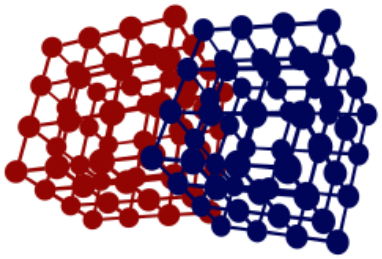
# DISEMM MANUAL

ALEXANDER HELDMANN[1]



## CONTENTS



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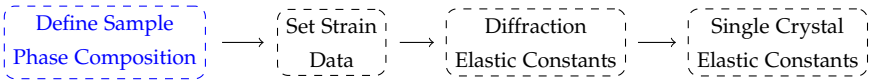
# 1 QUICK START

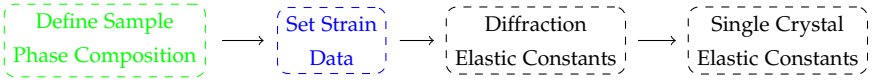
This section contains the quick start guide for a fast start and use of the Software. The standard settings will be used through out this section. More detailed instructions and descriptions are given in later sections.
The first window shown after starting the application is shown in figure 1. It contains the sample information necessary to perform an evaluation and allows to manage diffraction experiments. After first starting the program this window should not contain any information. In order to start the analysis the composition of the sample has to be declared.




TO START one selects *Crystallographic data* in the top menu. A list containing three items will appear. The first two *From file* and *Manual input* are both valid options to load the first crystallographic data of the phases contained by the sample. The top option allows to add the information by Crystallographic Information File[1] and the second allows a manual input.

**CAUTION** The crystallographic data is essential for all steps during the analysis. It is the first input and will enable the other features of the program including the save options. The most important parameters which need to be provided are: _cell_length_a, _cell_length_b, _cell_length_c, _cell_length_alpha, _cell_length_beta, _cell_length_gamma and _symmetry_Int_Tables_number, which contains all lattice information and the symmetry id of the space group. In case of a multi phase analysis the phase type and fraction needs to be declared as well.

**CAUTION** The Data may be changed in the main window or by selecting the third option in the menu *Show loaded data*. To delete the added crystallographic information one has to select add new phase. Answer the first prompt with *No* and then a second prompt will appear in which the user should select *Yes*.

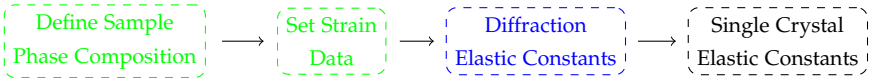



THE LATTICE STRAIN DATA acquired during in-situ tensile tests are required to fit the diffraction elastic constants (DEC) and the single-crystal elastic constants. There exists multiple ways to add the necessary data. First via File as shown in the Appendix 7.2. The second method evaluates the position of the peaks from added diffraction pattern. The pattern may be added via the top menu *File* and *load diffraction pattern* or via Drag and Drop directly into the *Diffraction Pattern* list from a Folder. While reading in the data from the files DISEMM performs an automated peak search based on the previously given crystal symmetries.

[1] More information on this format is provided on https://www.iucr.org/resources/cif/spec/version1.1, as well as an example in the appendix 7.1

**CAUTION** The correct wavelength during the diffraction measurements must be given before the diffraction patterns are added. Otherwise DISEMM will estimate the peak positions at wrong positions. If the wavelength is unknown the peaks may be associated manually or in the settings an alternate peak finding algorithm may be used. The use of an incorrect wavelength may alter the results, though.

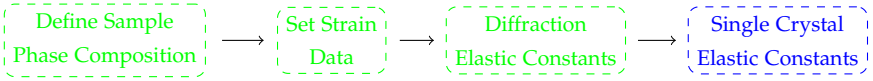
By default DISEMM fits the peak in the pattern with a pseudo Voigt function and calculates the necessary strain data automatically. A check of the fitting results is performed in a separate window accessible through the menu *Peak Fitting* then *Fitting Window*.




**THE DEC** are fit in a separate window accessible in the menu *Elastic calculation*, then *DEC calculation*. This contains all relevant information on the DECs. At first this window is empty besides the diffraction pattern and their peaks on the right side of the window. DISEMM implements and auto-association for the DEC, after clicking on *Auto association of DECs* it will create all possible DEC from the peak data loaded. Each DEC for each phase has then to be fit by selecting it from the list and click on *Refit DEC* to set $s_1$ and $\frac{1}{2}s_2$.

**CAUTION** The skip of this step is not advised since it offers the selection of the fitting data used to determine the single-crystal elastic constants.

**CAUTION** The auto-association feature will not distinguish between elastic and plastic data and will associate both to the DECs. It is advisable to add plastic deformation data after the DECs are fitted.



