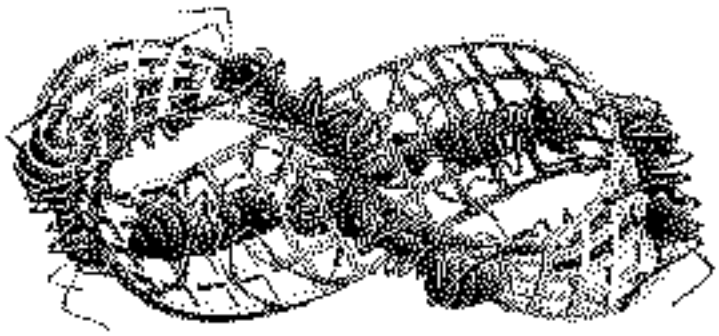
# xband



## A graphical user interface to run band structure programs

## Version 6.3

# 1 Introduction

**xband** is a graphical user interface (GUI) that supplies a number of basic functionalities to facilitate the use of a band structure program. The menu COMPILE PROGRAMS allows one to edit make, dimension and source files and to compile the available programs. With TIDY UP files needed no more can easily be deleted. One of the most tedious step of a band structure calculation is usually setting up the input file. **xband** simplifies this by creating via CREATE SYSTEM a system file, that contains all information on the atomic configuration and geometry of a system. Various ways of visualisation are supplied to document or check the created atomic configuration that makes use of the program **rasmol**. The system file is independent of the program package used and can be stored and retrieved again later via the SELECT/MODIFY SYSTEM menu. Calling a band structure program package allows one to set up specific input files using the information stored in a system file. In addition program execution can be prepared and initiated in various ways. The resulting output

files can be printed, catenated or edited while data files can be further processed using the program **plot** to create **xmgrace** graphics files. Although **xband** has been developed primarily to support the use of the **SPRKKR** package of H. Ebert et al., it can easily be modified to support other packages as well (see Customisation).

**xband** has been written in tcl language starting from the LaTeX GUI xtem of Lamprecht, Lotz and Weibezahn and can be used, copied, modified and distributed on the basis of the GNU licence rules (see the file copying). **xband** uses auxiliary FORTRAN programs (**plot**, **findsym** and **spheres**) written by H. Ebert and A. Perlov that are part of the **xband** distribution with the GNU licence rules applying. The program **spheres** is based on subroutines that stem from the Stuttgart LMTO-package and that have been developed by G. Krier, O. Jepsen and O.K. Andersen.[1] In addition **xband** uses programs (**emacs**, **xmgrace**, **rasmol** and **dataexplorer**) that are not part of the **xband** distribution, but can be obtained free (e.g. as part of a Linux distribution). For high quality 3D plotting of Bloch spectral functions the **DISLIN** library can optionally be used. It is a plotting library free of charge for academic use and has to be downloaded from http://www.dislin.de and installed as described there.

# 2 Installation

**xband** can be obtained from the web-page:
http://olymp.phys.chemie.uni-muenchen.de/ak/ebert/
To install **xband** create a directory (in the following ~ /band) and copy the package xband_DATE.tar.gz to that directory. Execute

```
gunzip xband_DATE.tar.gz
tar -xvf xband_DATE.tar
```

This step supplies all tcl-files and creates the subdirectory ~ /band/locals that contains all default settings in various files (*.vst) as well as three data files (*.dat). You may modify all files apart from ITXC_spacegroups.dat.

When you call **xband** it checks whether the programs **findsym**, **plot**, **spheres** and **glbox** are available. If not, it will try to create the executables. To supply **findsym** (**plot**, **spheres**, **glbox**) yourself, go to ~ /band/symmetry (~ /band/graphics, ~ /band/spheres, ~ /band/glbox) and call `make`. If the compilation failed, adapting the compiler name and options to your system in the makefile should remove the problems. You have to use Fortran 95 compatible compiler. We suggest to use Intel fortran compiler.In all makefiles variable FC is set to ifort. If necessery, please change it to your favor compiler.

Note that the executable **findsym** (**plot**, **spheres**, **glbox**) will be copied automatically upwards to ~ /band and named findsym_$(OSTYPE) (plot_$(OSTYPE), sphere_$(OSTYPE), glbox_$(OSTYPE)), i.e. for example findsym_linux or findsym_OSF1. This allows one to work with **xband** simultaneously under several operating systems.

If the **DISLIN** library is available on your computer and you want to use it for plotting, please edit the makefile in ~ /band/graphics and change the line USEDISLIN=0 to USEDISLIN=1.

[1] We thank these colleagues for the permission to use these subroutines.

**xband** is started by calling the Unix script **xband** that you'll find in ~ /band. Edit this script and specify the directory where the **xband** tcl-files can be found. E.g.: test XBANDPATH || $XBANDPATH=$HOME/band.

To use the script **xband** add the directory ~ /band to your PATH or copy **xband** to a directory that is included in your PATH (e.g. ~/bin or ~/com).

# 3 Calling xband

Call **xband** by

```
xband
```

or

```
xband &
```

If **xband** is called from a xterm window it will write some output to that window used for checking.

# 4 Main Menu

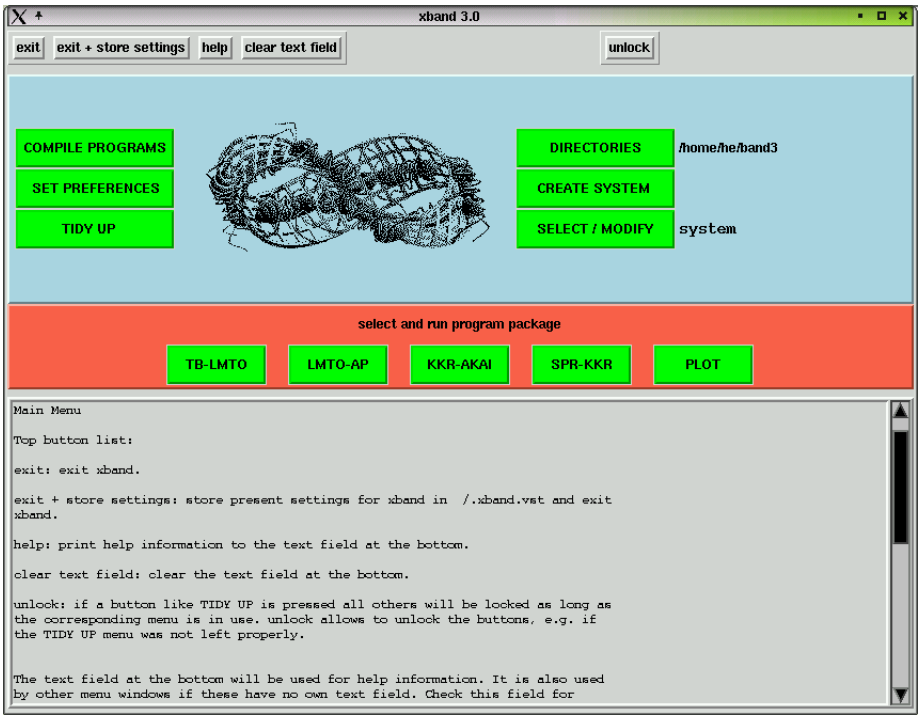



Figure 1: Screenshot main window

Starting **xband** the main window shown in Fig. 1 will be opened. The top button list supplies the following functionality:

exit: exit **xband**.

exit + store settings: store present settings for **xband** in ~ /.xband.vst and exit **xband**.

help: print help information to the text field at the bottom.

clear text field: clear the text field at the bottom.

unlock: if a button like TIDY UP is pressed all others will be locked as long as the corresponding menu is in use. unlock allows one to unlock the buttons, e.g. if the TIDY UP menu was not left properly.

The text field at the bottom will be used for help information. It is also used by other menu windows if these have no own text field. Check this field for hints if something seems to go wrong.

The central field of the main menu shows the **xband** logo and supplies two columns of menu buttons that will be described below. In addition the field displays on its right hand side the names of the working directory and system files after these have been set.

The field between the central one and the text field allows one to call the plot menu via PLOT. In addition it gives access to the program packages that are available to the user. The settings for this field are specified in the file ~ /band/locals/packages.vst. Pressing one of the program package buttons activates the RUN PROGRAM PACKAGE menu that has the same structure for all packages. For that reason only that for the **SPRKKR** package of H. Ebert et al. will be described below.

# 5 The SET PREFERENCES menu

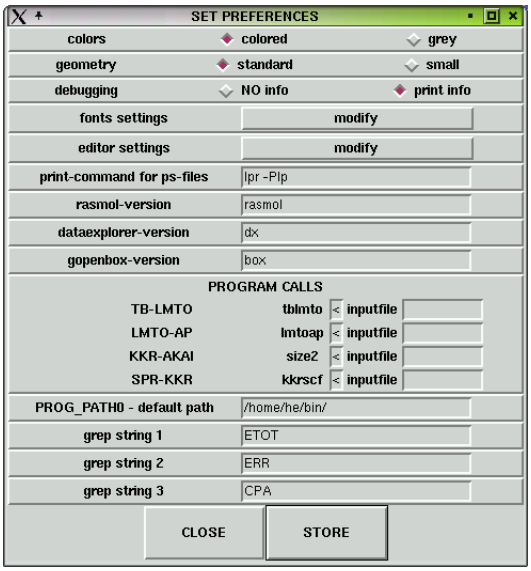



Figure 2: Screenshot SET PREFERENCES menu

When starting, **xband** presets all parameters with internal defaults. It then tries to read ~/.xband.vst if this is available. With SET PREFERENCES (see Fig. 2) you may specify the name of a program (e.g. **rasmol**) if it deviates from the default name.

In case of problems with the size of some menu windows one may reduce their size by changing the geometry setting. By default **xband** uses colours, that may be suppressed. All settings can be modified by editing the files ~/band/locals/geometry.vst and ~/band/locals/colors.vst.

The switch **debugging** controls whether debugging information is written to the xterm to start **xband**.

The button modify in the field **fonts settings** invokes a menu that allows one to select fonts. After you made your choice for all fonts in use, **xband** writes these to the file ~/band/locals/fonts.vst. You can edit this file any time and replace a font by another one. Calling the unix command xlsfonts gives you a list of all fonts available on your machine. Note: if **xband** is called the first time and it cannot find the fonts that have been preset, the font select menu will also be invoked to replace those fonts which are not available.

The button modify in the field **editor settings** invokes a menu that allows one to select an editor. If your favorite editor is not in the list you may add its specifications in ~/band/locals/editor.vst.

For every program package used one may specify how a program is invoked. This may be

program < inputfile

if the input is read from standard input, or

program inputfile options

if the program gets the name and options from the command line.

All settings will be stored in ~/.xband.vst using the button STORE to exit. The content of this file is shown in the info region at the bottom of the main window.

# 6 The COMPILE PROGRAMS menu

This menu is invoked by COMPILE PROGRAMS used to edit make, dimension and source files and to compile programs (see Fig. 3).

Directory list (centre region left): use left mouse click to change the directory. You may also type the name of the new directory in the entry field below the list for this purpose.

Makefile, dimension and source file lists: use left mouse click to select. Edit selected files using the edit buttons. Change listing mode by clicking alphabetic or last access. Allowed suffixes for the files are listed in the small windows above the file lists. These suffix lists can be modified by editing the corresponding file in ~/band/locals.

Selecting a source file automatically starts **emacs** for editing. Selecting a makefile gives a list of possible calls of `make` in the makefile window (top region). Use left mouse click to select a `make` call and execute the compilation.

