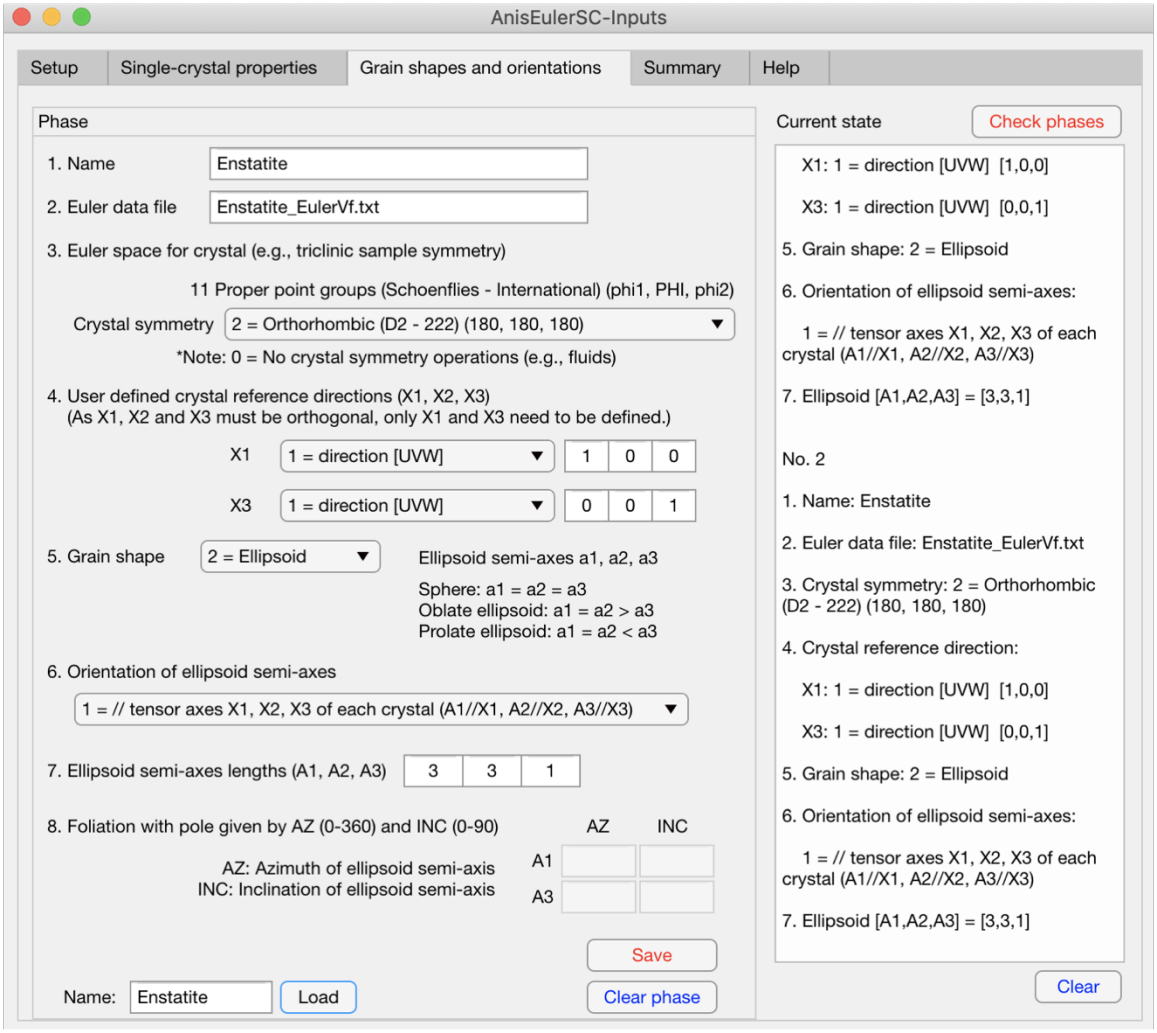


Figure 9. Grain shapes and orientations tab of AnisEulerSC-Inputs. For the second phase (enstatite), all input data are specified, saved and checked on the 'Current state' screen.

- Repeat for the next phase of Diopside.