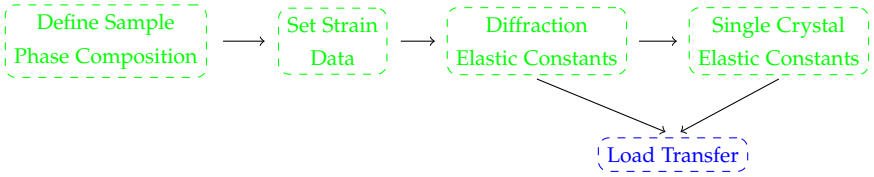

**THE SINGLE-CRYSTAL ELASTIC CONSTANTS** are accessed in the main window menu *Elastic calculation* then *Single-Crystal Elastic Constants*. This window displays the elastic properties in particular the single-crystal elastic constants but also shows the bulk properties as well as give different measures for the anisotropy. At this point of the evaluation the strain-data and if performed the DEC are known and will be Displayed in the upper right *List of measured DEC's*. The settings for the fit such as phase selection and grain-to-grain interaction model are placed in the center below the elastic constants. To fit the elastic constants with the selected setting just click *Fit tensor*

**CAUTION** Beware to provide suitable starting values for the single-crystal elastic constants before the fitting.

**CAUTION** Kroener's and De Wit's grain-to-grain interaction model might not stop at the minimum during the minimization. This is due to a lack of values in the image of the of the $\chi^2$-function and can fixed by changing the starting values slightly.

**CAUTION** Voigt's grain-to-grain interaction model has been proven to be very unstable during the evaluation due to the very flat fitting topology.

**TIP** Reuss grain-to-grain interaction model does seem to always find the global minimum during the minimization. It is advisable to first fit the constants with this model and use the values as starting values for the other grain-to-grain interaction models.




THE LOAD TRANSFER between two different Phases is calculated by the transition factors in the right lower corner. There are 4 different buttons: Just to calculate the stress factors from the currently selected tensor model click *Set transition factors*. The phase stresses are updated by *Reset Stress* and finally the DECs are reset by *Refit DEC*. Now, if the single-crystal elastic constants are refit by clicking on *Fit tensor* the constants are refit according to the new DEC. DISEMM is able to compute the this loop automatically until the elastic constants of each phase do not change anymore.

**CAUTION** The grain-to-grain interaction model, as well as texture and other settings are set the same way as for fitting the elastic constants itself.

# 2 MAIN WINDOW

The main window is the first window after starting DISEMM . It serves as the central unit from which every part is accessed. The basic concept of DISEMM is to handle diffraction data and accordingly the main window shows the sample composition with the crystallographic data of each individual phase shown in the red box in figure 1 and manages the diffraction data in the blue box.

THE TOOLBAR is indicated by the green box of figure 1 and its icons are mainly controlling the plotting area and allow the user to fix the viewing distance of the x-axis **1** and y-axis **2**.

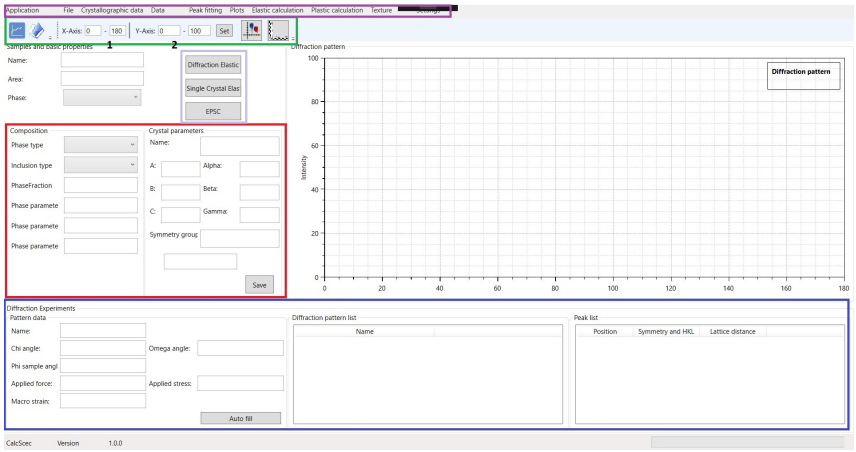



**Figure 1:** The main window of DISEMM after starting the application. It displays information on the shape, composition and crystallographic data of sample. It also allows to overview performed diffraction experiments and edit the automatic association of peaks.

THE MENU is indicated by purple in figure 1 and manages most settings of the application. It contains the quit and restart in *Application*. The second column contains most file relevant functions such as diffraction pattern import, peak data import, export of the sample data to .xlsx format. The save and load of the current data in the costom file format is also located here.

**CAUTION** It is advised to use the .scec format for saving the project data. In cases of large texture files other formats will show performance issues during the conversion.

DISEMM first input data is the crystallographic data of the sample. Added by accessing the top menu in the third entry *Crystallographic data*. The top option allows to add the information by Crystallographic Information File[2] and the second allows a manual input.

