

# **stRAinMAN**

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stRAinMAN is a computer program written for Windows operating systems to calculate strains from changes in Raman (or other phonon) mode wavenumbers, and vice-versa, using the concept of the phonon-mode Grüneisen tensor.

Details of the theory are provided in the manuscript provided in this distribution. This document provides a brief set of instructions for using the program.

stRAinMAN is currently supplied on a non-commercial basis. Therefore, you must acknowledge of the use of the program when you publish results that have been obtained with it. Relevant literature is:

- Program: Angel RJ, Murri M, Mihailova B, Alvaro M (2019) Stress, strain and Raman shifts. *Zeitschrift für Kristallographie*, 234, 129-140. Open access. doi:10.1515/zkri-2018-2112
- Grüneisen tensor components for quartz: Murri M, Alvaro M, Angel RJ, Prencipe M, Mihailova BD (2019) The effects of non-hydrostatic stress on the structure and properties of alpha-quartz. *Physics and Chemistry of Minerals* 46:487-499 doi:10.1007/s00269-018-01018-6
- Grüneisen tensor components for zircon: Stangarone C, Angel R, Prencipe M, Campomenosi N, Mihailova BD, Alvaro M (2019) Measurement of strains in zircon inclusions by Raman spectroscopy. *European Journal of Mineralogy* 31:685-694 doi:10.1127/ejm/2019/0031-2860
- Grüneisen tensor components for rutile: Musiyachenko KA, Murri M, Prencipe M, Angel RJ, Alvaro M (2021) A Grüneisen tensor for rutile and its application to host-inclusion systems. *Amer Min* 106:1586-1595. doi:10.2138/am-2021-7618

Strains of inclusions calculated with stRAinMAN can be used to calculate entrapment conditions with the EntraPT software at [www.mineralogylab.com/software/entrap/](http://www.mineralogylab.com/software/entrap/). Examples of how to use both programs have been published in:

- Bonazzi M, Tumiati S, Thomas J, Angel RJ, Alvaro M (2019) Assessment of the reliability of elastic geobarometry with quartz inclusions. *Lithos* 350-351:105201 doi:10.1016/j.lithos.2019.105201
- Gilio M, Angel RJ, Alvaro M (2021) Elastic geobarometry: how to work with residual inclusion strains and pressures. *Amer Min* 106:1530-1533 doi:10.2138/am-2021-7928
- Gilio M, Scambelluri M, Angel RJ, Alvaro M (2022) The contribution of elastic geobarometry to the debate on HP versus UHP metamorphism. *Journal of Metamorphic Geology* 40:229-242 doi:10.1111/jmg.12625 Open access.

### ***DISCLAIMER***

While we try to ensure that stRAinMAN software is free of bugs and errors, people use it at their own risk. We cannot accept any responsibility whatsoever for either incorrect results or for any physical, mental or other damage arising from use of this software, nor from errors in this documentation.

If you think you have found a bug, please send us complete details including input and log files.

# Version news

The stRAinMAN software was originally released in August 2018.

The current version is v2.03, released in Spring 2022. The calculations of strains from mode shifts and vice-versa remain unchanged, and users of the new version should get the same results as from the previous release (v2.0) of October 2019. In version 2.03 the following changes have been made:

- The format of the results to the output window and to the log file have been changed, to remove format overflows and to make the output easier to read. A complete set of results is always available in the log file.
- The GUI now appears correctly when the scaling of the display in Windows is changed from 100%.
- The inactive 'programs' tab has been removed from the GUI.

## Changes made in v2.0 (released October 2019):

- **New features:**
  - Input and output boxes for strains now support more decimal places.
  - Output window has been changed so that you see all of the recent output from the program in a single scrolling window, independent of the tab in which you are working.
  - This has enabled better logging of output to the log file.
  - More information is provided in the output from calculations.
  - Uncertainties of the peak shifts can be put in the peak-shift data file, and they will be used to weight the least-squares determination of strains.
  - The peak-shift data file can have missing values
  - Comments or labels can be added to each datum in the peak-shift data file, and they will be added to the output of the calculated strains.
  - Tabs and illegal characters in peak-shift data files are now ignored by the program.
- **Bug fixes:**
  - Corrected bug that made the weighted-chi-squared value incorrect from least-squares to determine strains from input shifts.
  - Fixed bug in opening log file.
  - Fixed incomplete resetting of input strain boxes in the calc\_shifts tab when a new cif was read in.