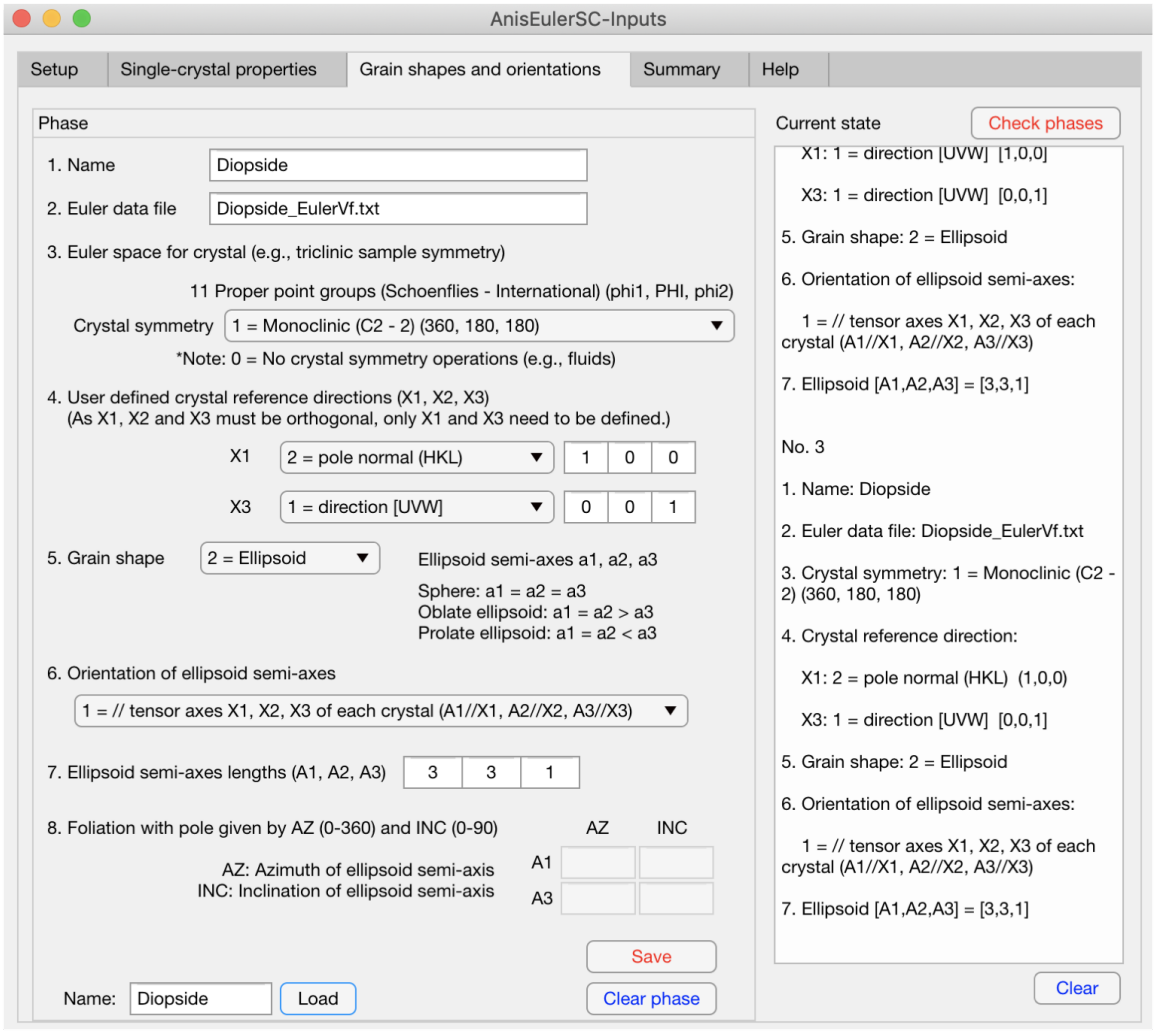


Figure 10. Grain shapes and orientations tab of AnisEulerSC-Inputs. For the third phase (diopside), all input data are specified, saved and checked on the 'Current state' screen.

