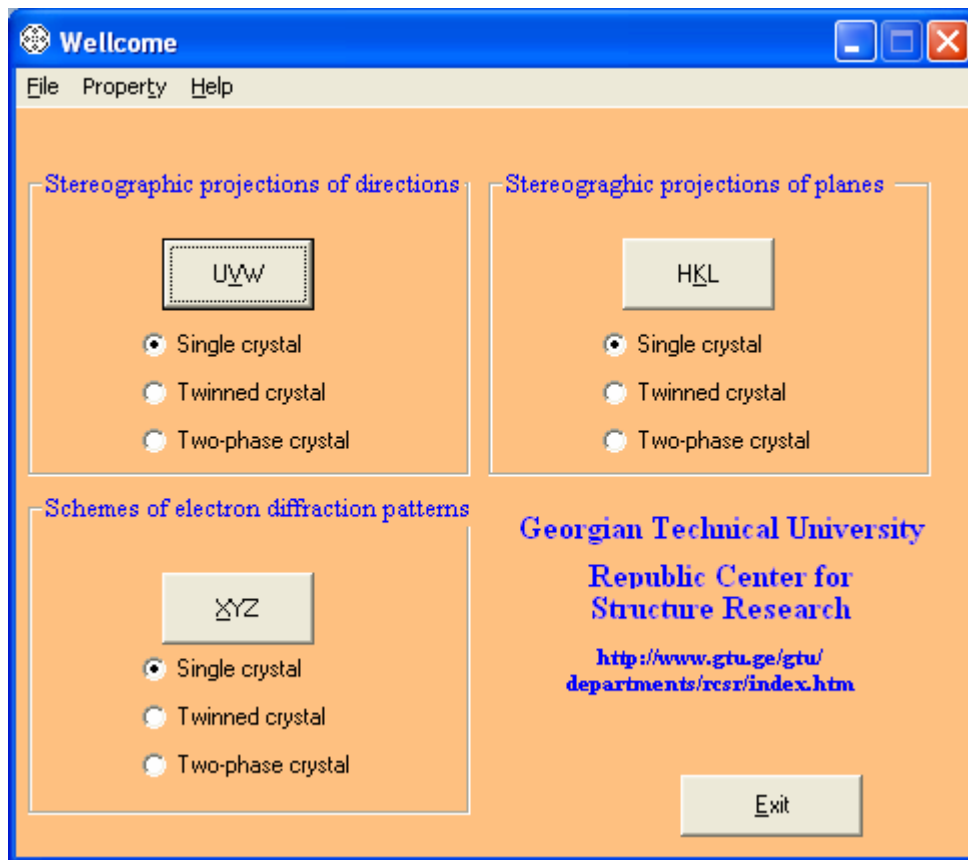# *ELDIST   Program   Guide*

Figure 1.

This startup window represents the   ELDIST's   abilities.

As an example, the use of two the most complex GUIs are explained below.

∗ ∗ ∗

The first one deals with the calculation and printing out of "Stereographic projections of planes" (gnomostereographic projections), option, "Two-phase crystal " (Fig.1).
As it is clear from the corresponding window, (Fig.2), there are two possibilities of projection. The user may specify the indices of the pole direction or the Miller indices of the plane of projection.

Orientation relationship between the phases are given in the common form of parallel directions and planes.