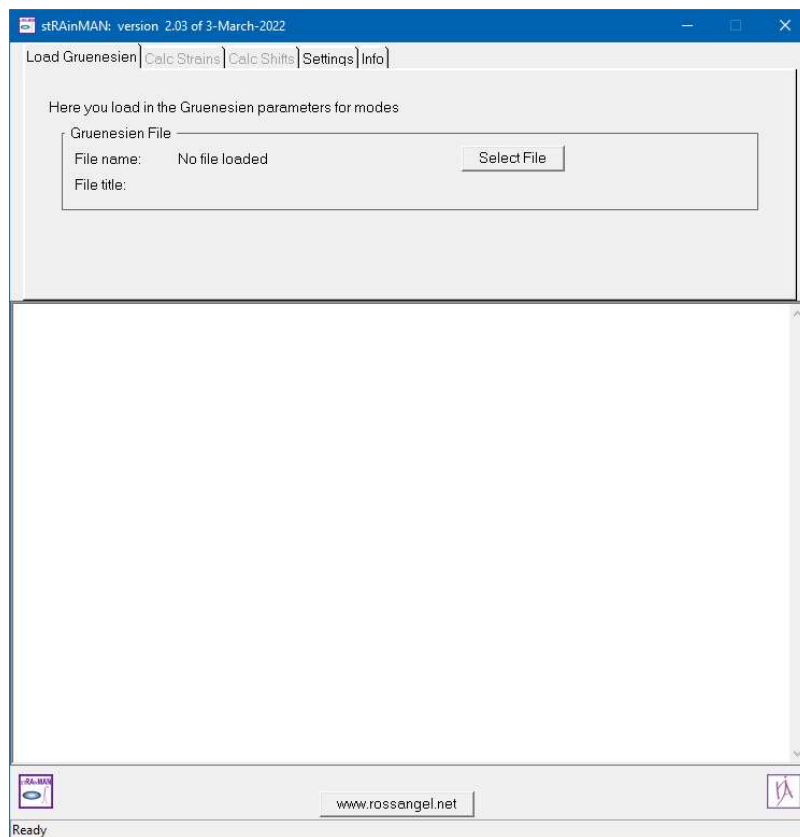
# Getting started

First read the paper in *Zeitschrift für Kristallographie* that describes the theory and methods. It is open access and can be found with the doi: 10.1515/zkri-2018-2112. A copy is included in this distribution.

Then follow this worked example, using the files for quartz provided in the distribution package. The example files and this manual are installed in the folder `c:\program files\strainman\examples`

We recommend copying all of the files from this folder to a folder under your own `\my documents`

Start the program. You should see this:

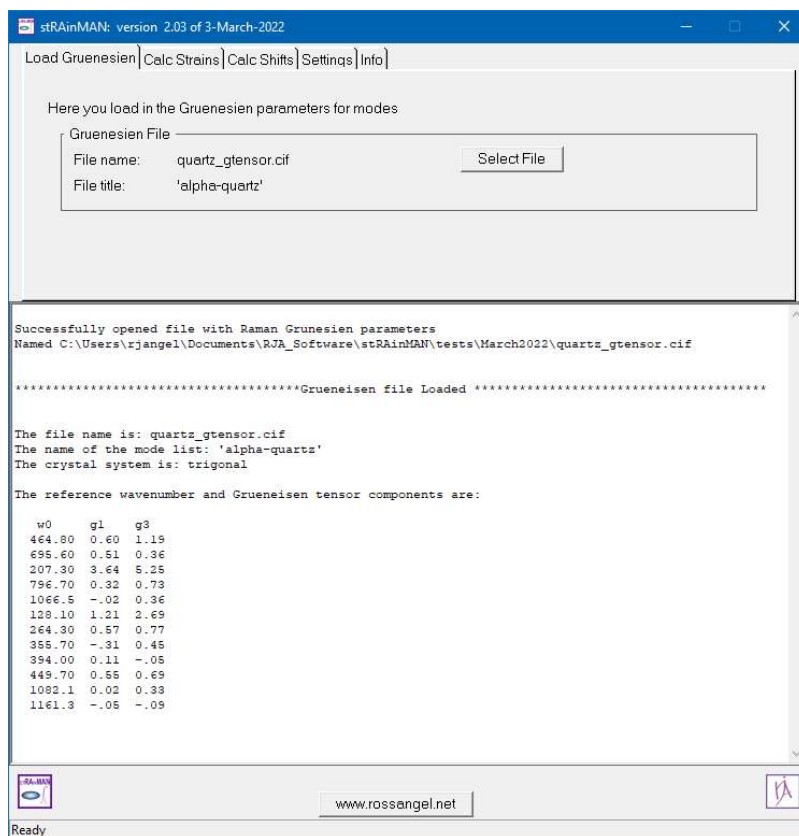


The Settings Tab allows you to modify a few aspects of the display, and to open a log file. The log file allows you to keep a permanent record of the calculations that you do in the program.