**CAUTION** DISEMM relies on the crystallographic data of the sample as the crystal structure defines many properties which are used during the analysis. Therefore it is required to load at least one set. The most important parameters which need to be provided are: _cell_length_a, _cell_length_b, _cell_length_c, _cell_length_alpha, _cell_length_beta,

[2] More information on this format is provided on https://www.iucr.org/resources/cif/spec/version1.1, as well as an example in the appendix 7.1

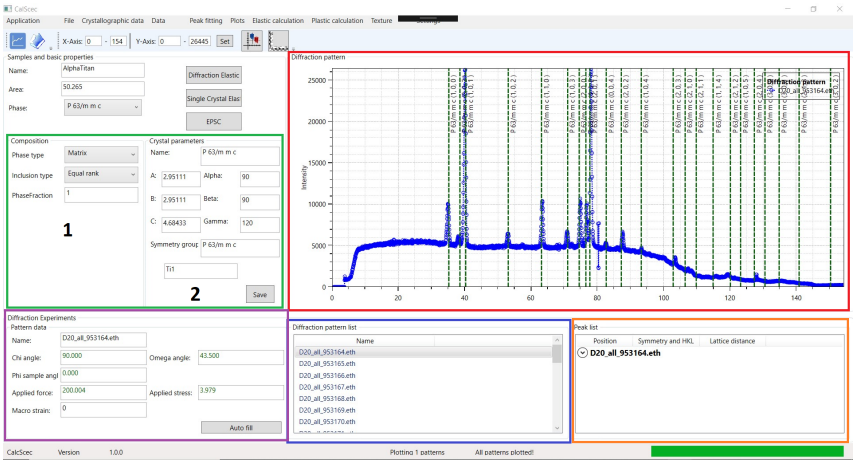



**Figure 2:** The main window of DISEMM after loading the sample informations. It displays information on the shape, composition and crystallographic data of sample. It also allows to overview performed diffraction experiments and edit the automatic association of peaks.

_cell_length_gamma and _symmetry_Int_Tables_number, which contains all lattice information and the symmetry id of the space group. In case of a multi phase analysis the phase type and fraction needs to be declared as well.

**TIP** It is advised to declare all phases of sample before adding diffraction pattern or peak data for the auto-association to add the peak information as well.

The column *Data* offers the possibility to edit the diffraction pattern information as well as the sample composition. The columns *Elastic calculation* and *Elastic calculation* are an alternative way to access the windows for the DEC, SEC and EPSC analysis. The last menu section contains the application settings. The entries will be explained at the sections when they are of interest.

THE CRYSTALLOGRAPHIC DATA is used throughout the hole evaluation. At least one phase needs to be defined in order to activate most of the functions implemented in DISEMM , this includes the save and export functions. While it is possible it is not advised to associate the peaks manually. To do so see the next paragraph ADDING DIFFRACTION PATTERN.

**CAUTION** DISEMM consists of many different automation tools for peak finding in diffraction pattern. The auto-association will only associate peaks to known crystal symmetries. The detection routines also require the lattice distances a, b and c including their angles. Any modification to these parameters should be performed prior to adding peaks or strain data.

To add the data one selects *Crystallographic data* in the top menu as described earlier. To change any parameters loaded in the user may use the interface provided in the main menu shown in figure 3 inside the green box. Marked by **1** the multi phase settings are found. Each phase has to be declared weather it is matrix or inclusion, as well as the phase fraction.

**CAUTION** DISEMM load partitioning approach for the SEC only supports two phases until now. One has to be declared as Matrix and the other should be set on inclusion.

**CAUTION** The parameters to define ellipsiod inclusion will only appear after the phase is defined as such.

**TIP** The composition does not necessarily be declared before adding diffraction pattern. But it should be defined before using the elastic load transfer or the EPSC models.

**TIP** To delete the added crystallographic information one has to select add new phase. Answer the first prompt with *No* and then a second prompt will appear in which the user should select *Yes*.

The crystal parameters are modified in box marked by **2**. It contains all essential parameters necessary to perform the analysis. More parameter are found in the menu *Crystallographic data* then *Edit*.

**CAUTION** DISEMM associates the crystal symmetry by the space group id[3]. Any changes to the space group id after starting the evaluation process may lead to unexpected results and should be avoided.

STRAIN DATA along different crystallographic directions may be added via File in the menu *File* then *Load reflex data*. The file format is prvoded in the appendix 7.2.

**NOTE** The following evaluation step is not necessary to calculate the DEC or SEC but is advised. By fitting the diffraction pattern in DISEMM it enables many different program features.

**TIP** DISEMM exhibits quite a collection of tools to handle pattern data and was developed to unify different aspects of Diffraction and mechanical modeling. Loading of the diffraction pattern also gives opportunity to refit selected peaks and improve the acquired results.

**TIP** At this point of the evaluation any changes to the strain data will NOT affect the evaluation. To apply the changes to the DEC and SEC the data only needs to be refit with the same settings

**CAUTION** Newly added peaks will not be auto-associated to the corresponding DEC they need to added manually before the refit.