2.2.4. Summary tab

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

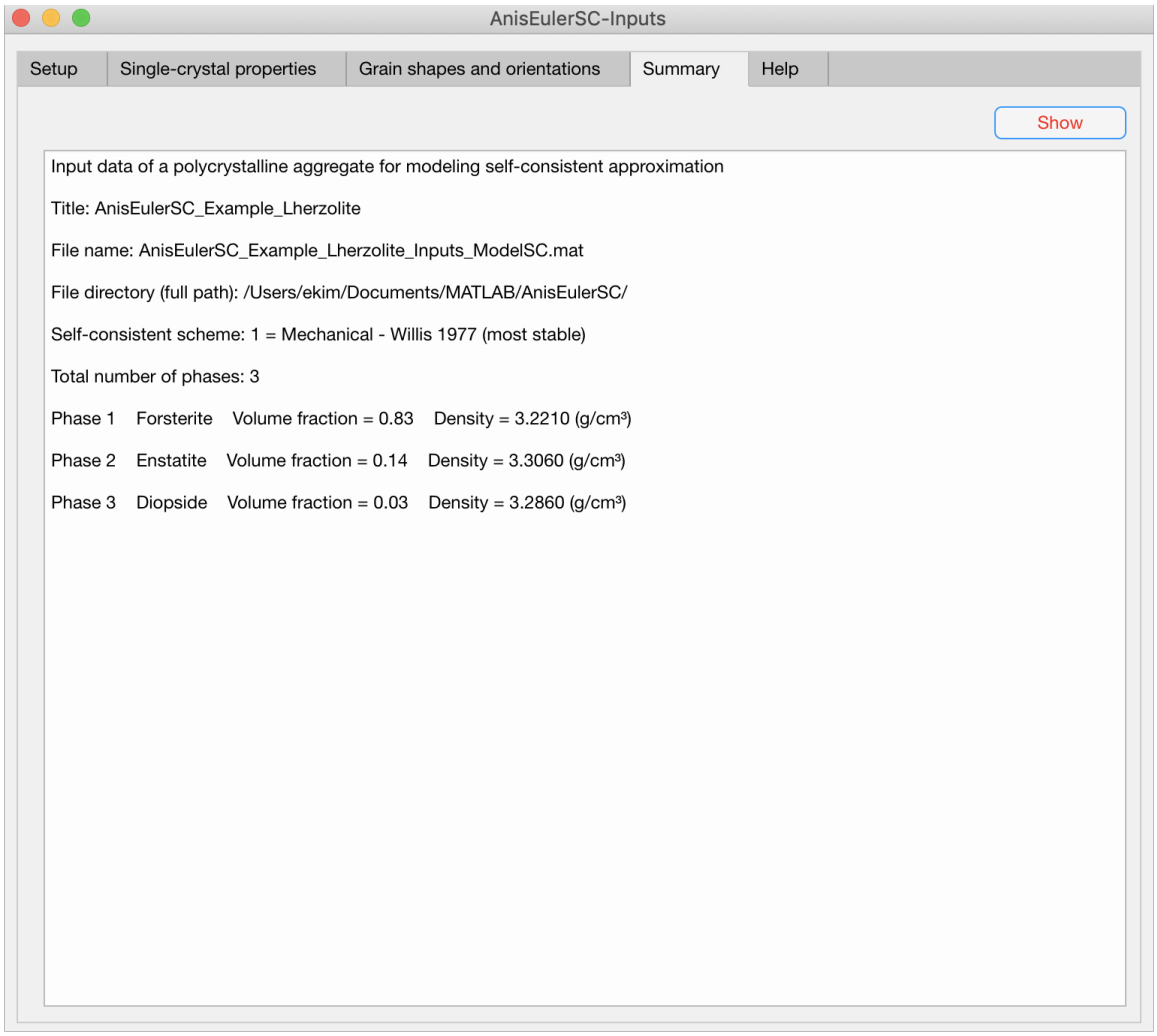


Figure 11. Summary tab of AnisEulerSC-Inputs.