The (hkl) indices of planes may be entered manually or generated automatically, limiting the maximal value of   h, k, l numbers in the box   "Max. hkl".
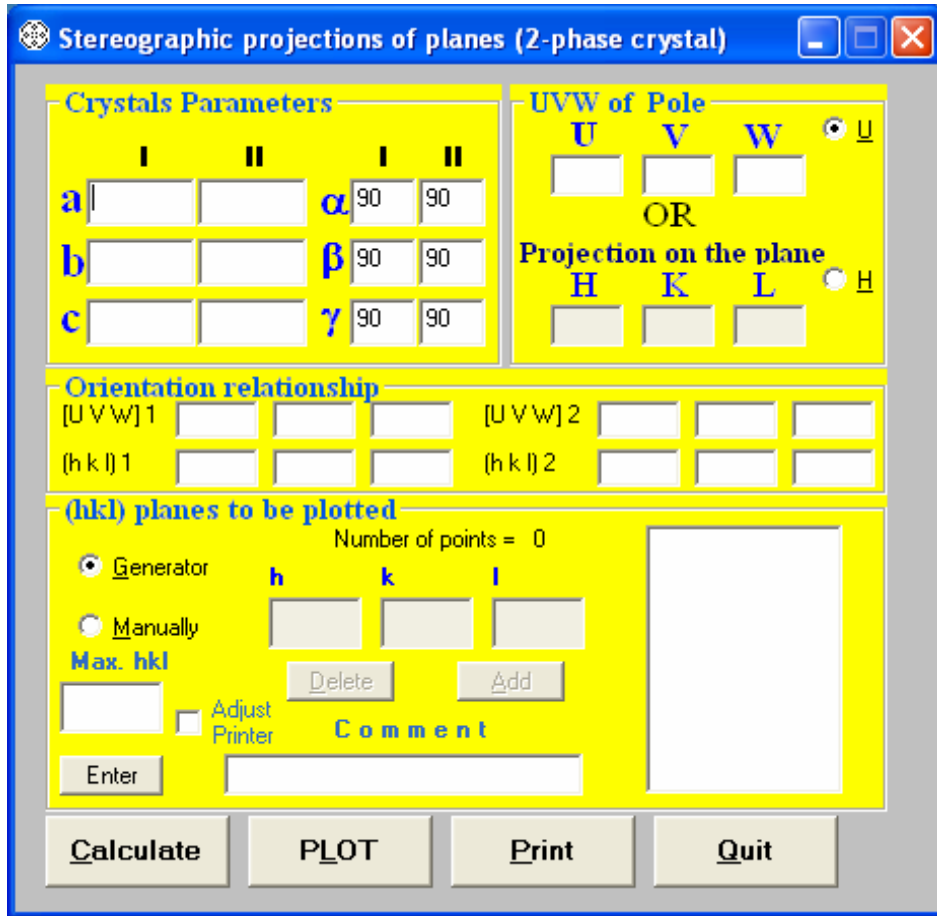
Figure 2.

The sequence of commands is as follows on in the window: from the left side to the right.
Since the projection is calculated and plotted [1] on the screen, after viewing, it may be printed out by clicking the "Print " button.

The "Adjust Printer" option allows to eliminate the printer's instrumental error.
This procedure should be conducted only once; after the program ELDIST is installed.
For this purpose one may use, for example, the program "Stereographic Projections of Directions", option: "Single Crystal". If the "Adjust Printer" option is switched, and all boxes are filled, clicking of the "Print " button provides the following window to appear (Fig.3):
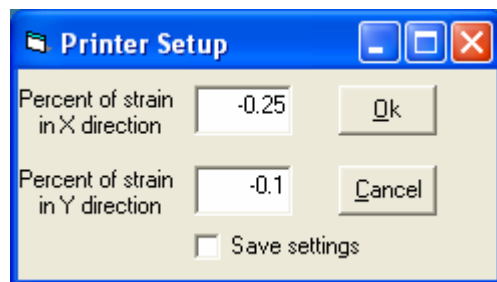

Figure 3.

Enter "0" (zero) in the both boxes and continue printing process by clicking the "Ok " button in this "Printer Setup" window (Fig. 3). After the actual values of projection circle's radiuses in the X (paper travel direction in the printer) and Y directions are carefully measured in the

printed out drawing, the differences between the required value of the radius (10cm) and the printed out one in X as well as in Y directions should be determined.

For example: let the values of the actual radius in X direction is equal to 98mm and to101mm in the Y direction. Since the radius of the standard projection sphere is equal to 100mm, the differences, therefore, are: -2mm and +1mm respectively. The "Percent of strain in X direction" is calculated as a relative displacement expressed in percents. The relative displacements are: -2/100 = -0.02 in the X direction and +1/100 = +0.01 in the Y direction. Consequently, to adjust the printer and align the drawing (projection circle), one should enter in the boxes above (Fig. 3) the values +2.00 and -1.00 respectively, and save the settings. After the above procedure user may check the performed adjustment by running this program again, and if necessary, repeat it.

