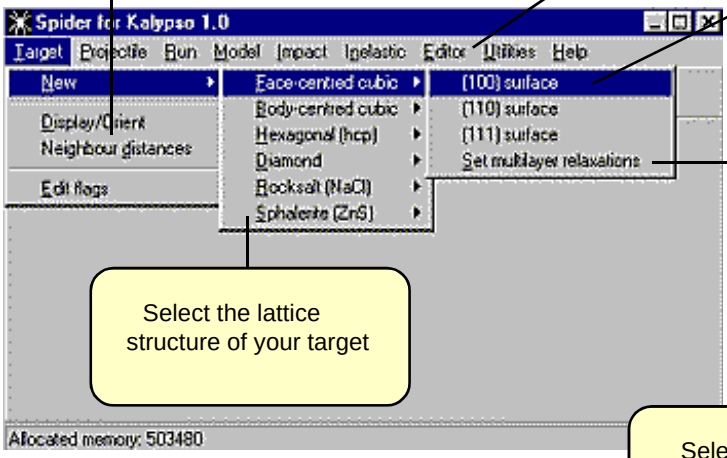
TARGET FILE DIALOG BOX

A number of target files with well-defined surface terminations can be created from menu commands, e.g. Cu(100). Frequently, further modification of the target files by the user is required. Things to consider, in addition to surface termination, are: (a) azimuthal target lattice orientation with respect to the projectile incident direction; (b) surface relaxation; (c) number of atoms in target, and its width and depth. If the required target file is that of a compound system such as Cu/Ni(100), or if it involves a non-standard orientation, considerably more work is required.

Display/Orient allows you to modify a target file. Neighbour Distances lists the distances of the neighbours of an atom you specify. Edit Flags is a specialised command which you probably will never use.

Editor menu offers a simple editor for viewing/changing input filesas text. The Utilities menu contains tools which perform useful calculations related to ion scattering.

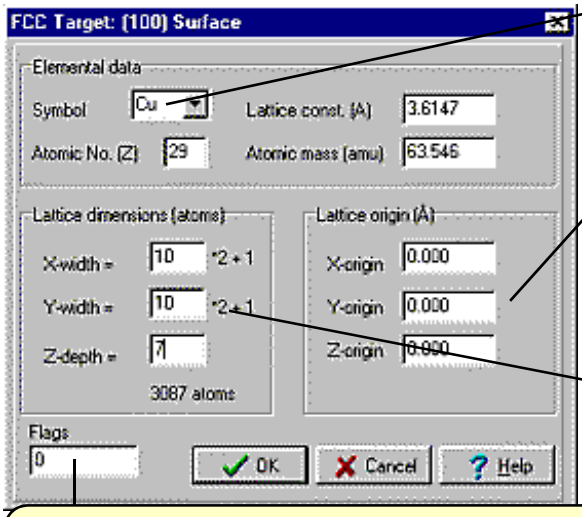
Use the submenu system to select a target file with the desired surface orientation.



Set multilayer relaxations, if required, for the target file. Applies to fcc targets only. (Bcc and others must be modified by hand.)

Select the lattice structure of your target

Select standard elements here, or enter elemental data by hand (from Spider Help).



Normally, lattice origin is at (0.0,0.0,0.0) but there are situations when you will want to displace it. This happens typically when you are creating part of a compound target file.