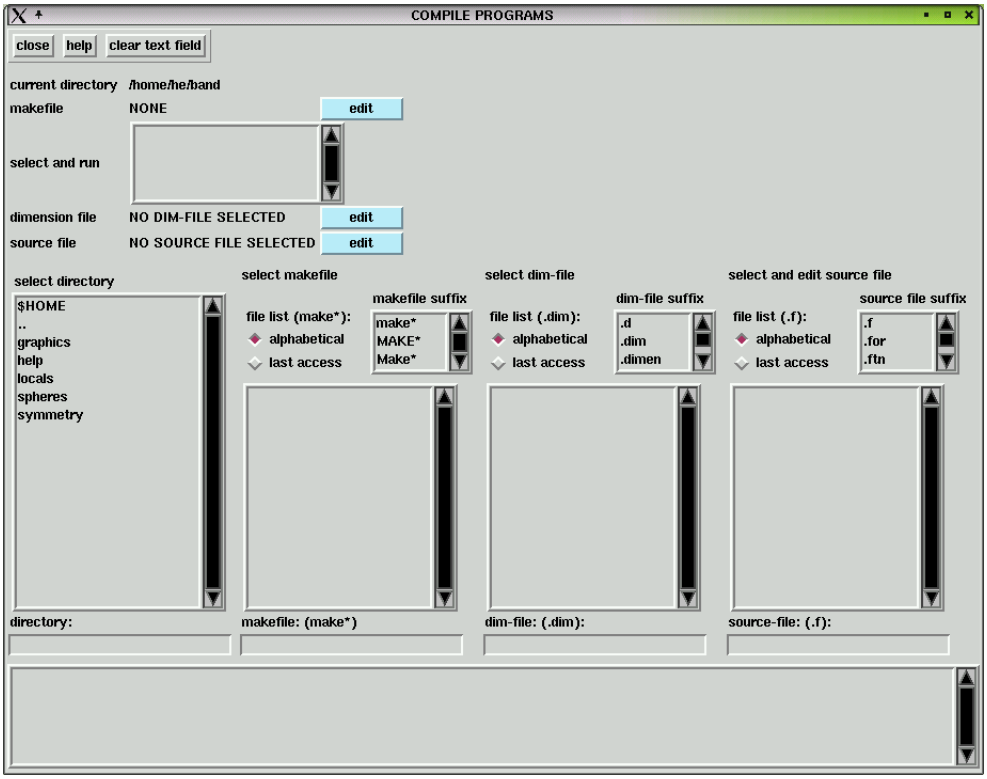



Figure 3: Screenshot COMPILE PROGRAMS menu

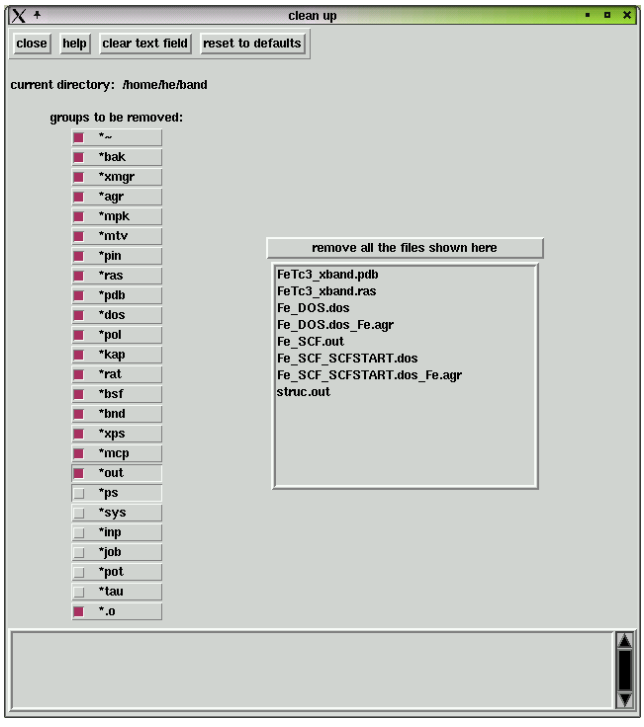



Figure 4: Screenshot TIDY UP menu

# 7 The TIDY UP menu

The left column of the menu (see Fig. 4) invoked with TIDY UP gives a list of suffixes (edit ~/.xband.vst to modify). Activate/deactivate the suffixes as needed and delete the files with activated suffixes by pressing the button remove all files shown here (right). The names of the deleted files are given in the text field at the bottom of the window.

# 8 The DIRECTORIES menu

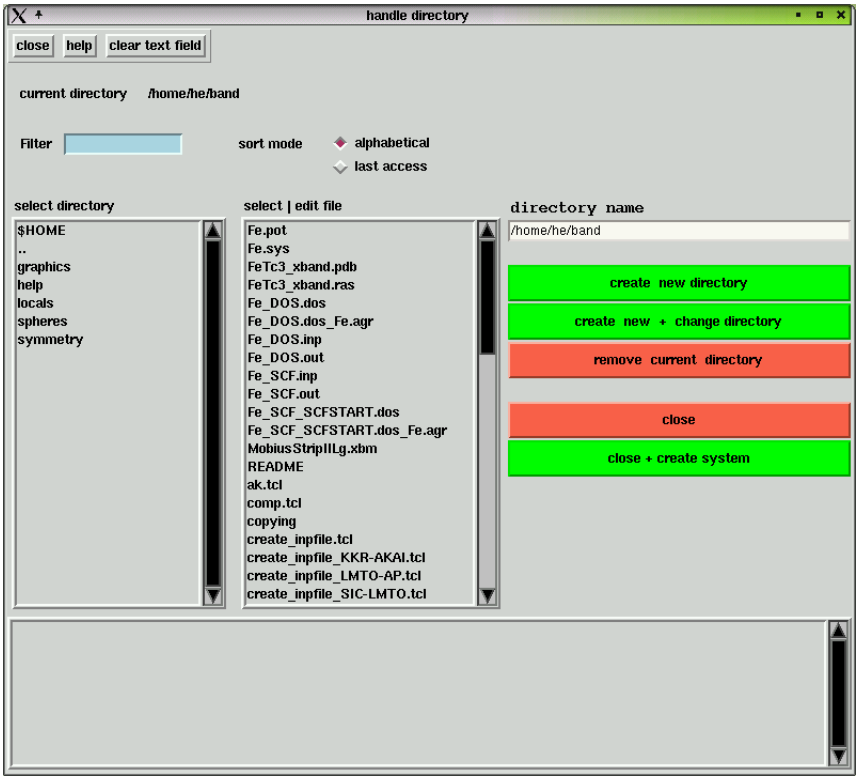



Figure 5: Screenshot DIRECTORY menu

The DIRECTORIES menu (see Fig. 5) invoked via DIRECTORIES allows one to create and remove directories.

Directory list (centre region left): use left mouse click to change the directory.

File list (centre): use left/middle mouse click to select/edit a file.

The column on the right hand side allows one to create and remove directories. To create a new directory modify the entry field at the top of the column and press the appropriate create button. To remove a directory press REMOVE CURRENT DIRECTORY. **xband** will take care that you remove only empty directories. Leaving the menu via the button close+create system invokes the create system menu without going via the main menu.

# 9 The CREATE SYSTEM menu

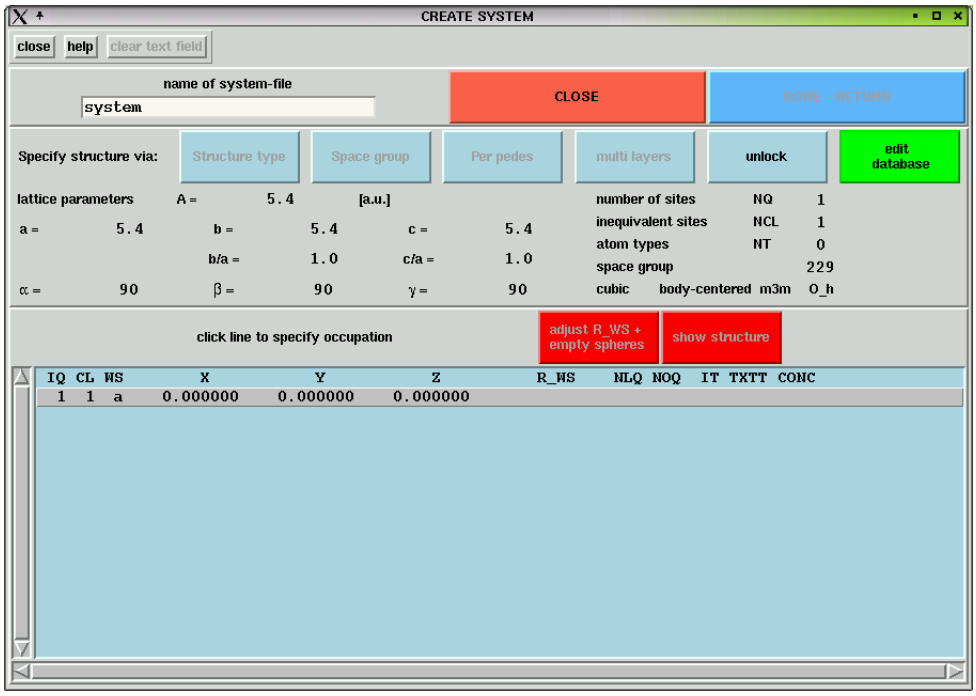



Figure 6: Screenshot CREATE SYSTEM menu

This menu (see Fig. 6) is used to create a system file that contains all geometrical information on a system. Leaving the menu activated by CREATE SYSTEM using the button DONE - RETURN writes the system file, while selecting a system using SELECT/MODIFY SYSTEM rereads it again (see below).

By default the CREATE SYSTEM menu allows one to set up 3D-structures. In addition one can set up 2D- and 0D-structures calling the corresponding menus via the buttons Create 2D-system and Create 0D-system (the 0D-feature will come in the next release), respectively.

There are four ways to specify a 3D-system:

Structure type supplies a list of predefined structure types that are specified in ~ /band/locals/ITXC_structure.dat (see edit database). Select by left mouse click. Specify the lattice parameters as requested. The next window lists all crystallographically inequivalent sites of the selected structure. If these have fixed coordinates, the button line is deactivated. If not, click line and specify coordinates as requested.

Space group supplies a list with all 230 crystallographic space groups. Some space groups are listed twice allowing to use a different choice of the basis vectors, orientation of the unique axis or origin. In doubt, select the space group with the c-axis as the unique axis or the second origin, respectively, because this will include the inversion as symmetry operation. Specify the lattice parameters as requested. The convention for the basis vectors

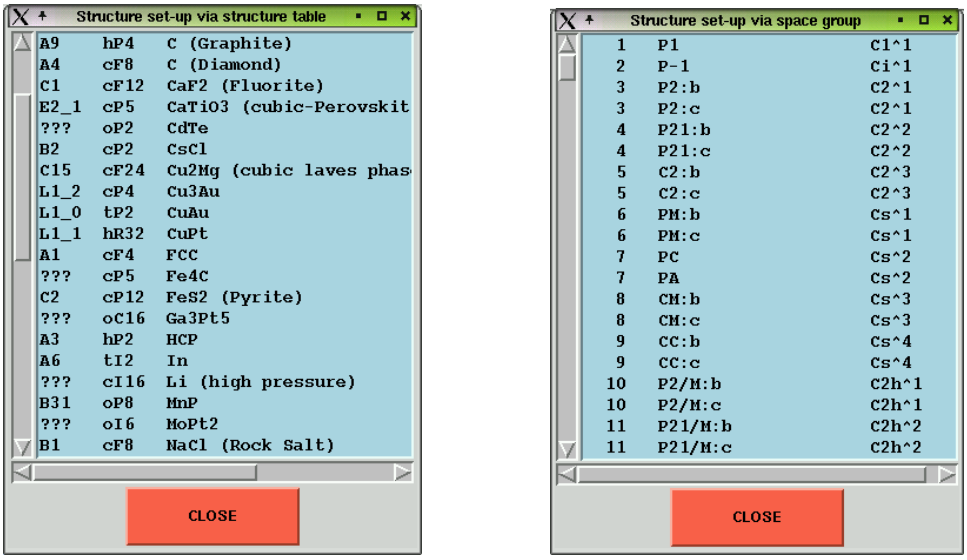



Figure 7: Screenshot structure type (left) and space group (right) listbox

and specification of the atomic positions are summarised in Table I. The next window lists all crystallographic inequivalent sites of the space group. Select a site by clicking the corresponding line. If the site has fixed coordinates, the button line will be deactivated afterwards. If not, specify the missing coordinates as requested. After specifying all sites of the system return pressing DONE - RETURN.