* * *

The second example of GUI deals with the "Schemes of electron diffraction patterns" (Fig.1), option "Two-phase crystal" (Fig.4).
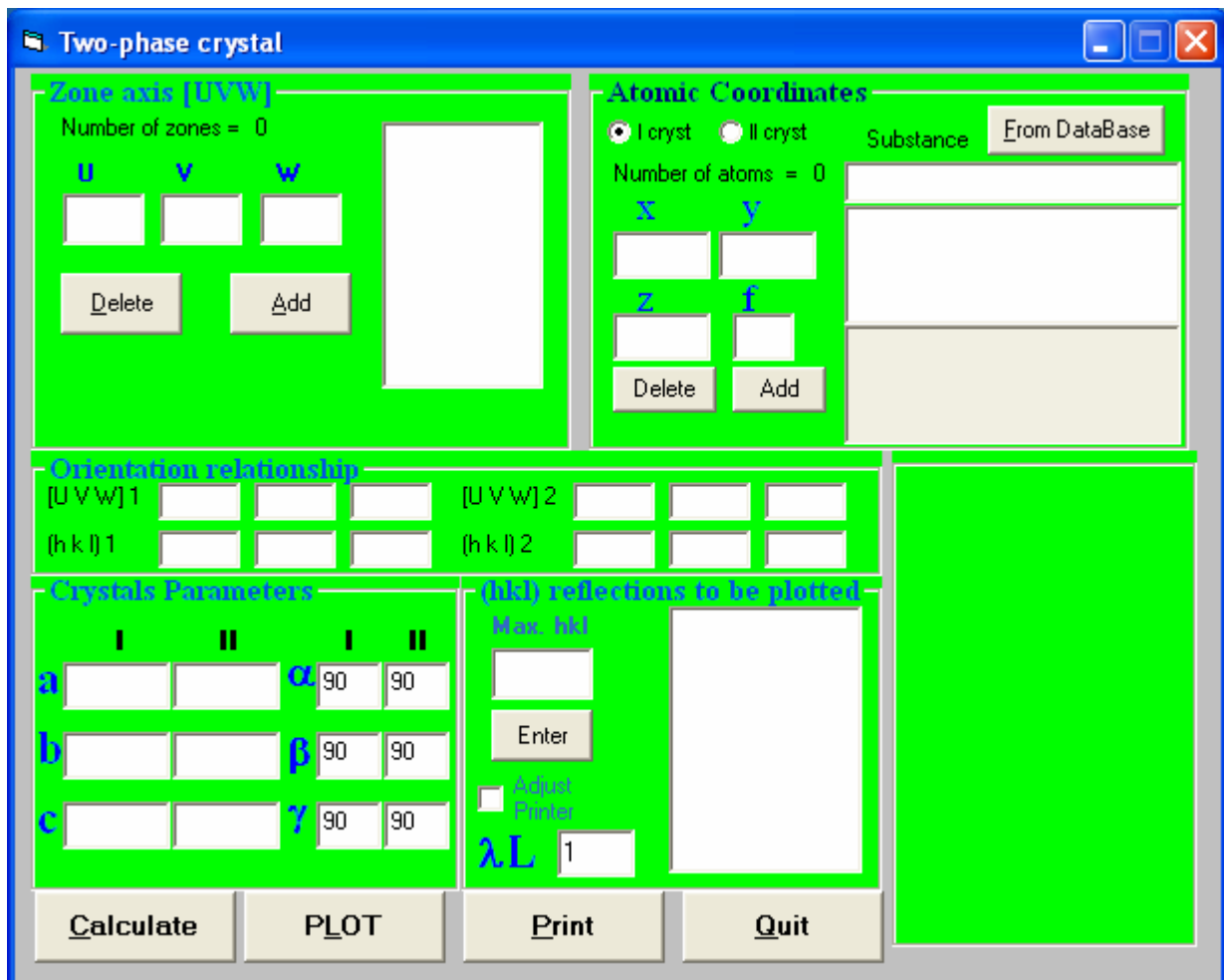

Figure 4.

At one session up to 50 interested zone axes UVW, may be entered in the U, V, W boxes.

The atomic coordinates x,y,z, for calculation of structure factors should be entered together with the respective atomic scattering factors "**f**" (Fig.4). However, since this program generates the allowable diffraction spots, with the intensity >0, paying no attention to their values, the user my enter any number for "**f**" (the same numbers for the atoms of the same kind and different numbers for different kinds of atoms to ensure difference in the atomic scattering factors). The program allows the atomic coordinates and the respective scattering factors be stored in the Data Base and taken from it as required (Fig. 4, 5).