Tabs for calculations only become active when the necessary information about the mode Grüneisen parameters have been loaded to the program. These are loaded from a file via a file browser launched from the *Load Grueneisen* tab.

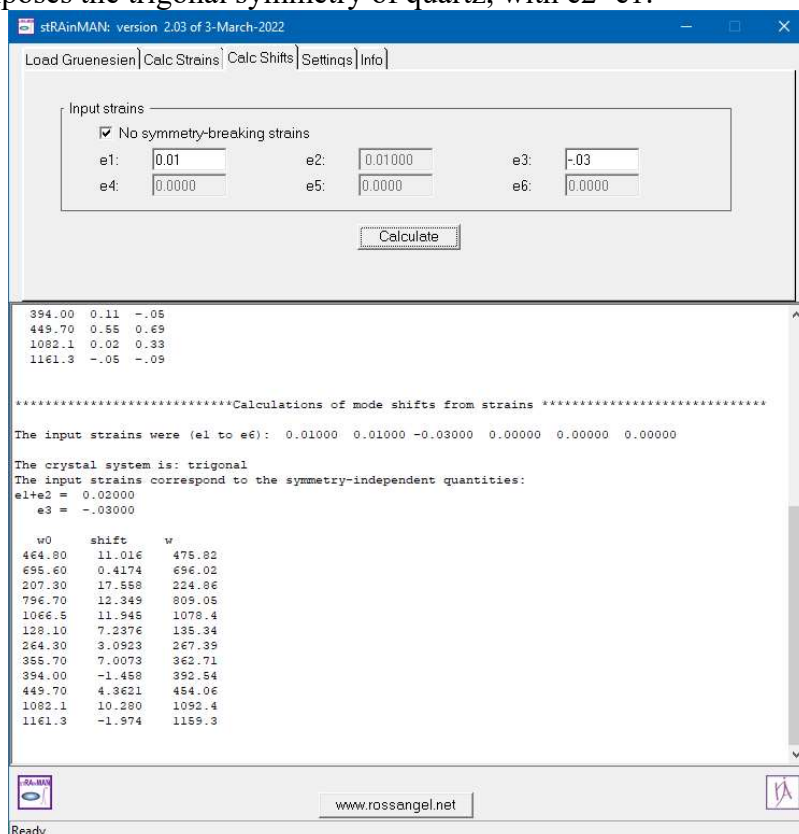
Click on the *Select File* button and use the file browser to navigate to the example files.

Open the file `quartz_gtensor.cif`. Information from the file will be listed in the GUI:



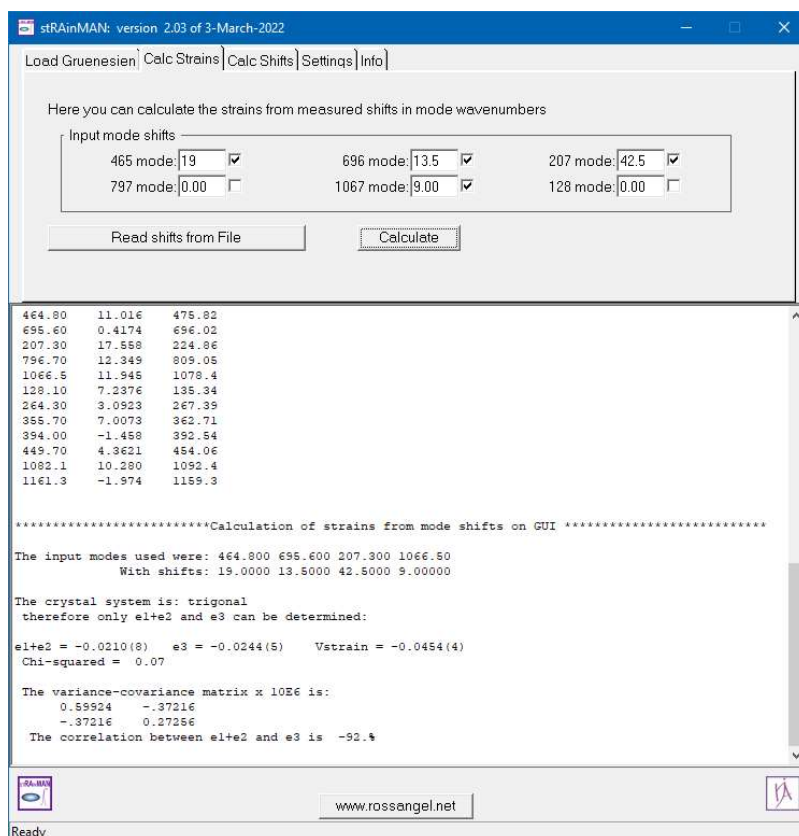
Now the calculation tabs are active. Go to the *Calc Shifts* tab. This lets you calculate the changes in the mode wavenumbers as a result of strains. Just type the strains into the boxes.