ADDING DIFFRACTION PATTERN to DISEMM is managed in the menu as well as in the window itself. DISEMM supports adding one or multiple pattern at once although each option is accessed separately in the menu. More comfort is provided by Drag and Drop the pattern files directly onto the list in the blue box in figure 3. The file structure is provided in the Appendix 7.3. DISEMM provides three different types of peak finding routines. The first searches for statistical anomalies and detects every small bump in the pattern. The second peak finder was developed by Zlokazov and find every peak accurately. The last calculates the positions by the added crystallographic data and automatically associates the peak to the corresponding (hkl) lattice plain. As default the peaks positions are estimated by their crystallographic structure. This setting is change in the menu *Settings*. DISEMM

[3] More information on the space group id is provided on http://img.chem.ucl.ac.uk/sgp/large/sgp.htm

's angular detection limits may be limited for the diffraction patterns in the settings.

TIP To change the current peak list select *Peak Fitting* then press *Select new Peak* and the option will be checked. Noe left click in the pattern on the desired position then click *Add New Peak*. The adding functionality only works on single pattern. If multiple are selected nothing will happen.

TIP To modify the (hkl) association pattern in the list shown in figure 3 in the blue box needs to be selected. Then select the peak in the orange box and open the context menu by clicking right then select *Change HKL association* or *Remove HKL association*

NOTE The pattern selection features multiple selections. By holding *shift* or *strg/ctrl* multiple entries may be selected.

After the postions and associations are determined DISEMM prepares the data for the fitting. It groups overlapping peaks into groups to properly fit them. By default DISEMM automatically fits the peak functions after the peak detection and grouping is finished for the pattern. This may be turned off in the menu under *Settings*. To manually adjust the fit and refit the peaks enter the menu *Peak fitting* then *Fitting Window*.
The experimental information like the orientation, applied load and current macro strain of the sample corresponding to the measured pattern are displayed in the purple box. The angles correspond to typical settings in Neutron diffraction experiments. To get a more detailed insight please read Heldmann et al. 2019. In case the number of pattern exhibits the possibility to add the data manually DISEMM offers basic auto fill options for pattern meta data. The auto fill windows tries to cover as many input combinations

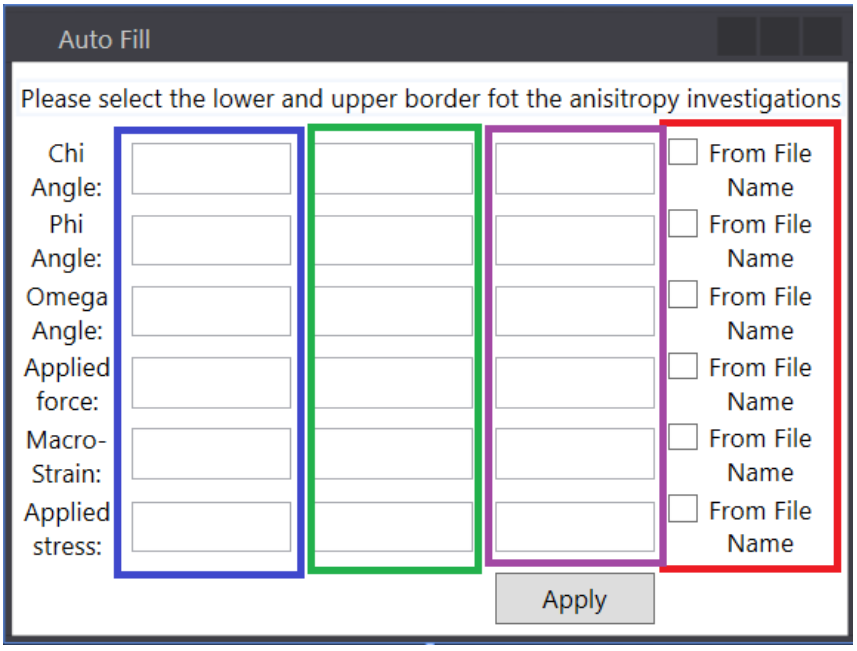



**Figure 3:** The auto-fill settings are devided into two options for auto completing the pattern information.

with as few settings as possible. There are two different modes to add the experimental information to the patterns. The first option is by the pattern

name which is generated with its filename. Just check the checkbox for the value in the red box and enter the index of the value in the blue box.

**TIP** To exclude a paramter from the auto-fill just enter "-1" in the according textbox in the blue box.

**NOTE** The separators are '.', '-', '_' used to divide the entries in the file name. For example Exp-Chi-90-appliedForce_500.dat leads to the list [Epx, Chi, 90, appliedForce, 500, dat]. The index of the chi value would be in this case 2 and the Index for the force would be 4.

**CAUTION** Die program defines the $\chi$ angle of the experiment between 90 (horizontal) and 180 (vertical) degrees.

**THE PLOTTING** of the diffraction pattern in the red box is triggered by hitting the *Enter* button after selecting one or more diffraction patterns in the blue box. There exist many different possibilities to customize the plot by changing marker size and form, stroke thickness and so on in the *Settings*.

# 3 PEAK FITTING WINDOW

This window manages the peak fit and region assignment. The top menu contains the plot settings in the first two columns. *Plot* manages settings such as the visibility of the σ line in the deviation plot or stroke thickness and point size. *Settings* contains the values for the grid line settings and y-axis maight be changed between linear and logarithmic. It also the settings to automatically adjust the starting values each time a peak is fit to improve the overall performance of the automated peak fitting.