For this purpose click the "From DataBase" button, (Fig. 4), scroll the "Substance" and select the desired substance by name or by formula (Fig.5 and 6).
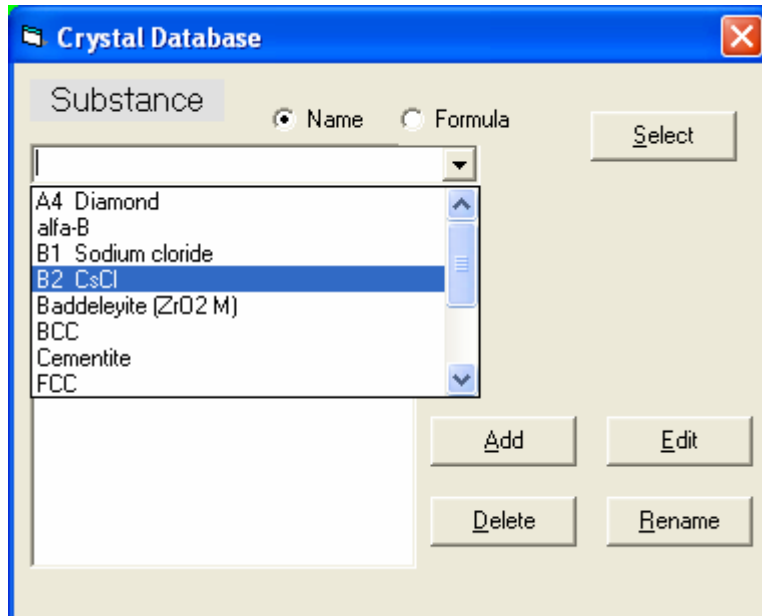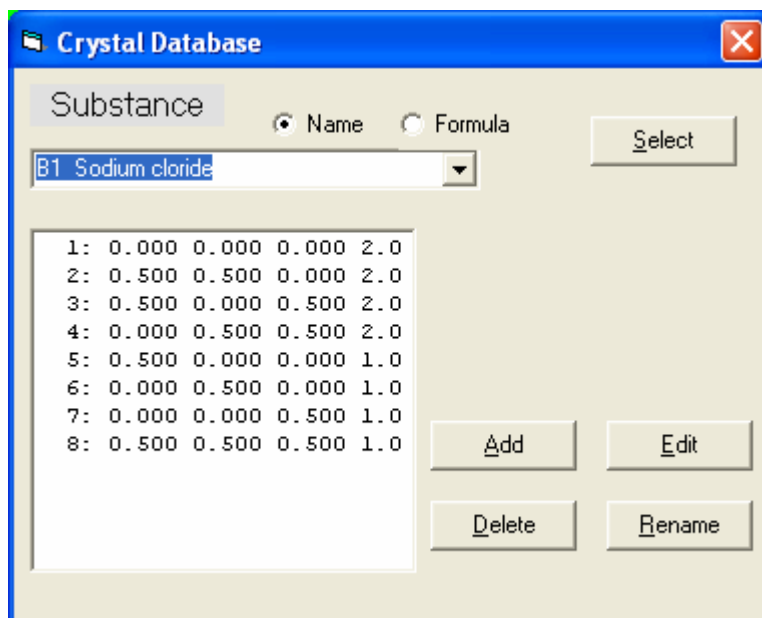

Figure 5.

Figure 6.

Then click the "Select" button and continue filling the rest of the boxes in the window shown in Fig.4.