Per pedes allows one to specify a system from scratch. Select the Bravais lattice or click the first line if it is unknown. The basis vectors, that are assumed by **xband**, are summarised in Table II. Give the total numbers of sites in the system and proceed. Supply the lattice parameters in the following window. Alternatively, you may skip this window and specify the primitive lattice vectors yourself in the next window. For all lattice sites the coordinates have to be given first. This can be done in Cartesian or crystallographic units. A radio button allows one to switch between these modes. You can use the copy button to copy the input from any line to the next empty line. reset will delete the input of a line. occupy calls the Specify occupation menu that is described below.

multi layers allows one to specify the structure for a number of frequently studied multi layer structures. Specify the common lattice parameter first and then select the multilayer system from the menu. Use the scales to specify the number of atom sites within the repeat unit. The restrictions due to three dimensional periodicity are automatically accounted for.

The left column of the menu allows one to create multilayer-systems with a homogeneous lattice, while the right column is used to create multilayers with the repeat unit consisting of two different but matching sublattices. In the latter case the inter-system distance can

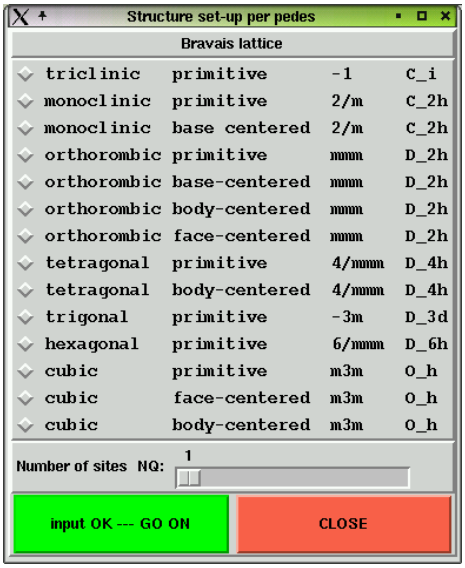



Figure 8: Screenshot per pedes dialog

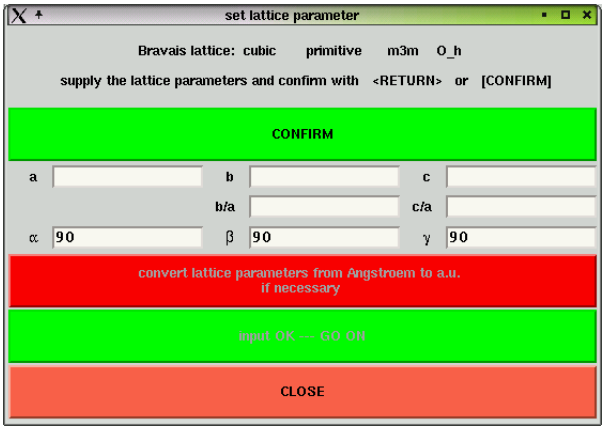



Figure 9: Screenshot set lattice parameter menu

be scaled in addition to the layer distance c of the sublattices. You may modify/extend the multilayer menu by editing the file ˜ /band/locals/multilayer.vst.

When leaving one of the submenus described above, the program **findsym** is called automatically. **findsym** uses the input file struc.ini and can also be run separately. In any case the result will be written to struc.out and standard output. After the automatic run of **findsym** the structure menu will be extended giving at the bottom a list of all the atomic sites in the system. Apart from specifying the system via Per pedes, these have to be occupied by left mouse clicking a line calling the Specify occupation menu. If there are more than one atoms present on a lattice site (in a substitutional disordered system) click button 2, 3 etc. in the header line to allow for 2, 3 etc. occupants. For every occupant specify its chemical symbol via specify occupant and its concentration using the scale. The corresponding Wigner-Seitz radius is taken from a table that is set up via the file ˜ /band/locals/rws.vst, if available. If no value for the Wigner-Seitz radius is predefined, this has to be supplied by the user. In case of

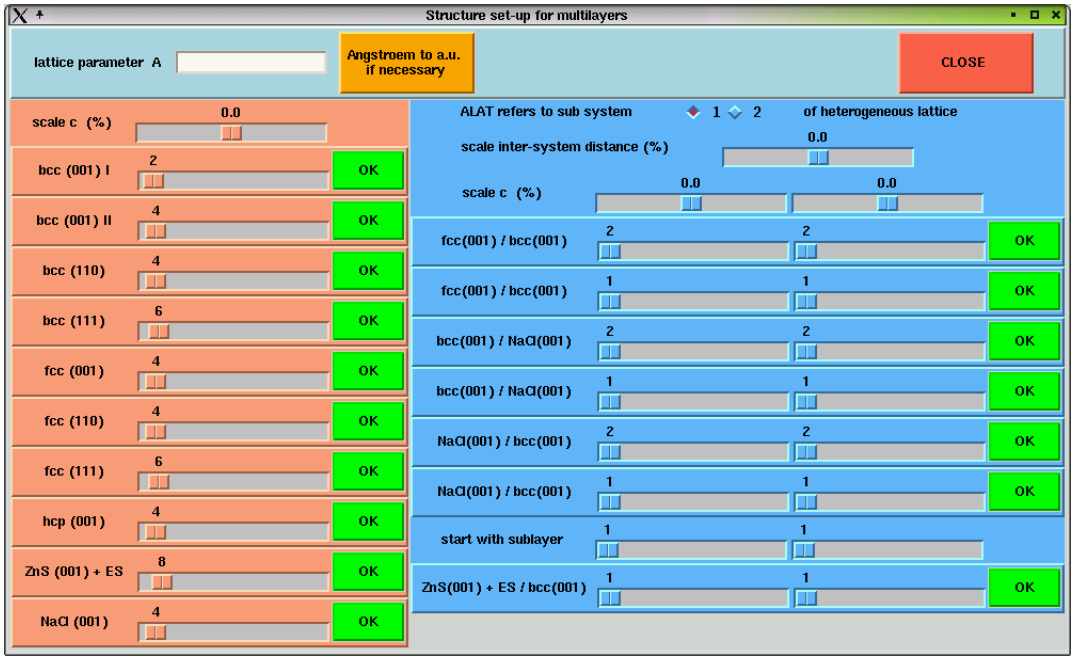



Figure 10: Screenshot multilayer menu

more than 1 occupant, the average Wigner-Seitz radius will be used that is obtained by summing up the concentration weighted individual radii. The name of an atomic type will be modified by **xband** if a chemical element occupies several crystallographically inequivalent lattice sites.

The Specify occupation menu occupies all equivalent sites simultaneously. After all sites have been occupied, or after setting up the system via Per pedes, the show structure and DONE - RETURN buttons get unlocked. Nevertheless, one may still modify the atomic configuration. When leaving via DONE - RETURN the atomic configuration is stored in the system file whose name is automatically generated and updated after every change of the configuration. Before leaving, however, the system file name may be modified using the entry in the top region of the window. The edit database button gives the possibility to add a structure to the database ~ /band/locals/ITXC_structure.dat. Left mouse click invokes the editor for the two ITXC-database files. Follow the instructions given in ITXC_structure.dat to add a new structure.

**xband** sets the Wigner-Seitz radii of the atoms according to the table in ~ /band/locals/rws.vst. Alternatively one may set the Wigner-Seitz-radii by pressing the button adjust R_WS + empty spheres. This will invoke the program **spheres** that sets the values according to a guess for the charge density. In addition one may add empty spheres. For these a lower and upper limit of their radii may be fixed. The program **spheres** should be invoked only after the structure has been completely specified. The symmetry of the system will not be modified by a run of **spheres**.

To check the generated configuration, input files for several visualizers can be created via show structure.

The menu (see Fig. 11) called that way allows one to display the atomic structure in four different ways by left mouse click on the corresponding buttons in the top row of the run visualizer menu window.

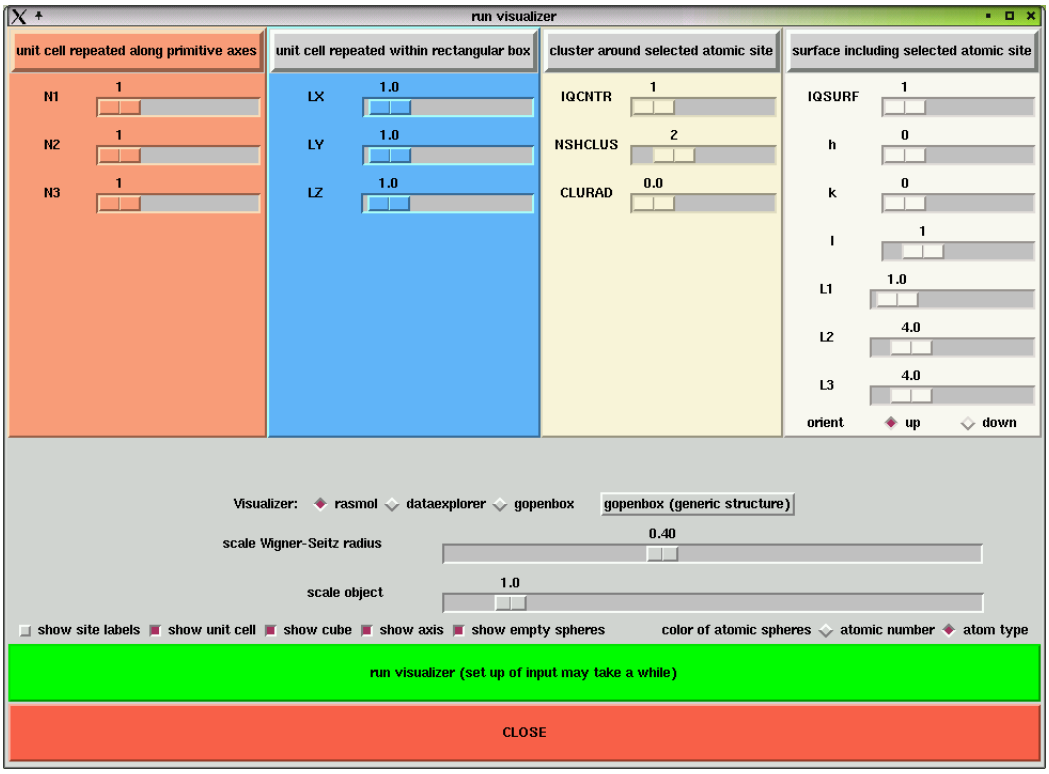



Figure 11: Screenshot run visualizer menu

unit cell repeated along primitive axes shows the lattice sites with the basis repeated along the three directions of the primitive basis vectors. The number of repetitions can be specified.

unit cell repeated within rectangular box displays the lattice sites with the basis repeated to fill a rectangular box. The side length of the box (in units of ALAT) can be specified.

cluster around selected atomic site sets up an atomic cluster centred at a specified lattice site IQ. The size of the cluster may be fixed by the number of neighbouring atomic shells or its radius (in units of ALAT).

surface including selected atomic site sets up a surface fragment for the Miller indices (h,k,l) going through site IQ with its width and lateral extensions specified in units of ALAT.

The current system can be visualized using three different programs, which have to be choosen in the visualizer-line: **rasmol dataexplorer** and A. Perlov's **gOpenBox**. Unavailabe parameters are grayed out correspondingly.

The button gOpenBox (generic structure) creates a generic input file for the **gOpenBox** program. None of the parameters set in the menu are therefore taken into account.