**TIP** The auto-adjustment of the starting values during fit best works if first a single pattern from the experiment is added to DISEMM . Then the fit and association of every peak is checked and corrected if necessary. After this step DISEMM will use the corrected starting values for the corresponding peaks and adjust them after each consequent fit if *Peak auto correction active* is activated.

**TIP** Later refitting does not influence the evaluation only the DEC and SEC need to be refit after change to adjust the values.

**NOTE** *Peak auto correction active* improves the overall performance of the automated fit and especially useful by treating large datasets and/or patterns with heavy overlaps.

**CAUTION** During the auto-correction only the peaks added to the program earlier will be found. This prevents the re adding of prior deleted peaks at the cost of not finding unexpected peaks.

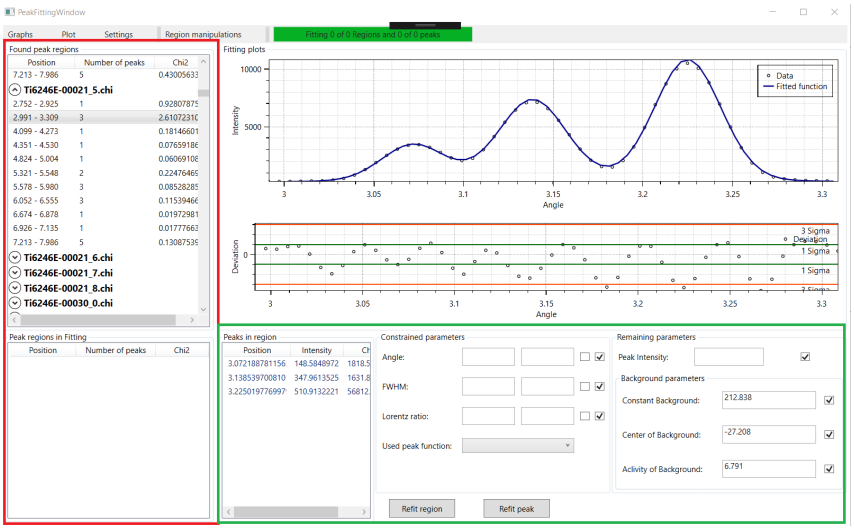



**Figure 4:** Screenshot of the peak fitting window of DISEMM during the evaluation. On the left in the red box there is a list of peaks contained in regions. The selected region is shown in the plot while the blue line indicates the fitted curve. In addition, each peak can be adjusted manually in the green box. Each fit is performed in its own thread, therefore a large number of regions can be fitted simultaneously. By adding a diffraction pattern to the *Sample Data* each pattern is searched for peaks, these are combined into regions and automatically fitted. Starting values are improved each time a peak is fitted.

The region manipulation is managed in the top menu. To perform an action first the corresponding option needs to clicked. This will enable the manipulation mode indicated by the checked menu entry. Then click on the plot to determine the position DISEMM will indicate the selection by a line. Then go back to the menu and click *Do Action* to perform the action.
The red box in figure 4 contains two lists. The top list contains all generated peak regions grouped into the pattern names. By clicking on them a list with regions found in the diffraction pattern will be displayed. It contains informations on the starting and ending angle, number of peaks inside the region as well as the combined $\chi^2$ value.

NOTE By structure DISEMM only accepts regions for the LMA implementation and therefore even single peaks are grouped into regions.

After selecting a peak region the peaks associated will be displayed in the green box on the right. To fix or constrain values of the peak during the fit or just to view the information a peak from the list needs to be selected. The corresponding parameters will be displayed in the text boxes of the right. The first box displays the parameter and the second shows the maximum distance from the parameter value which is allowed. The first checkbox activates the constraints during the fit. DISEMM also allows for excluding parameters for the fit by unchecking the second checkbox.

TIP DISEMM is implemented in a way that excluding parameters from the fit simplifies the topology of the fit and increasing performance.

NOTE The $\chi^2$ value shown in the peak list in the green box is calculated by the single peak function without any overlaps. Its deviation from the regional indicates the influence of the other peaks.

CAUTION DISEMM treats each parameter of every peak individually during the fit. Excluding or constraining a parameter in one peak will not affect the same values of the others.

To refit the region just click on *Refit Region*. DISEMM contains a designated thread pool to manage the regions during the fit. For each region a thread is created and then added to the thread pool. As soon as enough computational resources are available the thread is send for fitting to the CPU. The state of the regions added to the pool is shown in the list at the bottom of the red box in figure 4. The top menu shows the overall fitting progress with how many regions are currently fit.

NOTE Only large regions will take a notable time to be fit and some smaller regions will be finished without being noticed.

CAUTION The automated fit will add every generated region to the thread pool increasing the number of threads very fast.

CAUTION The resources are automatically allocated depending on their availability. Large numbers of threads will use up almost all of the CPU and will slow down your operating system significantly.

