Win_Strain
Users manual

A program to calculate strain tensors from unit-cell parameters.

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INTRODUCTION

The changes in unit-cell parameters of a crystalline material, whether induced by changes in pressure, temperature, composition, or a structural phase transition, are best expressed in terms of the fractional changes, or strains. The strains form a second-rank tensor which can be calculated directly from the two sets of cell parameters, given a definition of the type of strain, and a definition of a set of Cartesian reference axes on which the components of the strain tensor are defined.

Ohashi previously developed a program called *Strain*, which was described in Ohashi and Burnham (1973), and the code was listed in Hazen and Finger (1982). The Ohashi strain program calculated the Lagrangian infinitesimal strain tensor on a set of Cartesian axes with X // a* and Z // c which was the traditional orientation specified by the *IRE*. A full description of the calculations involved is given in Hazen and Finger (1982) and Schlenker et al (1978).

The Lagrangian strain tensor is specified with respect to the initial starting values. But the Eulerian finite strain, specified with respect to the final state is found to be a more appropriate for describing the high-pressure behaviour of materials. I have therefore re-written the program to allow the calculation of both the finite Lagrangian and both the infinitesimal and finite Eulerian strain tensors, as specified by Schlenker et al (1978). In practise, for small strains, these four tensors are indistinguishable at the level of typical experimental uncertainties. The appropriate property tensor (compressibility or thermal expansion) is also calculated for each strain definition.

In addition, I have added two further choices of Cartesian axial systems. The choice of Cartesian axial system only affects the values of the components of the strain tensor, not the orientation of its principal axes with respect to the crystallographic axes, nor the magnitudes of its principle axes, nor the strain ellipsoid. I have rewritten the code to be more robust in solving the eigenvalue problem of determining the orientation of the principal axes of the strain in the monoclinic and triclinic crystal systems. For orthorhombic and higher symmetries the orientation of the principal axes are constrained by symmetry to be parallel to the Cartesian axes and no explicit orientation calculation is performed. This reduces the quantity of spurious output from the program. and does not require calculation.

1. INSTALLATION

1. The win_strain.zip file contains the executable and this manual as a *pdf* file, along with three data files (*.dat) and the output files generated from them by running Win_strain.

2. Extract the win_strain.exe and the *pdf* file containing this manual into one folder. It is recommended that this folder is not used for data files.

3. Extract the example files to a working directory.

4. Create a shortcut to win_strain.exe either in the working directory, or on the desktop, by right-clicking on the file, dragging to the working directory or desktop and then selecting "create shortcut".

5. Run the program by double-clicking on the shortcut.

2. INPUT DATA FILE

The format of the input data file has been substantially modified and made more flexible than the format of the original strain program. Several examples are provided in the win_strain.zip distribution file.

The first lines of the data file consist of a keyword followed by information, as in this example:

TITLE   Albite at high pressure: Benusa et al (2005) Amer Miner 90, 1115-1120
LINES   1
LINE1   p sigp A SIGA B SIGB C SIGC ALPHA SIGAL BETA SIGBE GAMMA SIGga VOLUME SIGV
DATA
0.000001,0.0000001,8.1409,0.0008,12.7883,0.0005,7.1602,0.0007,94.251,0.007,116.586,0.007,87.676,0.006,664.777,0.085
0.455,0.007,8.1074,0.0010,12.7678,0.0005,7.1481,0.0006,94.246,0.009,116.683,0.008,87.717,0.007,659.272,0.090
1.438,0.007,8.0381,0.0012,12.7280,0.0005,7.1231,0.0007,94.246,0.008,116.839,0.010,87.794,0.007,648.461,0.104

TITLE allows a title to be put on the file. It does not get used by the program.

LINES specifies how many lines of the data file will be used for the cell parameter data for each temperature or pressure. The allowed values are 1 or 2.

LINE1 must always be given specifies the data that will be given on the first line for each temperature or pressure.

LINE2 is only allowed if **LINES 2** has been specified. It then describes the data that will be given on the second line for each temperature or pressure.

The example given above has one line for each data point. It specifies that each line will contain a value for the pressure (p), its uncertainty (sigp), and then all of the unit-cell parameters, with each followed by its standard deviation. The volume is not required for strain calculations, but may be given. The uncertainties are also not required but, if they are present, uncertainties in the magnitude and orientation of the strain ellipsoid will be calculated.