2.2.5. Help tab

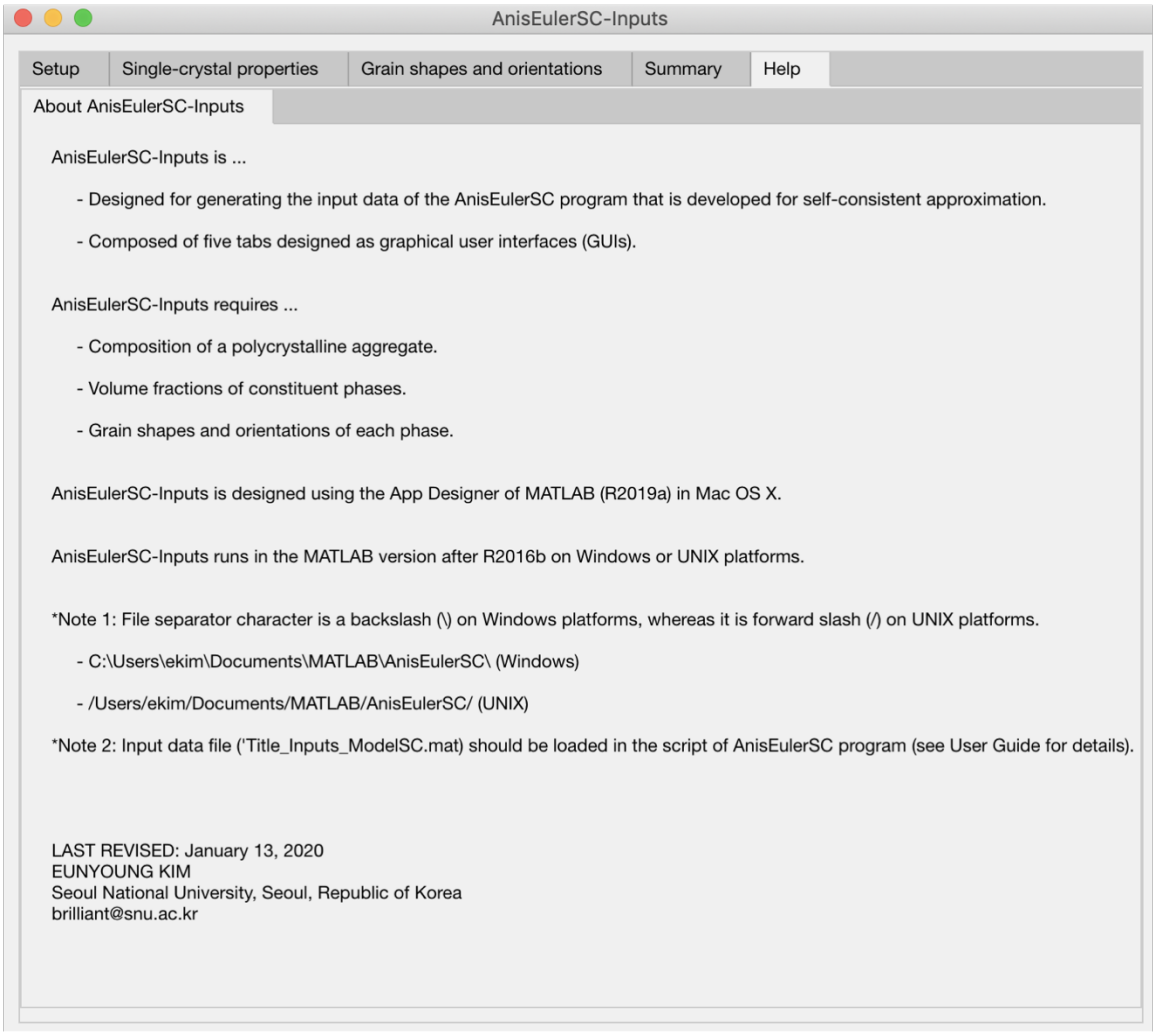


Figure 12. Help tab of AnisEulerSC-Inputs. The information of AnisEulerSC-Inputs is described in the About AnisEulerSC-Inputs tab.

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');
```

References

Gubernatis, J. E. & Krumhansl, J. A. (1975). Macroscopic engineering properties of polycrystalline materials: Elastic properties. *Journal of Applied Physics*, 46(5), 1875-1883. https://doi.org/10.1063/1.321884.

Hielscher, R. & Schaeben, H. (2008). A novel pole figure inversion method: specification of the MTEX algorithm. *Journal of Applied Crystallography*, 41(6), 1024-1037. https://doi.org/10.1107/S0021889808030112.

Mainprice, D. (1997). Modelling the anisotropic seismic properties of partially molten rocks found at mid-ocean ridges. *Tectonophysics*, 279 (1), 161-179. https://doi.org/10.1016/S0040-1951(97)00122-4.

Tommasi, A., Vauchez, A., & Ionov, D. A. (2008). Deformation, static recrystallization, and reactive melt transport in shallow subcontinental mantle xenoliths (Tok Cenozoic volcanic field, SE Siberia). *Earth and Planetary Science Letters*, 272(1), 65-77. /https://doi.org/10.1016/j.epsl.2008.04.020

Willis, J. R. (1977). Bounds and self-consistent estimates for the overall properties of anisotropic composites. *Journal of the Mechanics and Physics of Solids*, 25(3), 185-202. https://doi.org/10.1016/0022-5096(77)90022-9.