[4] If the angle parameters shows 1.0 degrees and distance is set to 0.5 the LMA will keep the value between 0.5 and 1.5 during the hole fit.

# 4 DEC WINDOW

The DEC window is divided into three parts. The plot in the brown box shows the fit of the selected DEC compared to the experimental data and below the deviation plot. The blue box contains the pattern related data set during the experiment in the same way as in the main window. The list in the lower half displays die peaks associated to the pattern and shares that information. The red box only contains two lists. The upper list displays the DEC and when selecting one the plot on the left fills and the peaks used for the fit are displayed in the list below.

**TIP** DISEMM uses the patterns and the associated peaks as main reference. Therefore changing any information will not influence the DEC data or evaluation process. To adjust the fits to the changes just refit the DEC.

**TIP** The plot of the DEC offers a great opportunity to spot any anomalies occurring in the data.

**NOTE** DISEMM was build to handle diffraction data and therefore uses patterns to create the strain data list. If the peaks are added by file each will generate a pattern containing the experimental information and might get a bit unhandy with the combobox.

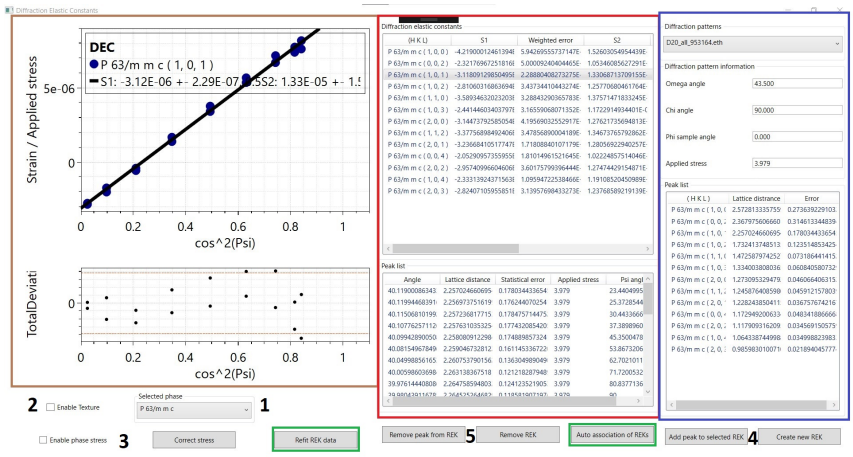



**Figure 5:** The DEC window of DISEMM after loading the sample informations. It displays two plots on the left, the upper shows the fit of DEC and the second displays its errors. After loading a fresh sample the List in "Diffraction Elastic Constants" is empty. The individual peak list used during the fit is listed right below the constants and will be displayed by selection a DEC in the list.

The buttons and settings are located at the bottom of the window. The phase selection is marked by 1. Each phase is stored individually and the steps to fit the DEC have to be completed for each phase. The texture is enabled by checking the checkbox marked by 2. The buttons marked in green are the fastest way to create the DEC. By clicking on *Auto association of DEC* DISEMM creates every DEC which associated lattice plane is measured in between the set pattern limits and associates the measured peaks, automatically. In general manual creation of the DEC and the respective association of peaks to them is possible by using the buttons marked by 4. To create a

new DEC select a peak from the peak list in the blue box and click *Create new DEC*. The adding of a peak to the DEC requires the selection of the DEC in the red box.

**CAUTION** The first peak added while creating the DEC serves as the reference for the strain calculation. The quality of the fit of this peak has the most influence on the result.

The buttons marked with 5 are to remove peaks from the DEC or the entire DEC. To remove the DEC just select the DEC in the red box and click *Remove DEC* and if only a peak needs to be removed select the peak in the list below the DEC and click *Remove peak from DEC*.

**CAUTION** The relative strains are calculated by the first peak as reference. Removing the peak peak greatly impacts the results.

The button and checkbox marked by 3 are to correct for the elastic difference of dual phase materials. DISEMM saves two individual values for the stresses applied during the experiment and the DEC. One for the undistributed values given by the user and a corrected value set by pressing *Correct stress*.

**TIP** The button *Correct stress* will cause to save the newly calculated stress and DEC values depending on the selection of the checkbox. This means if not necessary to keep the original stress values one can override the old ones just by not checking the checkbox without breaking the further analysis.

# 5 SINGLE-CRYSTAL ELASTIC CONSTANTS WINDOW

This window manages the SEC. The tensor of elasticity is displayed in the red box in Voigt's notation. To change from the elastic constants to stiffnesses or the phase in case of multiple phases select the corresponding option in the settings in blue box. DISEMM saves the SEC for each grain-to-grain interaction model individually and the SEC in the red box will change according to the selected model.

**TIP** The individual storage of the SEC in DISEMM offers the opportunity to manage up to five different sets of SEC. They may be used as save slots for individual inputs as well to compare and analyze existing data to one another in an easy fashion.

**CAUTION** The Voigt grain-to-grain interaction model only works by applying heavy restrictions on the parameters and is not recommended to use. However, it is left in DISEMM to provide a save slot for SEC during the evaluation.