If the data was measured as a function of varying temperature, this may be specified with 'T' with 'sigT' specifying the uncertainty.

If the crystal system is of higher symmetry than triclinic this may be specified with the keyword **SYSTEM**, for example:

SYSTEM TETRAGONAL

If the crystal system is specified in this way, then only the symmetry-independent unit-cell parameters have to be given. The program will set the remaining unit-cell parameters to correspond to the conventional setting of the crystal system. The monoclinic system is set with *b* unique.

The last keyword must be **DATA**, on a line on its own. The unit-cell data is then entered on the following lines, with the format specified by the information with **LINE1** and possibly **LINE2.** The order in which the different unit-cell parameters on each line or lines must always match the order specified on the **LINE1** and possibly **LINE2,** but can be in any order.

The order of the data points (e.g. increasing or decreasing pressure, or temperature) depends on the calculations you want to do. See the section on running the program.
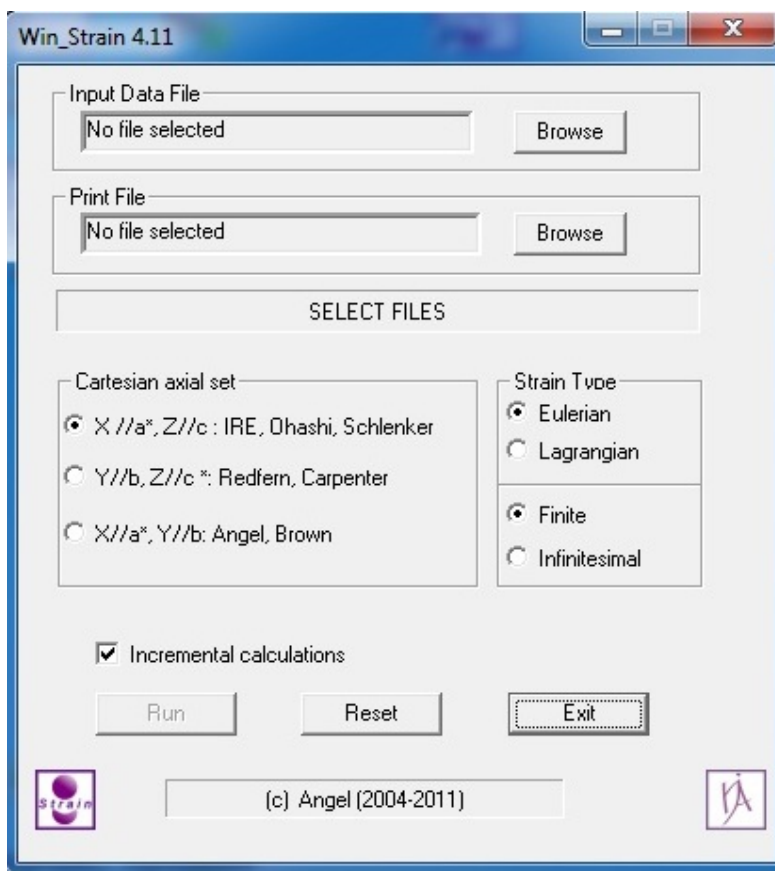
Here is an example for a tetragonal crystal with two lines for each data point, the first line with the temperature and the unit-cell parameters, and the second line with the uncertainties on the unit-cell parameters:

```
SYSTEM TETRAGONAL
LINES  2
LINE1  T A  C
LINE1   SIGA SIGC
DATA
300,4.9805,9.7923
0.0010,0.0019
320,4.9810,9.8017
0.0009,0.0020
```

In this case the program will use the information that the crystal system is tetragonal to set $b = a$ and $\alpha = \beta = \gamma = 90^\circ$.

3. RUNNING THE PROGRAM

Start the program by double-clicking on the shortcut. The Win_strain dialogue box will appear:

Some guidance as to what to do at each step is provided in the message window (that says "Select Files" in the example above).

Use the *Browse* buttons to select the data file with your unit-cell parameter data, and a file to which the results will be printed.

Then select the choice of Cartesian axial set on which the tensor components will be calculated.