The "Calculate" button provides a list (Fig.7) of calculated possible directions of the 2nd phase zone axis to be simultaneously presented in the scheme of diffraction pattern (Fig.8). In this list (Fig.7), in the fourth column the angles of deviation from the incident electron beam are

also given (i.e. the angles between the zone axes of the first and second phases). The user may select the suitable zone axis of the second phase judging from the values of the angles and the indices of the zone axes (rational indices).
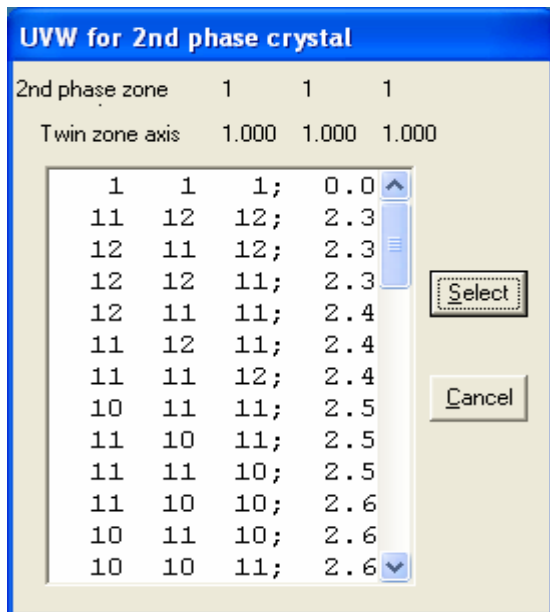

Figure 7.

The "P<u>LOT</u>" button (Fig.4) generates a scheme of the respective diffraction pattern on the computer screen. Appearance of such a scheme is shown in Fig.8.
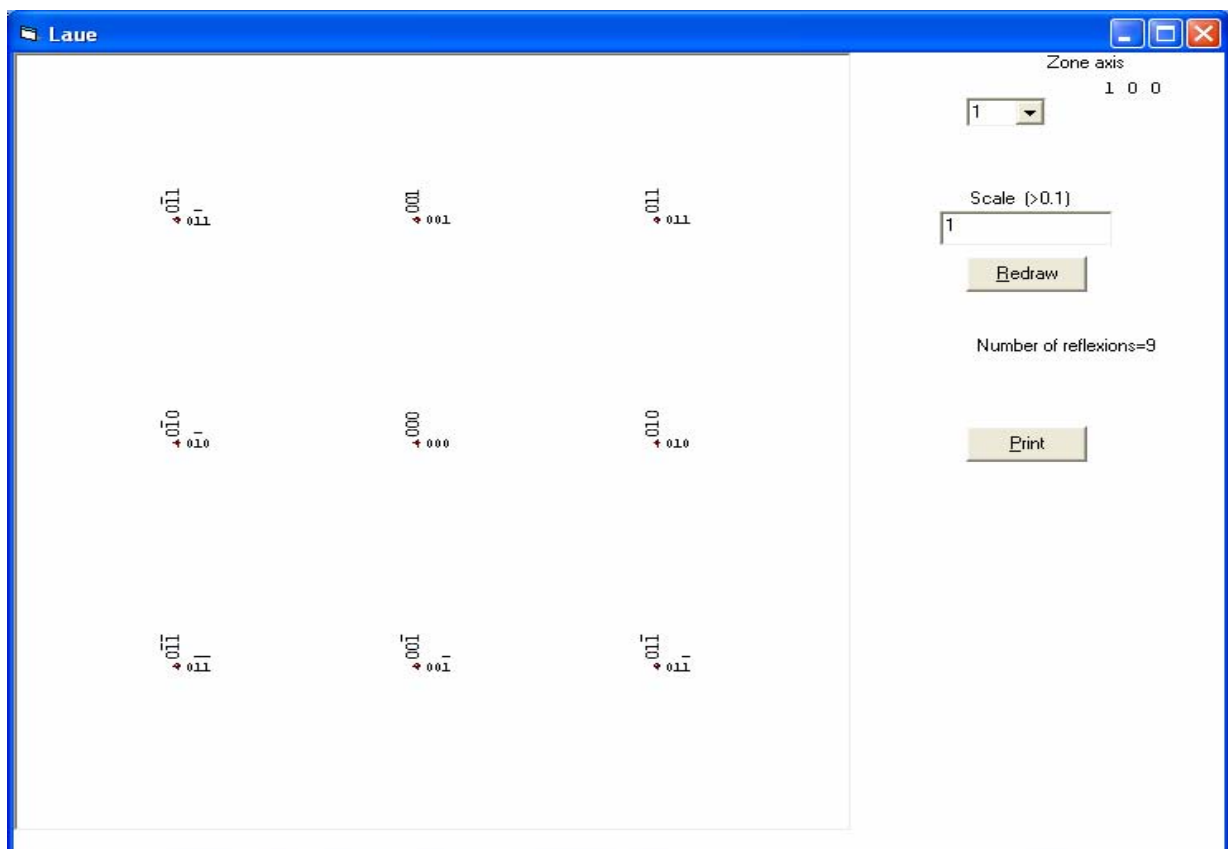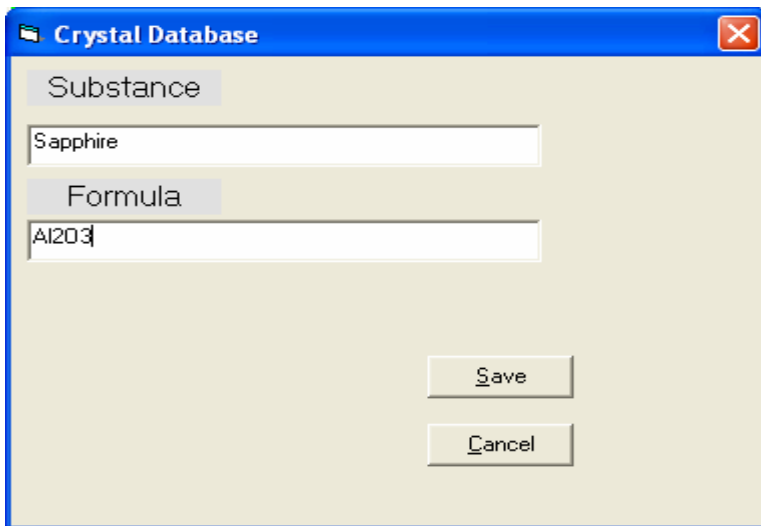