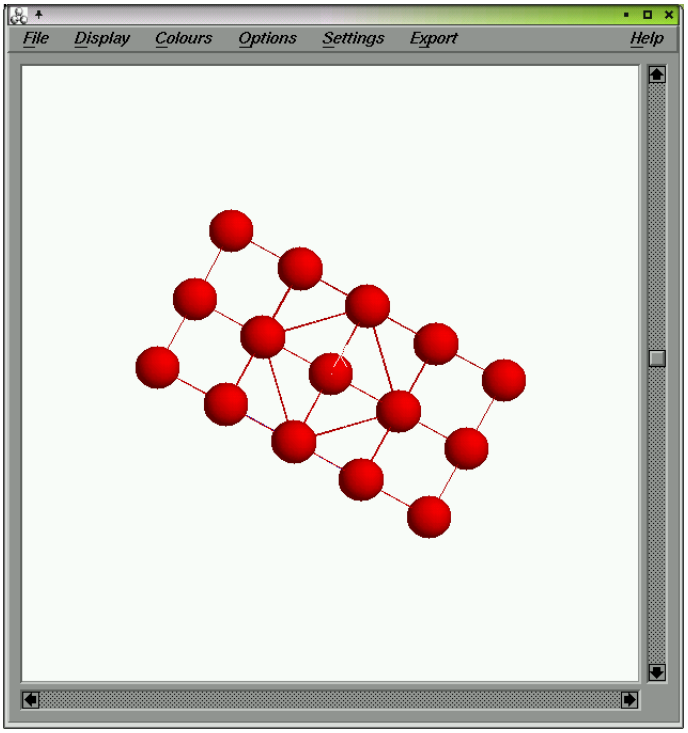



Figure 12: Screenshot **rasmol** as visualizer

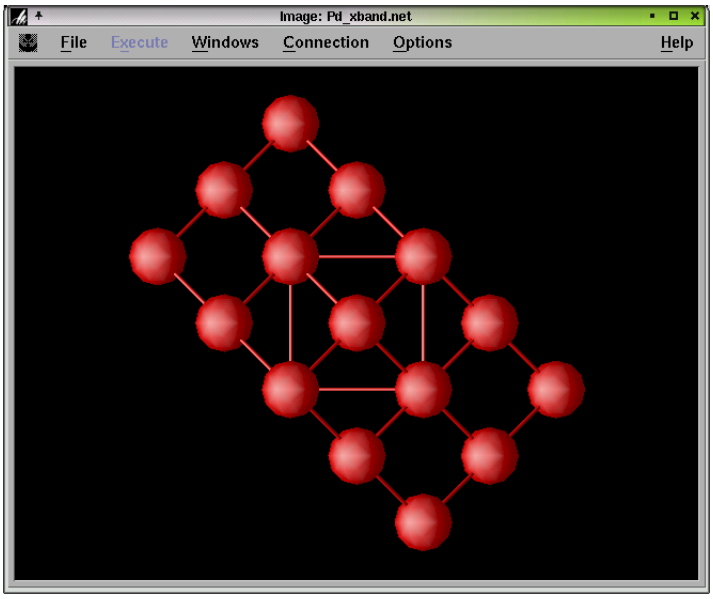



Figure 13: Screenshot **dataexplorer** as visualizer

The radius of a sphere representing an atom may be scaled up using the scale object parameter. The value 1 corresponds to the proper Wigner-Seitz radius. The checkbuttons at the bottom allow one to add labels to the lattice sites giving the atom type name TXTT, atom type number IT, and lattice site number IQ. A cube with side length ALAT, the crystallographic unit cell and the Cartesian axes may be shown as well.

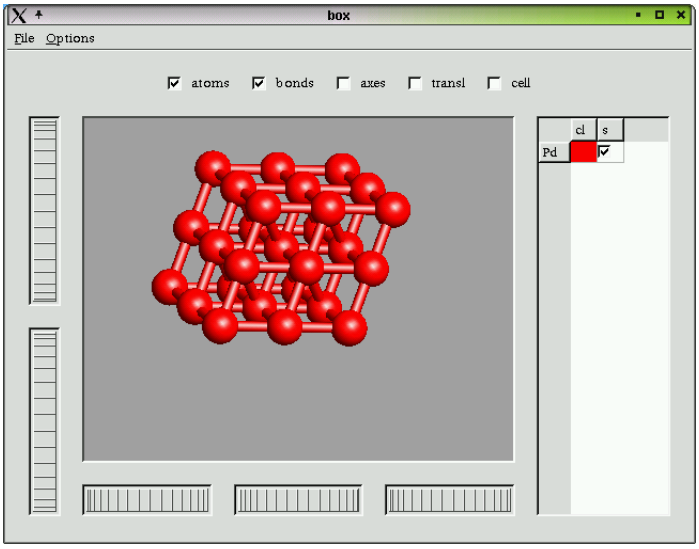



Figure 14: Screenshot **gOpenBox** as visualizer

Because **rasmol** was designed for molecules a number of geometrical restrictions are imposed. These can be circumvented in most cases by scaling the dimensions of the system up or down by the supplied scale (default value is 1).

After setting the mode and the required parameters the inputfiles for the chosen visualizer are created and the corresponding program is executed by clicking on the run visualizer button.

**rasmol** is using the data file X_xband.pdb together with the script file X_xband.ras. These can be used later on Unix level calling rasmol -script X_xband.ras.

**dataexplorer** is using the data file X_xband.dx together with the network file X_xband.net. These can be used if calling **dataexplorer** standalone.

**gOpenBox** is using the file X_xband.gopenbox or in generic structure mode the file X_xband.structure. Both can be used later on Unix level calling glbox X_xband.gopenbox or glbox X_xband.structure.

# 10 The CREATE 2D-SYSTEM menu

Calling the CREATE 2D-SYSTEM menu via the button Create 2D-system opens the window shown in Fig. 15. There are 4 ways to create a 2D-system.

homogeneous extended lattice: The corresponding menu shown in Fig. 16 allows one to set up extended 2d-systems with a homogeneous underlaying lattice. The system is assumed to consist of a periodic left (L) and right (R) bulk (specified by a corresponding unit cell), and a spacer in between. The occupation of all layers may be symmetric or not and bulk (L) may be identical to bulk (R) (symmetric systems need less input from user). The unit cells may be enlarged along the in plane a and b axis (e.g. to simulate disordered systems). The bulk unit cells may be larger than the structure unit. The interlayer distance may

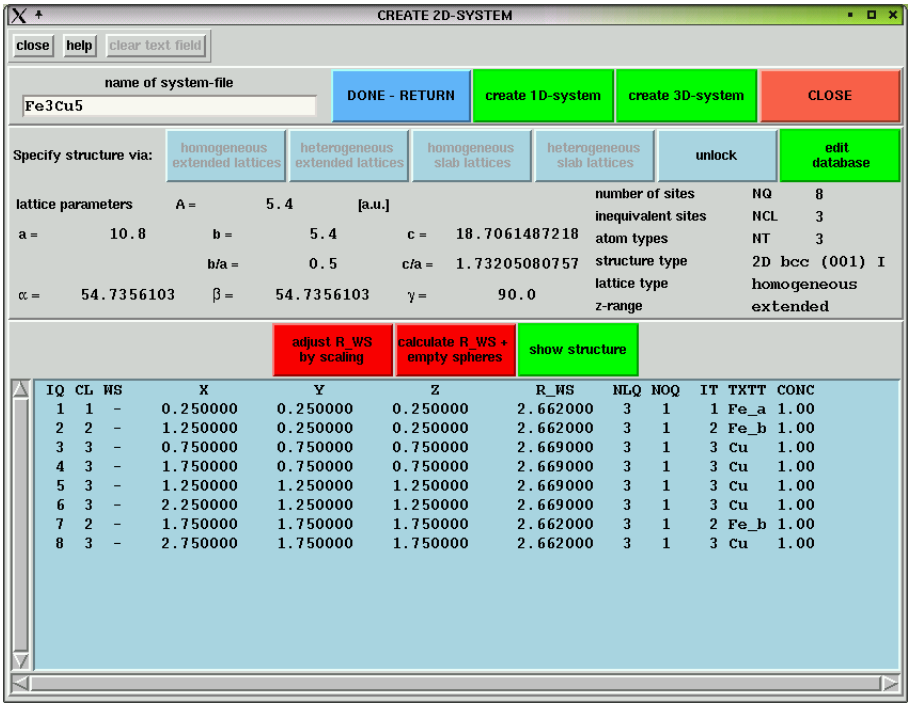



Figure 15: Screenshot create 2D system menu


Figure 16: Screenshot structure set-up menu for layered system with homogeneous extended lattice

be scaled by scaling the parameter c. The right column of the menu allows one to select among various predefined structures (see 2D_structure.dat For each 2D-structure the number of layers in the basic structure unit (that will be repeated) is given and the total number of layers can be chosen consistently with a scale. The following occupation menu called by

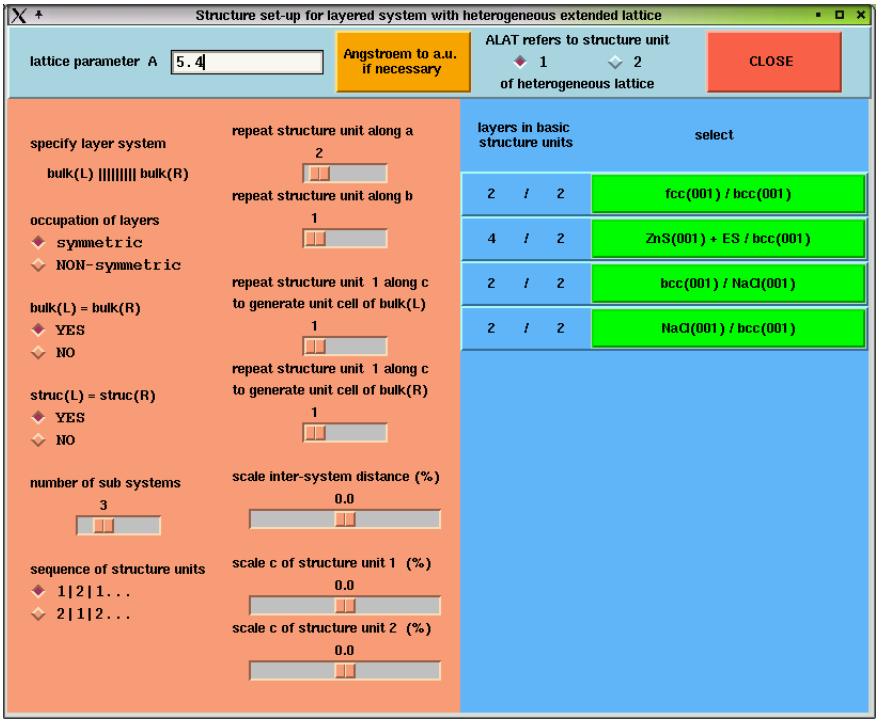



Figure 17: Screenshot structure set-up menu for layered system with heterogeneous extended lattice

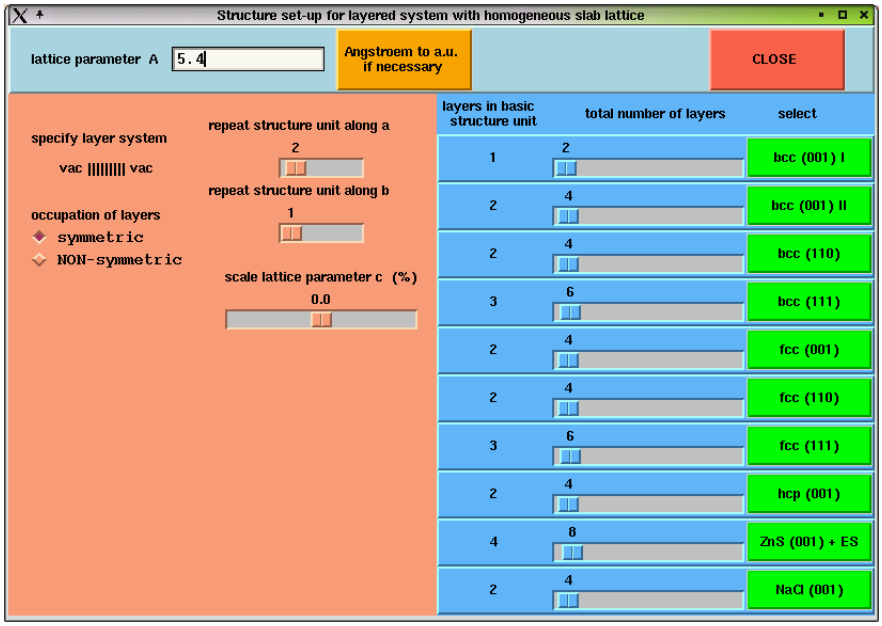



Figure 18: Screenshot structure set-up menu for layered system with homogeneous slab lattice

the right hand button is desribed below.

heterogenous extended lattice: The menu invoked by this button is very similar to the


Figure 19: Screenshot structure set-up menu for layered system with heterogeneous slab lattice