If you select *No symmetry-breaking strains* then the program imposes the symmetry of the crystal on the strains, as in the example below. Here the input was  $e1=0.01$  and  $e3=-.03$ , and the program imposes the trigonal symmetry of quartz, with  $e2=e1$ :



The *Calc strains* tab of the stRAInMAN GUI allows the user to calculate the strains in a crystal from the measured changes in wavenumbers of several modes.

The GUI lists the first six modes from your Grüneisen file. If you did not measure all of them, just select the measured modes with the tick boxes. Insert the measured changes in mode wavenumbers into the boxes, and hit the *Calculate* button:



The strains are listed in the output window. If you have input more mode shifts (in this example 4) than the number of independent strain components (2 for quartz) then you will see some additional information in the output as shown here:

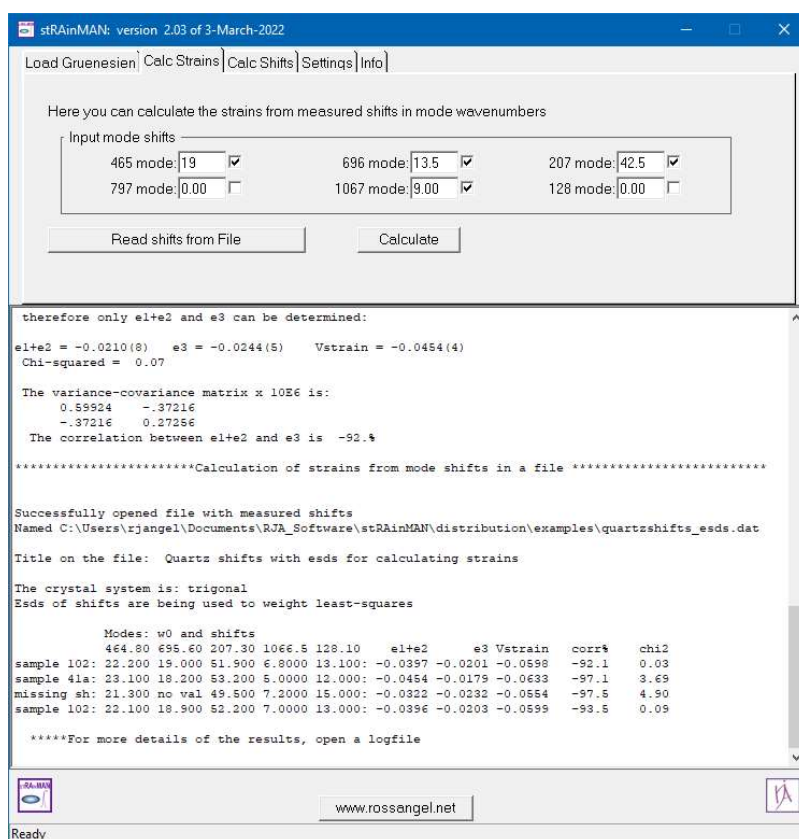
- Estimated uncertainties on the strains, as calculated by least-squares.
- The chi-squared value of the least-squares fit of the strains.
- If there are only two strains, the variance-covariance matrix and the % correlation between the strain values.

If you have measured a lot of Raman spectra, you can put the changes in Raman mode wavenumbers into a *peak-shift* data file.

- The format of this file is described at the end of this document.
- The *peak-shift* data file can also include the uncertainties in the peak shifts. They will be used to weight the least-squares determination of the strains.
- The file quartzshifts.dat shows you the file format without the uncertainties for the shifts.
- The file quartzshifts\_esds.dat shows you the file format with the uncertainties for the shifts.

First, open a log file to record the results: go to the *Settings* tab.