Figure 8.

After viewing the scheme on the computer screen, user may change (adjust) the scale of the indexed scheme (Fig.8), redraw it and print it out ("**Print** " button, Fig.4 or Fig.8).

The number in the upper box in Fig.8 shows a serial number of the zone axis [UVW] initially entered in the window Fig.4. User may repeat the above procedure for any other zone axes of the second phase given in Fig.7, so simulating a tilting of crystalline sample in the column of electron microscope.
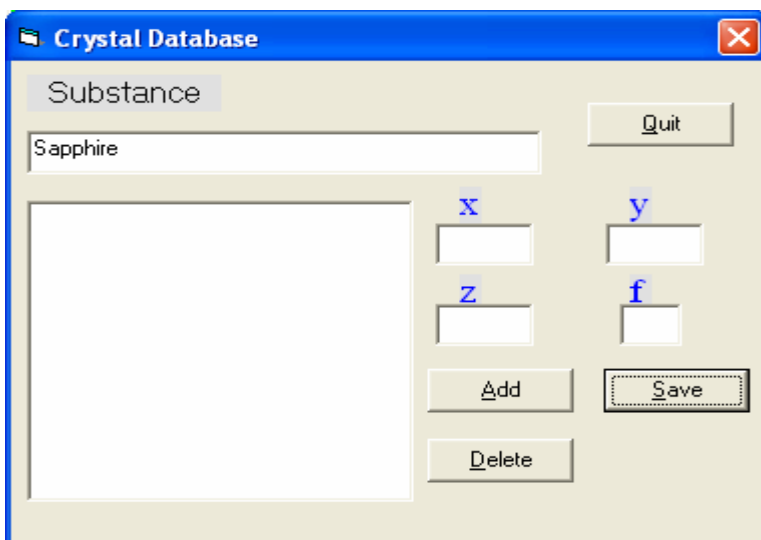
$$* \ * \ *$$

In order to add new data in the Data Base of atomic coordinates, ("From DataBase"), click the "Add " button (Fig.5 or 6) and enter a name and formula of the new substance (Fig.9), click "Save" , and then the "Edit " button in the window (Fig.5) which activates the storing option (Fig. 10).

Figure 9.

Enter the atomic coordinates and the respective scattering factors in the boxes (Fig.10).

Figure 10.

Save the entered data. This data base may be updated as required, depending on the investigated materials.

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1) **Note**

If during execution of the program (when you click on P⎽LOT button) you receive a message: "Component 'comctl32.ocx' or one of its dependencies not correctly …" you need to run a regserv.bat file, which is available in the program pack.