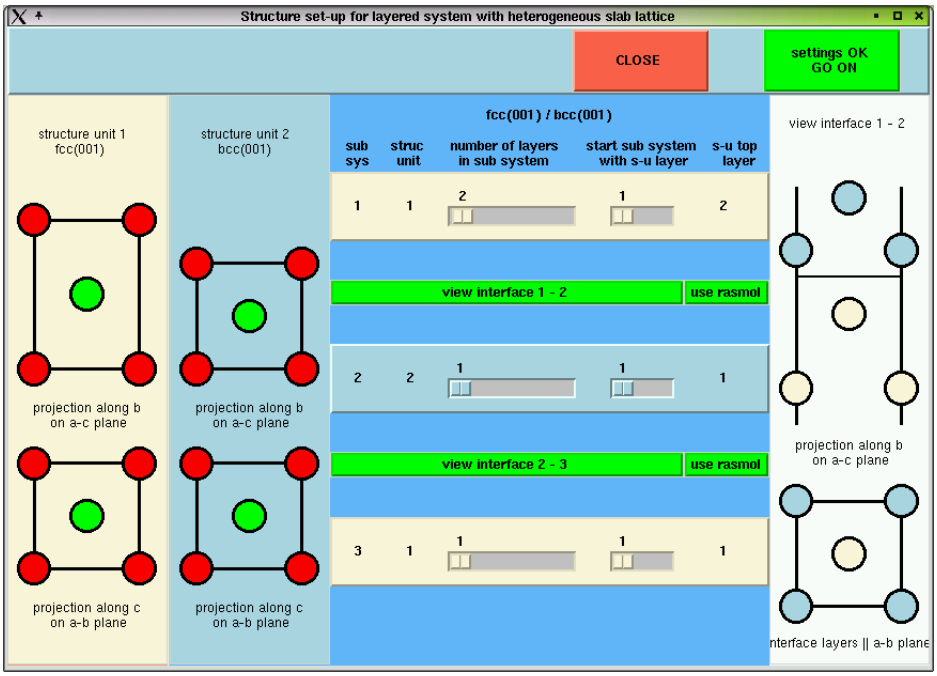



Figure 20: Screenshot structure set-up menu for layered system with heterogeneous slab lattice

previous one (shown in Fig. 17) but allows one to set up layered systems set up of two different structure units. Accordingly the structure of bulk (L) and bulk (R) (struc (L) and struc (R), respectively) may be the same or different. The total structure may consist of many subsystems having alternating structure unit 1 and 2, starting with unit 1 or 2. All relevant interlayer distances may be scaled seperately. The right hand column gives the various

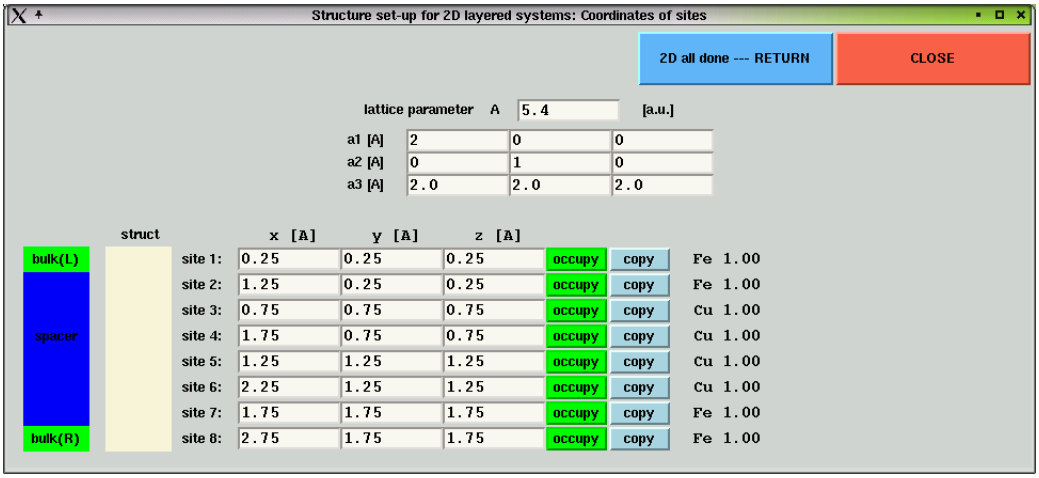



Figure 21: Screenshot coordinates of sites set-up menu for layered system

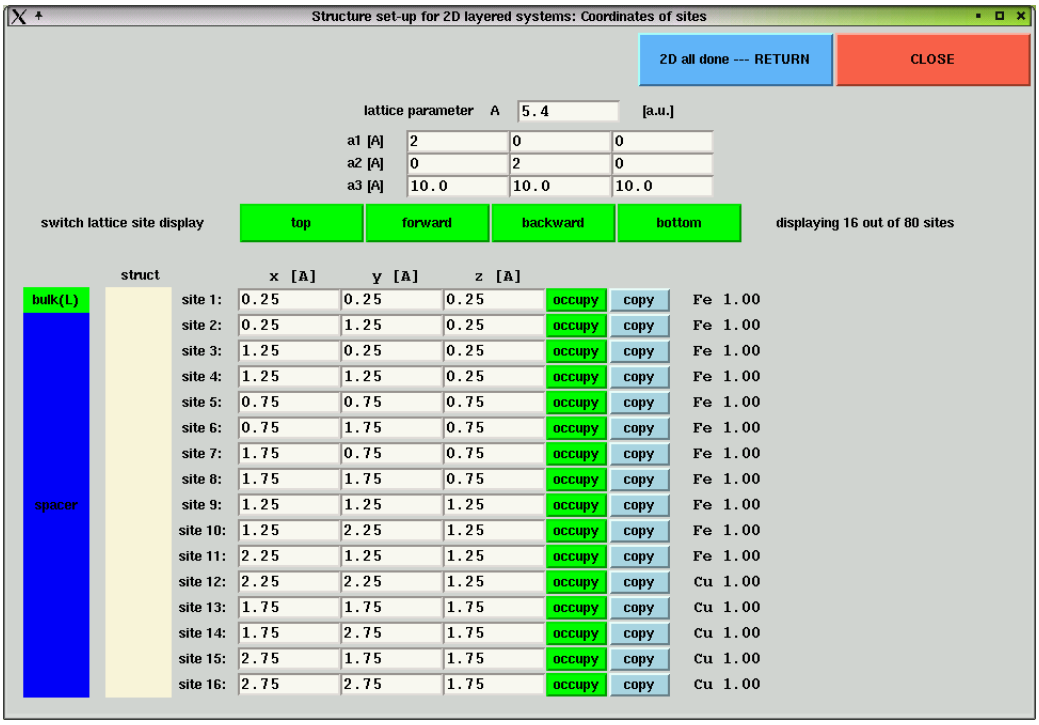



Figure 22: Screenshot coordinates of sites set-up menu for layered system

structures available (see 2D_structure.dat) together with the number of layers in the two basic structure units (left). Selecting a 2D-structure invokes the menu shown in Fig. 20. The two columns to the left (with different coloured background) give a projection from top and side of the two basic structure unit. The following menu following to the right allows one to specify the various numbers of layers in the subsystems (In Fig. 20 there are 3 subsystems having - from top - structure 1, 2 and 1 as indicated by the background color). The number of layers in the subsystem can be chosen together with the index of the starting layer. The latter option is necessary to have a proper matching of the subsystems. This can be visualised on

the right hand side by a projection pressing the view interface button. Alternatively the 4 layers around the interface can be viewed via rasmol using the use rasmol button. The following occupation menu described below is called by the Settings OK - GO ON button.

homogeneous slab lattice: The corresponding menu is completely analogous to the one for extended systems and is shown in Fig. 18. The only difference is that bulk (L) and bulk (R) is missing now; i.e. the slab has a finite extension perpendicular to the layers and is surrounded by vacuum.

heterogenous slab lattice: Again the menu shown in Fig. 19 is analogous to its counterpart for extended systems.

Having set up a 2D-structure using one of the various menus, the lattice sites may be occupied via the menu shown in Fig. 21. Go through the table from top to bottom and specify occupation of a site via the occupy button. Pressing one of the copy button of the occupied sites copies its occupation to the next empty sites. For symmetric systems the occupation is mirrored automatically.

If there are too many sites to be shown on the screen only a subset is displayed. One can go through the list by paging using one of the buttons above the list. This situation applies to the screenshot shown in Fig. 22 that shows 16 sites for an extended 2D-system with 80 sites in total (including bulk (L) and bulk (R)).

# 11 The CREATE 0D-SYSTEM menu

0D-systems, i. e. impurities and deposited clusters are set up via the CREATE 0D-SYSTEM button. Before pressing this button, one has to select the system file of the underlying structure (e. g. 3D bulk or 2D surface) first. One will be prompted to choose an existing system file or to create a new one if no system is currently selected. Otherwise the create 0D-system step A menu (see Fig. 23) will open. Here one can specify how big the underlying structure is chosen to later modify it with the 0D system, and around which site the system should be centered. Specify how many unit cells the system is expected to be. Click Occupy to continue. This brings up the create 0D-system step B menu (see Fig. 24). There are three views of the underlying sysems, one for a view along each axis. The view on the right is the one for the z-axis and only shows three different layers of the system. Small atoms represent atoms with the lowest z-value of these three layers. On the right hand one can adjust which layers are shown with the prev layer and next layer buttons.

Now one or more additional occupation types have to be created in the usual way. These appear in the list of occupation types together with the types of the underlying lattice. If a occupation type is selected, atoms of the underlying lattice can be set to this type by clicking on the atom in the z-axis view. The atom is also selected. To select an atom without changing the type or to unselect an atom, use the middle or right mouse button, respectively. At any time one can check the structure by pressing the Show 3D button. Selected atoms have a bigger radius than unselected lattice sites in this visualization. One can easily select all atoms surrounding the so far selected atoms by using the add relaxation zone button. Either the number of surrounding shells or a radius has to be supplied to do so.

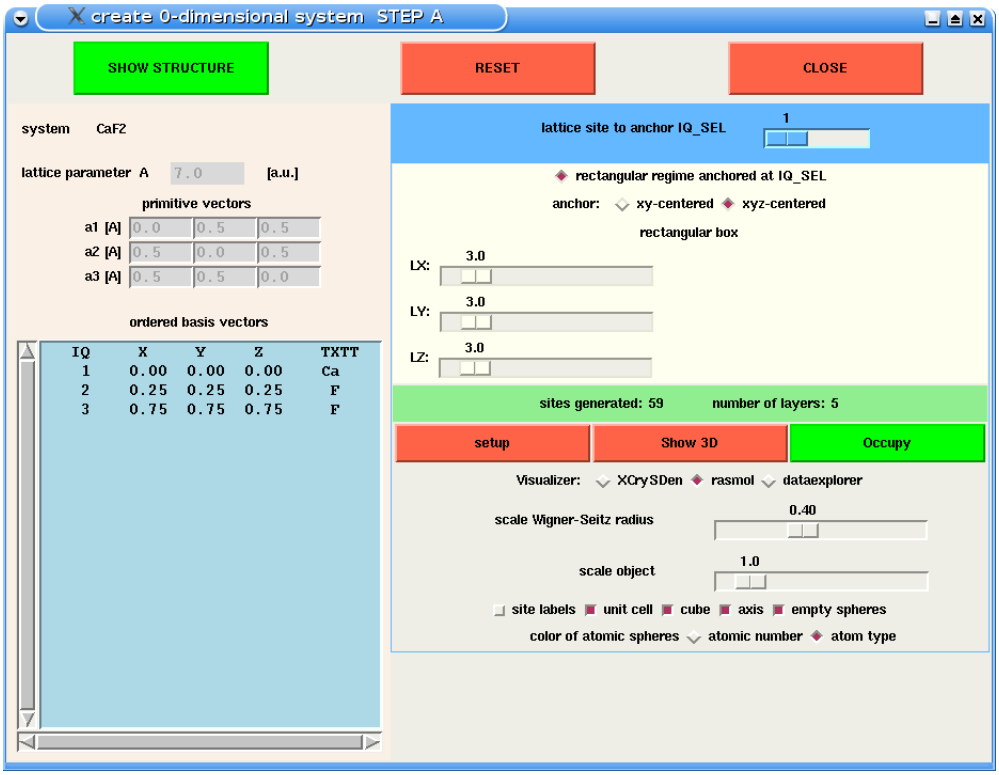



Figure 23: Screenshot Create 0D-structure, step A

If the system is set up, click Done and enter a new filename to save the system.