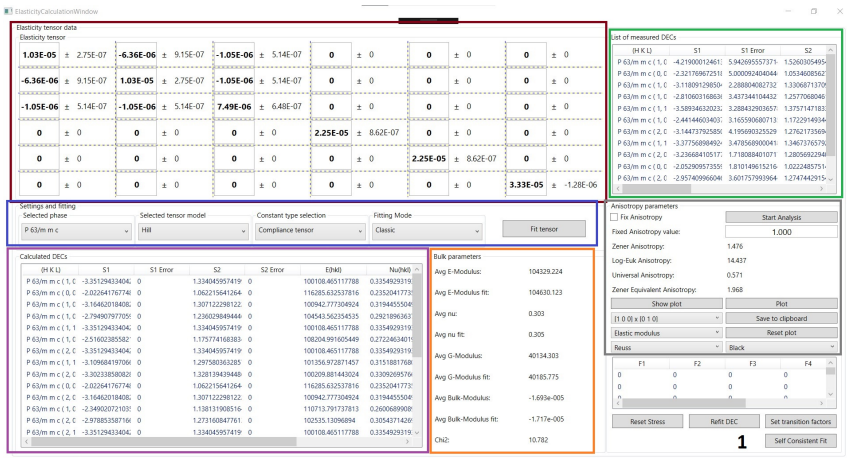



**Figure 6:** The single-crystal elastic constants are displayed in this window. It contains various settings for fitting the constants and information on the DEC calculated from the constants.

In the green box the DEC determined earlier are displayed if the classic fitting mode is selected DISEMM will minimize the difference between them and the ideal DEC calculated from the SEC shown in the purple box. The orange box to the right shows the bulk elastic properties for the selected phase and grain-to-grain interaction model. The values calculated from the diffraction values are marked by fit.

**NOTE** The ideal bulk properties obtained by Reuss and Hill as well as the $\chi^2$ value will match only the SEC should differ.

The gray box contains all values regarding the elastic anisotropy. Fixing the anisotropy will lead to a fixed Zener value and is therefore only applicable for cubic symmetries. By clicking on *Start Analysis* DISEMM will fit the elastic constants with fixed anisotropy while varying the Zener value with a predefined step between an user set upper and lower limit. The options below allow to plot parameters like shear or Young's modulus for different crystallographic direction. To show the plotting area click *Show Plot*.

**TIP** It is possible to plot the bulk parameters for every grain-to-grain interaction model for every set of given SEC by selecting the grain-to-grain interaction model at the bottom of the gray box.

The load transfer in dual-phase alloys in managed below the gray box. The list contains the transition factors and below are the buttons to perform every step manually and below the self-consistent approach implemented in DISEMM to set the values automatically. To perform the correction manually fit both phases with desired grain-to-grain interaction model then click *Set transition factors*. This will set the transition factors. Now the stresses need to reset by clicking *Reset Stress* then adjust the DEC to the new values by clicking *Refit DEC*. Then use *Fit tensor* to refit the SEC.

**TIP** The setting for the fit of the SEC using the self-consistent load transfer approach are the same as for clicking *Fit tensor* and are set in the blue box.

**CAUTION** Clicking on *Refit DEC* and *Self Consistent Fit* will override the existing values.

# 6 TROUBLESHOOT

It might occur that datafiles containing peak or diffraction data is not loading properly. In this case check the decimal separator. It DISEMM uses a format like this “0.0”. Please make sure your regional setting are set accordingly.