To read the shifts from a *peak-shift* data file and calculate the strains, return to the *Calc\_strains* tab, and push the *Read shifts from File* button. After opening the file, you will see the strains calculated for every spectrum in the file:



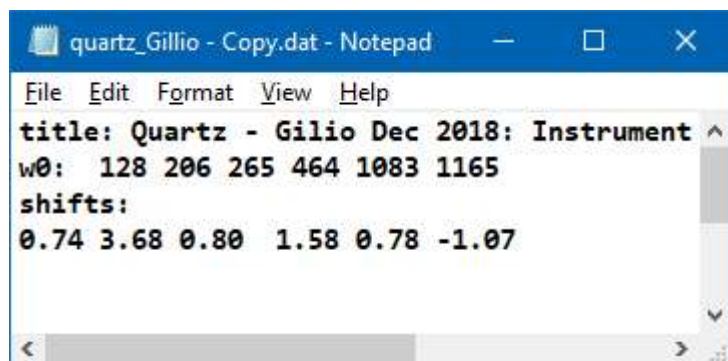
More results from the calculation, including the esd's of the strains, are written into the log file.

## Peak-shifts Data File Format

As described in the worked example, peak-shift data can be provided to the program in a text file, and the strains corresponding to each set of shifts will be calculated. The data can be cut-and-pasted from an Excel spreadsheet (or other software) directly into a text file.

### Data file format

The old datafile format without esd's will still work. It looks like this:



```
quartz_Gillio - Copy.dat - Notepad
File Edit Format View Help
title: Quartz - Gilio Dec 2018: Instrument
w0: 128 206 265 464 1083 1165
shifts:
0.74 3.68 0.80 1.58 0.78 -1.07
```

Keywords are distinguished by having a colon ':' at the end.

All data files must have the first three lines:

- Title:
- w0: Approximate values of wavenumbers of the lines under zero strain. These must be within 1 or 2 wavenumbers of the values in your *cif* with the Grüneisen tensor information. The numbers from this line are not used in any calculations, they are only used to identify which tensor components to use from the *cif*.
  - The order of the shifts in each data line in this file must be the same as the order of the modes in this line.
  - The order of modes here does not have to be the same as the order in which they appear in your Grüneisen *cif*.
- Shifts: This indicates the start of the data lines.

Each of the following lines contain the data of peak shifts from one Raman spectrum:

- One line per set of shifts.
- Each line should contain the shifts of modes in the same order as those in the line w0:

Optional features that you can use in the data file are illustrated below:

- Missing values can be indicated by a text string with no spaces inside it. For example, the file shown below has the value for the 696 shift missing from the 3<sup>rd</sup> data line, indicated by the text 'nv'.



- Data can be labelled by text at the end of the line, following a #. It is not required to label data lines.

```

quartzshifts.dat - Notepad
File Edit Format View Help
title: Quartz shifts for calculating strains, no esds
w0: 128 206 464 696 1067
shifts:
13.1 51.9 22.2 19.0 6.8 #sample 102
12.0 53.2 23.1 18.2 5.0 #sample 41a
15.0 49.5 21.3 nv 7.2 #missing shift
13.0 52.2 22.1 18.9 7.0 #sample 102a
Ln 1, Col 1 100% Windows (CRLF) UTF-8

```

If you want to use the esd's in the mode shifts, add the word 'esds:' after the word 'shifts:' (note that both words **must** have a colon after them as shown below).

And then on each line, list the esd of each shift after the value of the shift, so each line of data has shift, esd, shift, esd, .....

```

quartzshifts_esds.dat - Notepad
File Edit Format View Help
title: Quartz shifts with esds for calculating strains
w0: 128 206 464 696 1067
shifts: esds:
13.1 0.5 51.9 0.5 22.2 0.5 19.0 0.5 6.8 0.5 #sample 102
12.0 0.5 53.2 0.7 23.1 0.3 18.2 3.0 5.0 1.0 #sample 41a
15.0 0.7 49.5 0.8 21.3 0.5 * * 7.2 1.5 #missing shift
13.0 0.6 52.2 0.8 22.1 0.7 18.9 0.9 7.0 0.9 #sample 102a
Ln 1, Col 31 100% Windows (CRLF) UTF-8

```

You can still have as many measurements or spectra as you like in one file, with one spectrum per line.

Note that if you have missing data (e.g. the 3<sup>rd</sup> data line) you need *two* text strings to indicate the missing shift *and* the missing esd. In the example the first \* is for the missing shift of the 696 line, the second \* for the missing esd.

You must input esd's for *every* shift, if you use this option to read esd's.

The program will then use the esd's to weight the shift data in the least-squares determination of the strains.