# 12 The SELECT/MODIFY SYSTEM menu

The button SELECT/MODIFY SYSTEM invokes a menu to select and possibly to modify a system file that has been created earlier.

Directory list (centre region left): use left mouse click to change the directory. You may also type the name of the new directory in the entry field below the list for this purpose.

System and potential file lists: use left mouse click to select and middle mouse click to select and quit. Edit selected files using the edit buttons in the top region. Change listing mode by clicking alphabetic or last access. Allowed suffixes for the files are listed in the small windows above the file lists. These suffix lists can be modified by editing the corresponding file in ~ /band/locals.

Having selected a system file one may quit or modify the system pressing the modify button. This step invokes the menu shown in Fig. 26. In the top region the old settings for the lattice parameter and primitive vectors are given followed by the present or new settings. To the right a number of buttons are available that allow to scale the primitive vectors or to stretch or compress the system along the Cartesian axes. The bottom table gives the old and new coordinates of the lattice sites. This can be given in Cartesian or crystallographic units. This table allows one to modify the basis vectors individually. Leaving the modify menu

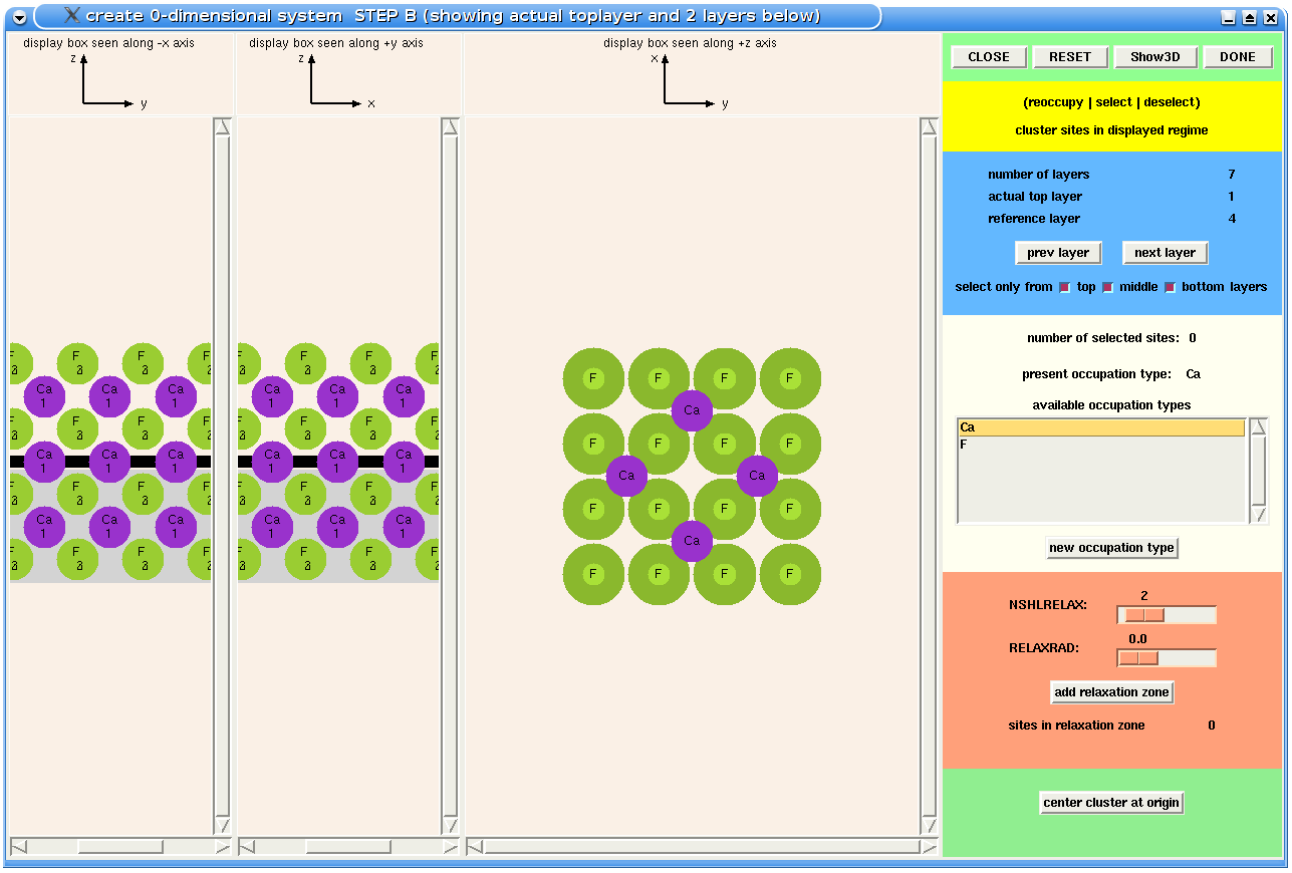



Figure 24: Screenshot Create 0D-structure, step B

displays the resulting system data via the window shown in Fig. 27. If the modifications influence the symmetry of the system this will be automatically accounted for.

# 13 The RUN PROGRAM PACKAGE menu

If the button SPR-KKR or any other program button is pressed the corresponding RUN PROGRAM PACKAGE menu is activated.

Directory list (centre region left): use left mouse click to change the directory. You may also type the name of the new directory in the entry field below the list for this purpose.

Input, job and output file lists: use left mouse click to select and middle mouse click to select and edit using **emacs**. Edit selected files using the edit buttons in the top region. Change listing mode by clicking alphabetic or last access. The filter allows one to select certain subsets of the files to be listed. Allowed suffixes for the files are listed in the small windows above the file lists. These suffix lists can be modified by editing the corresponding file in ~ /band/locals.

With an input, job or output file selected or created the corresponding pull down menu (column of buttons in the middle of the top region) gets unlocked. This menu allows one to

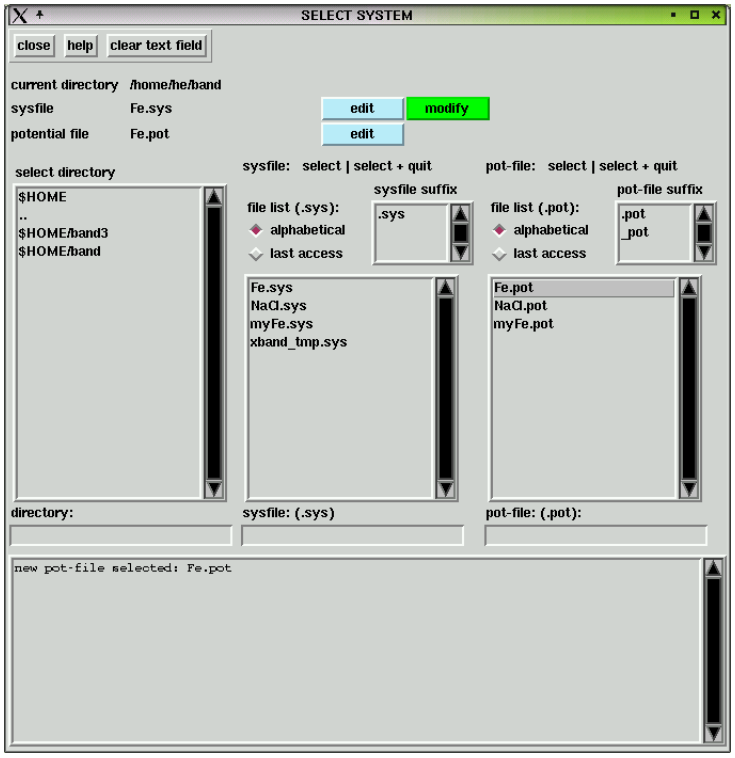



Figure 25: Screenshot SELECT SYSTEM menu

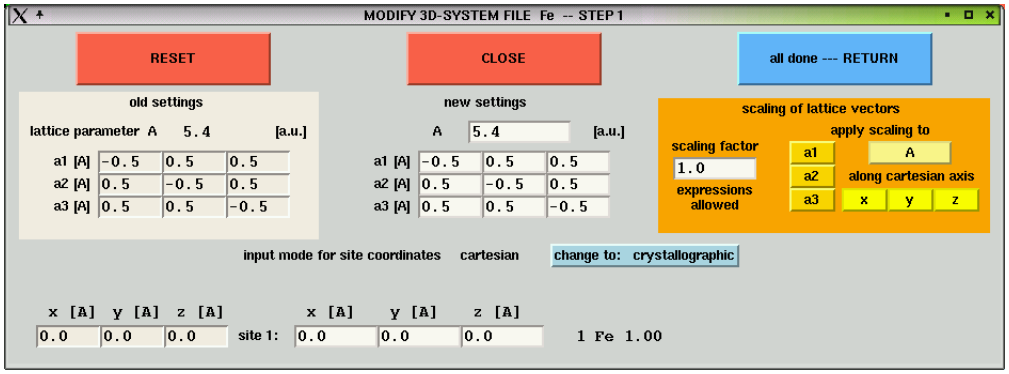



Figure 26: Screenshot modify system menu step 1

edit, copy, move, delete, catenate or print the files and supplies some more functionality.

Selecting an input file allows one to run the various programs of the package. A new input file can be created via create input. For this purpose, the system information has to be available. This is the case if a system was selected or created via SELECT/MODIFY SYSTEM or CREATE SYSTEM before calling SPR-KKR. If create input is pressed without a system specified, the user will be asked to select or create a system file. The next call of create input should be successful and activate the input menu, that is of course dependent on the package.