Select the strain definition you want to use – Lagrangian or Eulerian. Select finite or infinitesimal. For high-pressure data it is normal to use Euelrian finite strain to be consistent with the common forms of equations of state (e.g. Birch-Murnaghan).

Choose the mode in which to do the calculations:

1. If *Incremental* is **checked** then the strains will be calculated from each data point to the next one.

2. If *Incremental* is **not checked** then the strains will be calculated from the first data point in the input file to each of the subsequent data points. This is useful for calculating the strains from zero pressure to each high-pressure data point.

Then push the *Run* button to run the calculations and produces several output files.

The print file contains the results of all of the calculations. For each calculation from a pair of unit-cell parameters the output is:

- the unit cell parameters,
- the reciprocal unit-cell parameters,
- the relative orientation of the Cartesian and crystal axial systems,
- the S matrices for transformations between the crystal axial system and Cartesian,
- the selected strain tensor calculated from the cell parameters, and the corresponding property tensor (thermal expansion or compressibility)
- the esd's on the strain and property tensors (if esd's for the unit-cell parameters were provided)
- If the crystal system is monoclinic or triclinic the orientation of the strain ellipsoid is given as well as the uncertainties in its orientation and the lengths of its principal axes (if uncertainties for the unit cell parameters were provided in the input data file).

Additional output files are created by the program to provide the results in formats suitable for import in to plotting programs:

_strain.cal contains on each line the components of the strain tensor. The column 'mid pt' gives the average of the pressures or temperatures of the two data points used to calculate the strain. The file has two columns for each component; the value followed by the esd.

_tensor.cal contains on each line the components of the compressibility or thermal expansion tensor. That is, the components of the strain tensor divided by difference in pressure or temperature between the two unit-cell parameter measurements. The column 'mid pt' gives the average of the pressures or temperatures of the two data points used to calculate the strain. The file has two columns for each component; the value followed by the esd.

_prin.cal is only produced for calculations in the monoclinic and triclinic crystal systems. For each strain calculation it has 3 lines of output, one for each principal strain. It contains on each line the lengths of one of the principal axes of the strain and the tensor property, plus the angles of this principal axis to the Cartesian and unit-cell axes.

4. EXAMPLE FILES

The distribution zip contains the input and output files for three examples:

- Kalsilite is a hexagonal material that undergoes a high-pressure phase transition without a symmetry change (Gatta et al. 2011). The example files have the Eulerian finite strains calculated at each pressure relative to the zero-pressure datum (i.e. *not* incremental). There is no calculation of the orientation of the strain ellipsoid, because it is fixed by symmetry.
- $LiGaSi_2O_6$ is a monoclinic pyroxene which undergoes the $P2_1/c$ to $C2/c$ phase transition (Camara et al. 2009). In this example the Lagrangian infinitesimal incremental strains from one data point to the next are calculated in the output files.
- AlbiteHP is an example of a triclinic unit-cell under compression. Data from Benusa et al. (2005). The incremental Eulerian finite strains from one data point to the next are calculated in the output files. The print file includes the description of the orientation of the ellipsoid with respect to the chosen Cartesian axial set, and to the unit-cell axes. This information is also written to the *albiteHP_prin.cal* file.

REFERENCES

Benusa M, Angel RJ, Ross NL (2005) Compression of albite, $NaAlSi_3O_8$. *American Mineralogist* 90:1115-1120.

Camara F, Nestola F, Angel RJ, Ohashi H (2009) Spontaneous strain variations through the low temperature displacive phase transition of $LiGaSi_2O_6$ clinopyroxene. *European Journal of Mineralogy* 21:599-614.

Gatta GD, Angel RJ, Rotiroti N, Zhao J, Alvaro M, Carpenter MA (2011) Phase-stability, elastic behavior and pressure-induced structural evolution of kalsilite: a ceramic material and high-T/high-P mineral. *American Mineralogist* 96:1363-1372.

Hazen RM, Finger LW (1982) *Comparative Crystal Chemistry.* John Wiley and Sons.

Ohashi Y, Burnham CW (1973) Clinopyroxene lattice deformations: The roles of chemical substitution and temperature. *American Mineralogist* 58, 843-849.

Schlenker JL, Gibbs GV, Boisen MB (1978) Strain tensor components expressed in terms of lattice parameters. *Acta Crystallographica* A34, 52-54.