# 7 APPENDIX

## 7.1 .cif File Example

data_53451-ICSD
#copyright 2015 by Fachinformationszentrum Karlsruhe, and the U.S. Secretary of
#Commerce on behalf of the United States. All rights reserved.
_database_code_ICSD 53451
_audit_creation_date 2003/04/01
_audit_update_record 2012/08/01
_chemical_name_systematic 'Iron - Alpha'
_chemical_formula_structural Fe
_chemical_formula_sum Fe1
_publ_section_title ;
Ueber die Temperaturabhaengigkeit der Gitterparameter von Eisen, Kobalt und Nickel im Bereich hoher Temperaturen ;
loop_
_citation_journal_id_ASTM primary 'Zeitschrift fuer Angewandte Physik' 1967 23 245 249 ZAPHAX 2 'Transactions of the Metallurgical Society of Aime' 1965 233 1519 1525 TMSAAB 3 'Golden Book of Phase Transitions, Wroclaw' 2002 1 1 123 GBOPT5
_publ_author_name ;
Kohlhaas, R.;Duenner, P.;Schmitz-Pranghe, N. ;
_cell_length_a 2.8665
_cell_length_b 2.8665
_cell_length_c 2.8665
_cell_angle_alpha 90.
_cell_angle_beta 90.
_cell_angle_gamma 90.
_cell_volume 23.55
_cell_formula_units_Z 2
_symmetry_space_group_name_H-M 'I m -3 m'
_symmetry_Int_Tables_number 229
loop_ _symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 'z, y, -x' 2 'y, x, -z' 3 'x, z, -y' 4 'z, x, -y' 5 'y, z, -x' 6 'x, y, -z' 7 'z, -y, x' 8 'y, -x, z' 9 'x, -z, y' 10 'z, -x, y' 11 'y, -z, x' 12 'x, -y, z' 13 '-z, y, x' 14 '-y, x, z' 15 '-x, z, y' 16 '-z, x, y' 17 '-y, z, x' 18 '-x, y, z' 19 '-z, -y, -x' 20 '-y, -x, -z' 21 '-x, -z, -y' 22 '-z, -x, -y' 23 '-y, -z, -x' 24 '-x, -y, -z' 25 '-z, -y, x' 26 '-y, -x, z' 27 '-x, -z, y' 28 '-z, -x, y' 29 '-y, -z, x' 30 '-x, -y, z' 31 '-z, y, -x' 32 '-y, x, -z' 33 '-x, z, -y' 34 '-z, x, -y' 35 '-y, z, -x' 36 '-x, y, -z' 37 'z, -y, -x' 38 'y, -x, -z' 39 'x, -z, -y' 40 'z, -x, -y' 41 'y, -z, -x' 42 'x, -y, -z' 43 'z, y, x' 44 'y, x, z' 45 'x, z, y' 46 'z, x, y' 47 'y, z, x' 48 'x, y, z' 49 'z+1/2, y+1/2, -x+1/2' 50 'y+1/2, x+1/2, -z+1/2' 51 'x+1/2, z+1/2, -y+1/2' 52 'z+1/2, x+1/2, -y+1/2' 53 'y+1/2, z+1/2, -x+1/2' 54 'x+1/2, y+1/2, -z+1/2' 55 'z+1/2, -y+1/2, x+1/2' 56 'y+1/2, -x+1/2, z+1/2' 57 'x+1/2, -z+1/2, y+1/2' 58 'z+1/2, -x+1/2, y+1/2' 59 'y+1/2, -z+1/2, x+1/2' 60 'x+1/2, -y+1/2, z+1/2' 61 '-z+1/2, y+1/2, x+1/2' 62 '-y+1/2, x+1/2, z+1/2' 63 '-x+1/2, z+1/2, y+1/2' 64 '-z+1/2, x+1/2, y+1/2' 65 '-y+1/2, z+1/2, x+1/2' 66 '-x+1/2, y+1/2, z+1/2' 67 '-z+1/2, -y+1/2, -x+1/2' 68 '-y+1/2, -x+1/2, -z+1/2' 69 '-x+1/2, -z+1/2, -y+1/2' 70 '-z+1/2, -x+1/2, -y+1/2' 71 '-y+1/2, -z+1/2, -x+1/2' 72 '-x+1/2, -y+1/2, -z+1/2' 73 '-z+1/2, -y+1/2, x+1/2' 74 '-y+1/2, -x+1/2, z+1/2' 75 '-x+1/2, -z+1/2, y+1/2'

76 '-z+1/2, -x+1/2, y+1/2' 77 '-y+1/2, -z+1/2, x+1/2' 78 '-x+1/2, -y+1/2, z+1/2' 79 '-z+1/2, y+1/2, -x+1/2' 80 '-y+1/2, x+1/2, -z+1/2' 81 '-x+1/2, z+1/2, -y+1/2' 82 '-z+1/2, x+1/2, -y+1/2' 83 '-y+1/2, z+1/2, -x+1/2' 84 '-x+1/2, y+1/2, -z+1/2' 85 'z+1/2, -y+1/2, -x+1/2' 86 'y+1/2, -x+1/2, -z+1/2' 87 'x+1/2, -z+1/2, -y+1/2' 88 'z+1/2, -x+1/2, -y+1/2' 89 'y+1/2, -z+1/2, -x+1/2' 90 'x+1/2, -y+1/2, -z+1/2' 91 'z+1/2, y+1/2, x+1/2' 92 'y+1/2, x+1/2, z+1/2' 93 'x+1/2, z+1/2, y+1/2' 94 'z+1/2, x+1/2, y+1/2' 95 'y+1/2, z+1/2, x+1/2' 96 'x+1/2, y+1/2, z+1/2'
loop_
_atom_type_symbol
_atom_type_oxidation_number Feo+ 0
#End of data_53451-ICSD

## 7.2 Peak File Structure and Example

The column in the peak file must be separated by the signs: ";", "," or tabulator.
The order of the columns is: [0] HKL; [1] Position; [2] FWHM; [3] Area in $cm^2$; [4] Chi; [5] Omega; [6] Phi; [7] Load in kN;

**CAUTION** DISEMM will associate the peaks according to the selected phase in the Main Window.

## 7.3 Diffraction Pattern File Structure and Example

Comments are noted by '%', '#' or '
' and columns must be separated by ' '; The order of the columns is: [0] Angle; [1] Count; [2] Error

**CAUTION** The error in the third column will be calculated automatically determined via the poission distribution if not present in the data.