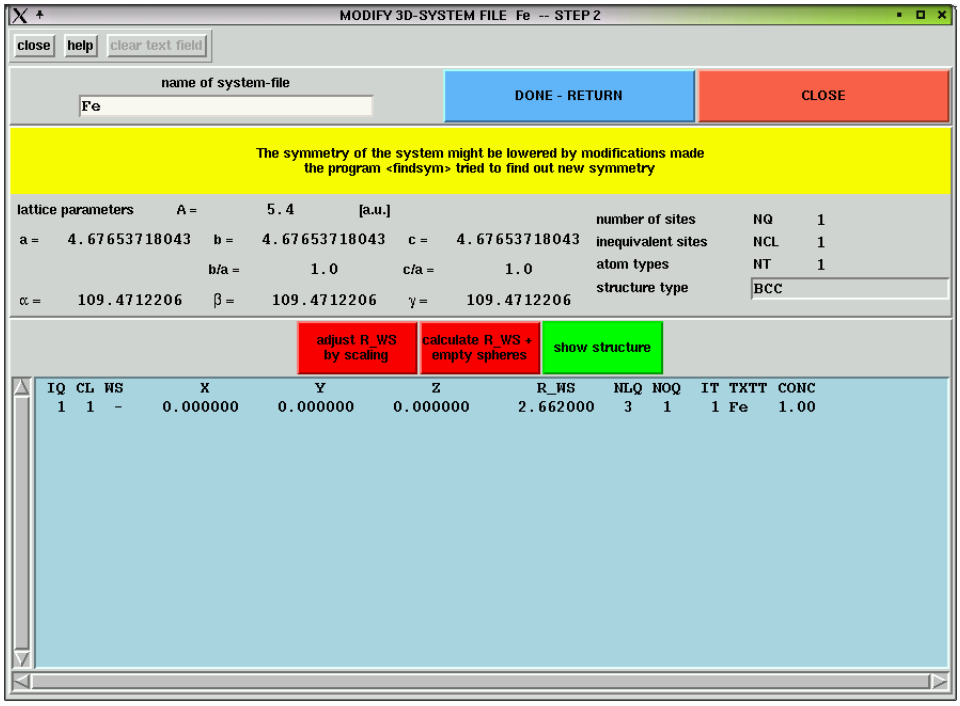



Figure 27: Screenshot modify system menu step 2

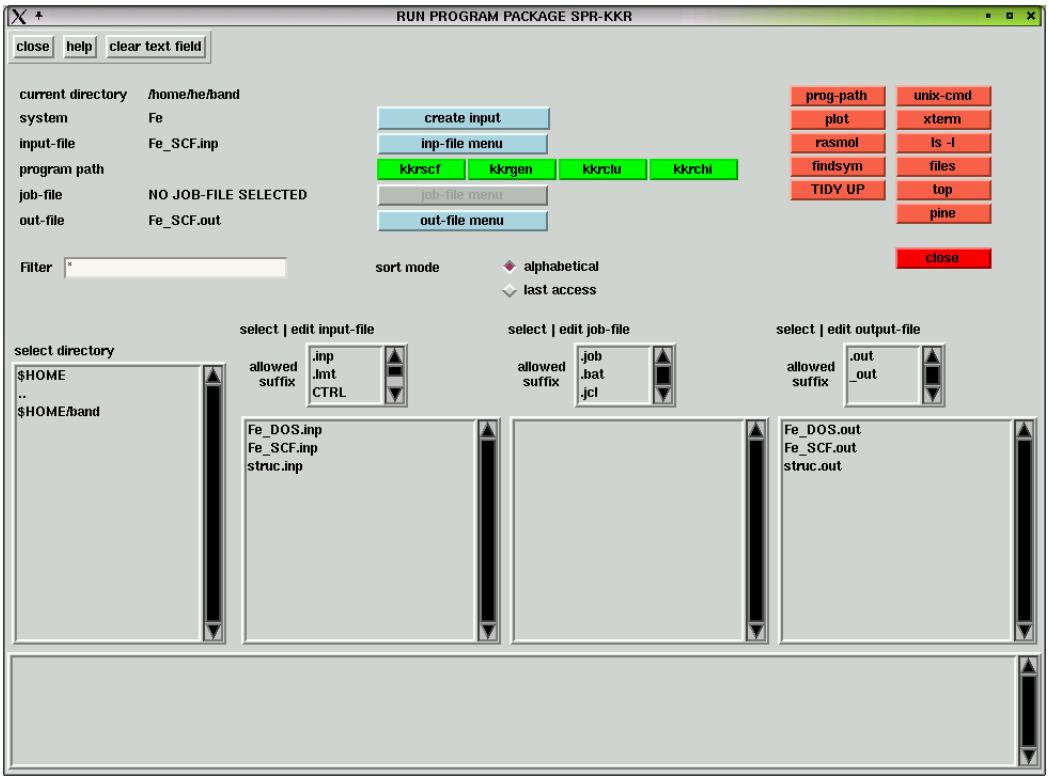



Figure 28: Screenshot RUN **SPRKKR** PACKAGE menu

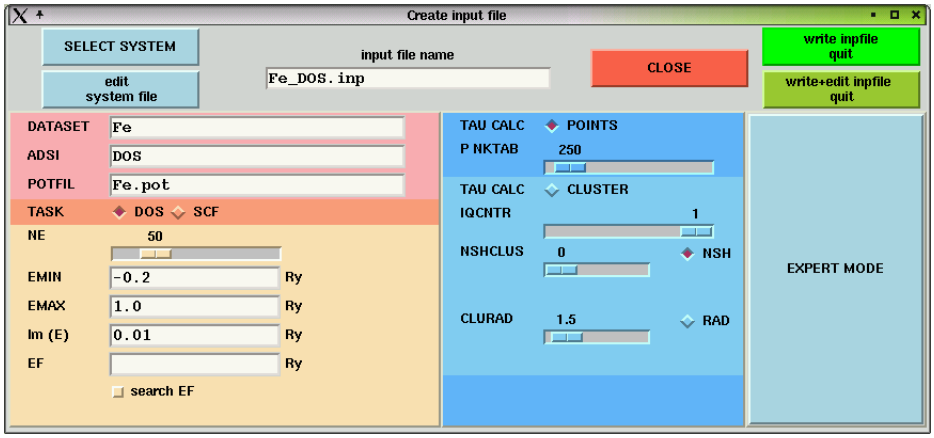



Figure 29: Screenshot **SPRKKR** create input menu

For the **SPRKKR** package create input allows one to create input files to run **kkrscf** and **kkrgen** to calculate the potential self-consistently and the DOS, respectively. The menu automatically creates the name of the input and potential files according to the system name and TASK. Before leaving the menu you may change these names as you like. Using the menu go through step by step by first selecting the TASK. This will in general create suggestions for the remaining entries.

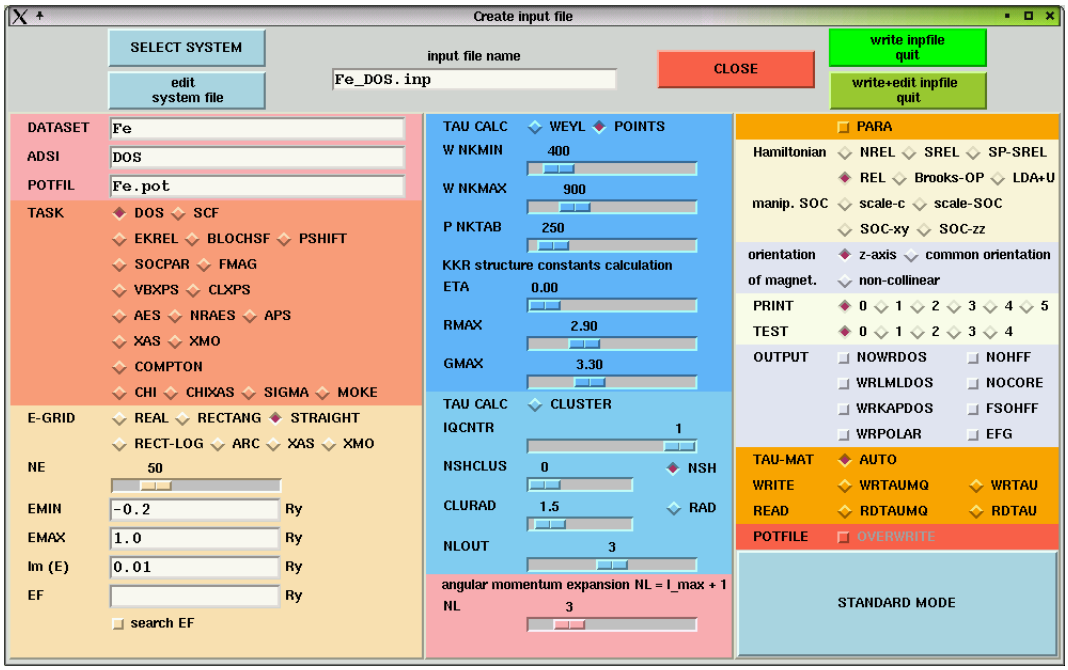



Figure 30: Screenshot **SPRKKR** expert create input menu

If you change to the EXPERT MODE you will have a long list of possible tasks. For several of them you will be asked to set specific parametrs, e.g. to select an atom type for which the

X-ray absorption spectrum has to be calculated. If necessery you can modify the parameters fixing the energy grid (left bottom). The top part of the middle column allows one to select the mode how the $\tau$-matrix is calculated - either via Brillouin zone integration or in the cluster mode. This implies you later using either **kkrgen** (**kkrscf**) or **kkrclu**. The right hand column of the menu offers a lot of ways to control the calculations and the output. A detailed description of the many parameters can be found in the **SPRKKR** manual.

With an input file selected or created the program buttons get unlocked. The corresponding pull down menu allows among others to run the programs interactively, to submit a local batch job, to submit a job to the queue system (using qsub) and to create a job file, that can be executed or submitted later in an Unix window. Interactive execution of the program is done in a Unix xterm window with the output appended to X.out. A message will be given on the screen after the run has been completed.

When running a program or creating a job file connected with this, **xband** checks whether the executable is available. If it cannot be found in the default directory PROG_PATH0 **xband** will give a warning and stop execution. To enable execution of the program the user can copy the executable to PROG_PATH0, change PROG_DIR0 via SET PREFERENCES or set the program directory explicitly via PROG PATH.

The RUN PROGRAM PACKAGE menu supplies in its top right corner two columns of buttons. Those on the left column allow one to call other **xband** menus and services while those on the right hand side supply a shortcut to some Unix commands. The button files alows to handle files in many different and specific ways.

# 14 The PLOT DATA menu

The PLOT DATA menu invoked via PLOT is meant to simplify data handling when plotting the results of a band structure program. The menu uses the program **plot** that supplies an interface between the **SPRKKR**-program package of H. Ebert et al. and **xmgrace**. If you use another band structure package you have to supply your own version of **plot** or modify the one supplied. The file ~/band/graphics/xmgr.f contains all necessary routines to create a **xmgrace** file with the most important parameters, i.e. label, legends and so on, set starting from an arbitrary data table.

Directory list (centre region left): use left mouse click to change the directory. You can also type the name of the new directory in the entry field below the list for this purpose.

data, pin and xmgrace file lists: use left mouse click to select and invoke corresponding program execution.

Edit selected files using the edit buttons in the top region. Change listing mode by clicking alphabetic or last access. Allowed suffixes for the files are listed in the small windows above the file lists. These suffix lists can be modified by editing the corresponding file in ~/band/locals.

Left mouse click on a data file selects the file and invokes **plot** that creates the corresponding **xmgrace** file(s).

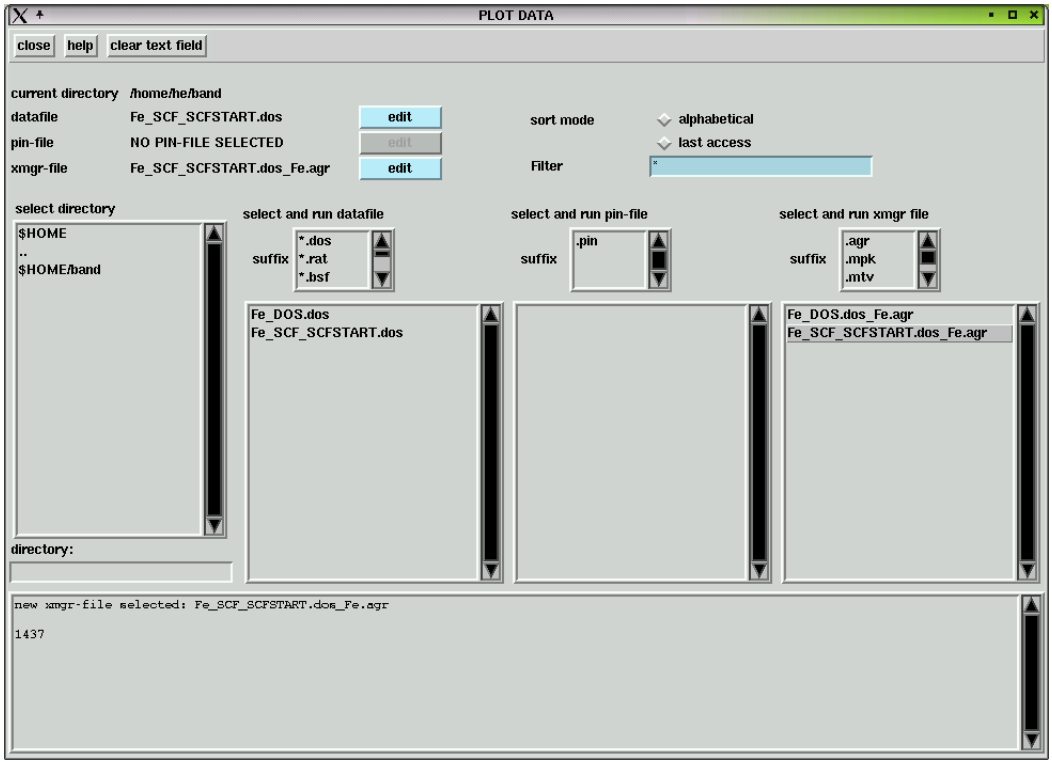



Figure 31: Screenshot PLOT DATA menu

Left mouse click on (one of) the new file(s) in the right file list calls **xmgrace**.

All other files listed in the rightmost listbox could also be displayed by left mouse click. The appropriate programm, like **xmatrix** or **ghostview** which is bound to the extension is executed automatically.

**plot** allows one to supply an additional **plot** input file (*.pin) that is read prior to the data file. Middle mouse click on a data file invokes a menu that allows one to give additional parameters for plotting and broadening. A corresponding **plot** input file is created when leaving the menu. This file is fed to **plot** by left mouse click in the pin-file list. The subsequently created **xmgrace** file can be viewed by invoking **xmgrace** via left mouse click in the **xmgrace** file list.

The Bloch spectral function is plotted using the **xmatrix** program from the **MATHPACK** library or by utilizing the **DISLIN** library. Using the latter opens either a view-only window which could be closed as indicated in the window title or creates a postscript file which can be displayed using **ghostview**. The required input for **xmatrix** is a pair of files with the extensions mpk (datafile) and xmv (visualisation). Due to limited capabilities of **xmatrix**, labeling is incomplete.

# 15 Customisation

Customisation of **xband** can be done on three different levels.

Use SET PREFERENCES to switch between supplied default settings and specify your print command, default program directory and program names. All settings made will be stored in ~/.xband.vst.

**xband** sets all parameters first using internally stored defaults and then tries to read updates from ~/.xband.vst and additional default files in the directory ~/band/locals. While ~/.xband.vst may be updated via SET PREFERENCES the other files remain always untouched. The only exception is the file ~/band/locals/ITXC_structure.dat that may be modified via edit database within the CREATE SYSTEM menu by the user.

If **xband** should deal with a new program package, this can be done by editing the file ~/band/locals/packages.vst. Follow the description given there to add the new program package to the main menu. Alternatively, you may modify ~/.xband.vst after it has been created. If no further action is made **xband** will not be able to write a specific input file but will just copy the content of the selected system file X.sys to the input file X.inp. To enable creation of a specific input file supply in ~/band a corresponding tcl-file create_input_NEWPACK.tcl with NEWPACK the name of the new program package. Copy for example create_input_KKR-AKAI.tcl to create_input_NEWPACK.tcl and use it as a template. There are two procedures in this file to be adapted. The first one has to be called create_input_NEWPACK and supplies the input mask for all additional variables to be transferred to the input file. Writing of the input file is done by the second procedure that has to be called write_input_NEWPACK and which is invoked by pressing one of the various quit buttons in the create input menu. Thus, creating your own specific input file via write_input_NEWPACK, you may use all information stored in a system file. The various variables are tabulated in Table III. All other information needed to run the new package can be supplied via an appropriate input mask setup in the procedure create_input_NEWPACK.

H. Ebert Munich, June 2012

# Table I

Conditional basis and atomic position vectors according to the convention of the International Tables of X-ray crystallography.

## Conditional vectors (Natural coordinate system):

Triclinic, Monoclinic, Orthorhombic, Tetragonal, Cubic:

$$\begin{array}{lccc} \vec{T}_1=( & 1 & 0 & 0) \\ \vec{T}_2=( & b/a\cos\,\gamma & b/a\sin\,\gamma & 0) \\ \vec{T}_3=( & c/a(\cos\,\beta-\cos\,\alpha\cos\,\gamma)/\sin\,\gamma & -c/a*\cos\,\alpha & \sqrt{(c/a)^2-T_{3,x}^2-T_{3,y}^2}) \end{array}$$

Hexagonal and trigonal (in hexagonal axes):

$$\begin{array}{lccc} \vec{T}_1=( & \sin\,\gamma & \cos\,\gamma & 0) \\ \vec{T}_2=( & 0 & 1 & 0) \\ \vec{T}_3=( & 0 & 0 & c/a) \end{array}$$

Rhombohedric:

$\cos\,\theta=\sqrt{\frac{2}{3}(1-\cos\,\alpha)}$,

$\alpha$ : angle between vectors.

$$\begin{array}{lccc} \vec{T}_1=( & \frac{1}{2}\cos\,\theta & -\frac{\sqrt{3}}{2}\cos\,\theta & \sin\,\theta) \\ \vec{T}_2=( & \frac{1}{2}\cos\,\theta & \frac{\sqrt{3}}{2}\cos\,\theta & \sin\,\theta) \\ \vec{T}_3=( & -\cos\,\theta & 0 & \sin\,\theta) \end{array}$$

All atomic position vectors must be given in multiples of $\vec{T}_1$, $\vec{T}_2$ and $\vec{T}_3$

## Basis vectors:

For space groups, where the first letter is **P** (*primitive*) (Triclinic, Monoclinic, Orthorhombic, Tetragonal, Cubic, Hexagonal, Rhombohedric)

$\vec{a}_1=\vec{T}_1$

$\vec{a}_2=\vec{T}_2$

$\vec{a}_3=\vec{T}_3$

first letter is **I** (*body centered*) (Orthorhombic, Tetragonal, Cubic)

$\vec{a}_1=-\frac{1}{2}\vec{T}_1+\frac{1}{2}\vec{T}_2+\frac{1}{2}\vec{T}_3$

$\vec{a}_2=\frac{1}{2}\vec{T}_1-\frac{1}{2}\vec{T}_2+\frac{1}{2}\vec{T}_3$

$\vec{a}_3=\frac{1}{2}\vec{T}_1+\frac{1}{2}\vec{T}_2-\frac{1}{2}\vec{T}_3$

first letter is **F** (*face centered*) (Orthorhombic, Cubic)

$\vec{a}_1=\frac{1}{2}\vec{T}_2+\frac{1}{2}\vec{T}_3$

$\vec{a}_2=\frac{1}{2}\vec{T}_1+\frac{1}{2}\vec{T}_3$

$\vec{a}_3=\frac{1}{2}\vec{T}_1+\frac{1}{2}\vec{T}_2$

first letter is **B** (*base (AC) centered*) (Monoclinic,Orthorhombic)

$\vec{a}_1=\frac{1}{2}\vec{T}_1-\frac{1}{2}\vec{T}_3$

$\vec{a}_2=\vec{T}_2$

$\vec{a}_3=\frac{1}{2}\vec{T}_1+\frac{1}{2}\vec{T}_3$

first letter is **C** (*base (AB) centered*) (Monoclinic,Orthorhombic)

$\vec{a}_1=\frac{1}{2}\vec{T}_1+\frac{1}{2}\vec{T}_2$

$\vec{a}_2=-\frac{1}{2}\vec{T}_1+\frac{1}{2}\vec{T}_2$

$\vec{a}_3=\vec{T}_3$

first letter is **R** (*rhombohedric in hexagonal axes*)

$\vec{a}_1=\frac{2}{3}\vec{T}_1+\frac{1}{3}\vec{T}_2+\frac{1}{3}\vec{T}_3$

$\vec{a}_2=-\frac{1}{3}\vec{T}_1+\frac{1}{3}\vec{T}_2+\frac{1}{3}\vec{T}_3$

$\vec{a}_3=-\frac{1}{3}\vec{T}_1-\frac{2}{3}\vec{T}_2+\frac{1}{3}\vec{T}_3$

# Table II

Basis vectors $\vec{a}_1$, $\vec{a}_2$ and $\vec{a}_3$ assumed by **xband** for the input mode Per Pedes according to the user selected Bravais lattice. Note that the International Tables of X-ray crystallography allows for some Bravais lattices more than one choice of the basis vectors.

| Bravais lattice | basis vectors used by **xband** |
|---|---|
| 1) triclinic primitive | $(a, 0, 0)$<br>$(b\cos\gamma, b\sin\gamma, 0)$<br>$(c(\cos\beta - \cos\alpha\cos\gamma)/\sin\gamma, -c\cos\alpha, a\sqrt{(c/a)^2 - a_{3,x}^2 - a_{3,y}^2})$ |
| 2) monoclinic primitive | $(a, 0, 0)$<br>$(b\cos\gamma, b\sin\gamma, 0)$<br>$(0, 0, c)$ |
| 3) monoclinic base-centered | $\frac{1}{2}(a + b\cos\gamma, b\sin\gamma, 0)$<br>$\frac{1}{2}(-a + b\cos\gamma, b\sin\gamma, 0)$<br>$(0, 0, c)$ |
| 4) orthorombic primitive | $(a, 0, 0)$<br>$(0, b, 0)$<br>$(0, 0, c)$ |
| 5) orthorombic base-centered | $\frac{1}{2}(a, b, 0)$<br>$\frac{1}{2}(-a, b, 0)$<br>$(0, 0, c)$ |
| 6) orthorombic body-centered | $\frac{1}{2}(-a, b, c)$<br>$\frac{1}{2}(a, -b, c)$<br>$\frac{1}{2}(a, b, -c)$ |
| 7) orthorombic face-centered | $\frac{1}{2}(0, b, c)$<br>$\frac{1}{2}(a, 0, c)$<br>$\frac{1}{2}(a, b, 0)$ |
| 8) tetragonal primitive | $(a, 0, 0)$<br>$(0, a, 0)$<br>$(0, 0, c)$ |
| 9) tetragonal body-centered | $\frac{1}{2}(-a, a, c)$<br>$\frac{1}{2}(a, -a, c)$<br>$\frac{1}{2}(a, a, -c)$ |
| 10) trigonal primitive<br>$\cos\theta = \sqrt{\frac{2}{3}(1 - \cos\alpha)}$ | $a(\frac{1}{2}\cos\theta, -\frac{\sqrt{3}}{2}\cos\theta, \sin\theta)$<br>$a(\frac{1}{2}\cos\theta, \frac{\sqrt{3}}{2}\cos\theta, \sin\theta)$<br>$a(-\cos\theta, 0, \sin\theta)$ |
| 11) hexagonal primitive | $\frac{1}{2}(a\sqrt{3}, -a, 0)$<br>$(0, a, 0)$<br>$(0, 0, c)$ |
| 12) cubic primitive | $(a, 0, 0)$<br>$(0, a, 0)$<br>$(0, 0, a)$ |
| 13) cubic face-centered | $\frac{1}{2}(0, a, a)$<br>$\frac{1}{2}(a, 0, a)$<br>$\frac{1}{2}(a, a, 0)$ |
| 14) cubic body-centered | $\frac{1}{2}(-a, a, a)$<br>$\frac{1}{2}(a, -a, a)$<br>$\frac{1}{2}(a, a, -a)$ |

# Table III

Variables stored in and supplied by any 3D system file, respectively. For additional information used to deal with 2D-structures: see the file write_read_system.tcl.

| Variable | Description |
|---|---|
| BRAVAIS | number specifying the Bravais lattice (see table II) |
| TABBRAVAIS($BRAVAIS) | name of the Bravais lattice with number BRAVAIS |
| SPACEGROUP | ITXC space group number |
| SPACEGROUP_AP | space group number in A. Perlov's table |
| STRUCTURE_TYPE | name of structure type |
| ALAT | lattice parameter A [a.u.] |
| BOA | ratio of lattice parameters b/a |
| COA | ratio of lattice parameters c/a |
| LATPAR($i) | lattice parameters a, b, c for $i=1,..,3 [a.u.] |
| LATANG($i) | lattice angles $\alpha$, $\beta$, and $\gamma$ [deg] |
| RBASX($i) | x-component of primitive basis vectors for $i=1,..,3 [A] |
| RBASY($i) | y-component of primitive basis vectors for $i=1,..,3 [A] |
| RBASZ($i) | z-component of primitive basis vectors for $i=1,..,3 [A] |
| NQ | number of lattice sites |
| RQX($IQ) | x-component of atomic position $IQ=1,..,$NQ [A] |
| RQY($IQ) | y-component of atomic position $IQ=1,..,$NQ [A] |
| RQZ($IQ) | z-component of atomic position $IQ=1,..,$NQ [A] |
| RWS($IQ) | Wigner-Seitz-radius for atomic position $IQ=1,..,$NQ [A] |
| NLQ($IQ) | angular momentum expansion $l_{max}+1$ for atomic position $IQ=1,..,$NQ |
| NOQ($IQ) | number of occupants on site $IQ for disordered systems |
| ITOQ($IO,$IQ) | number of atomic type of occupant $IQ on site $IQ |
| NCL | number of inequivalent lattice sites, i.e. classes |
| WYCKOFFCL($ICL) | Wyckoff symbol for lattice sites of class $ICL |
| NQCL($ICL) | number of lattice sites in class $ICL |
| IQECL($IE,$ICL) | lattice site number of $IE-th site in class $ICL; $IE=1,..,$NQCL |
| NT | number of atomic types |
| ZT($IT) | atomic number of atomic type $IT |
| TXTT($IT) | chemical symbol of atomic type $IT; eventually extended |
| CONC($IT) | concentration c of atomic type $IT ($0 \leq c \leq 1$); i.e. probability to find it on a site $IQAT (see below) |
| NAT($IT) | number of lattice sites occupied by atomic types $IT |
| IQAT($IA,$IT) | lattice site number of $IA-th site occupied by atom type $IT; $IA=1,..,$NAT |