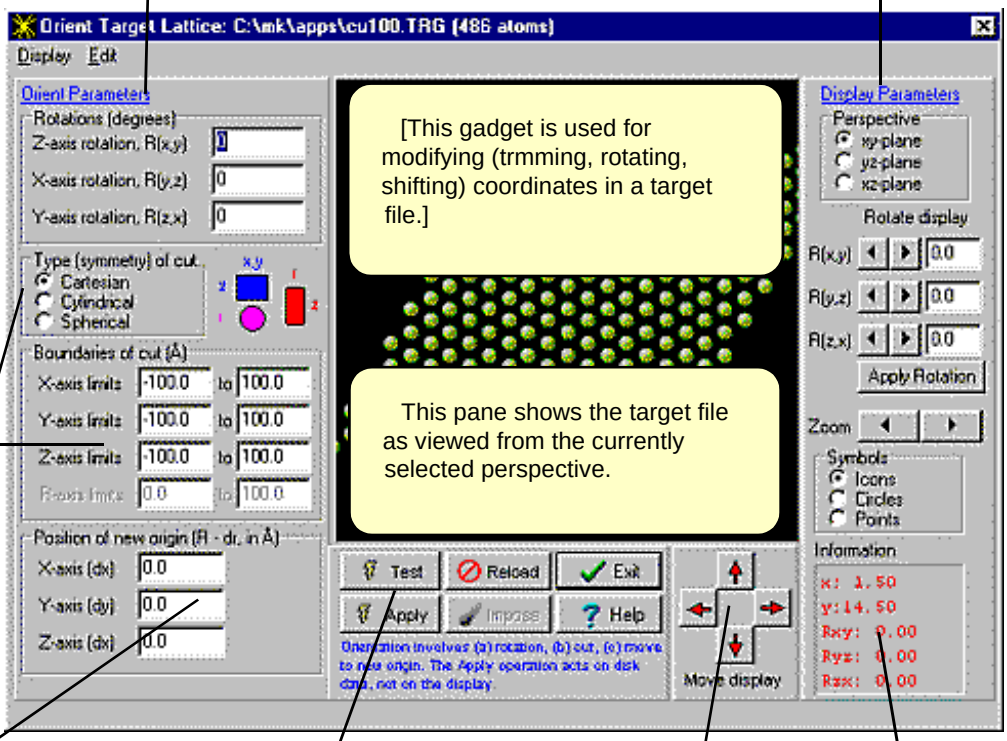
The lattice dimensions are specified here. The width of the lattice in this example is 21 atoms in both *x* and *y* directions.

The Flags parameter should be left at '0' for an element. For a compound, it might be '1' or '0' (see documentation).

DISPLAY/ORIENT TARGET

The options on this side are used to modify the target file. No changes are made until the Test or Apply buttons are hit.

Various display options are on this side. No change is made to the target file.



[This gadget is used for modifying (trmming, rotating, shifting) coordinates in a target file.]

This pane shows the target file as viewed from the currently selected perspective.

Cut edges of various shapes from target file (Cartesian is normal).

Translation of coordinates in target

Use Apply to commit changes to disk, or Test to test the results of the editing operations. Use Reload to go back to the freshly loaded file display.

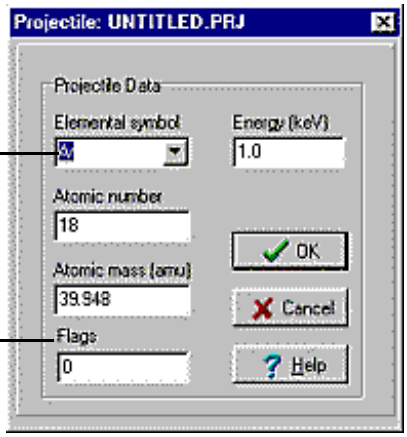
Move display (also can use arrow keys.)

Current display informa-tion.

PROJECTILE FILE DIALOG BOX

Enter projectile data by hand, or select from drop-down list. Enter kinetic energy in keV.

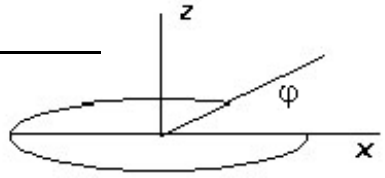
Leave flags at '0', unless your simulation refers to a 'self-bombardment' experiment, in which case use the same flags value as used for that type of atom in the target file (see Simula-tion Primer).



RUN FILE DIALOG BOX

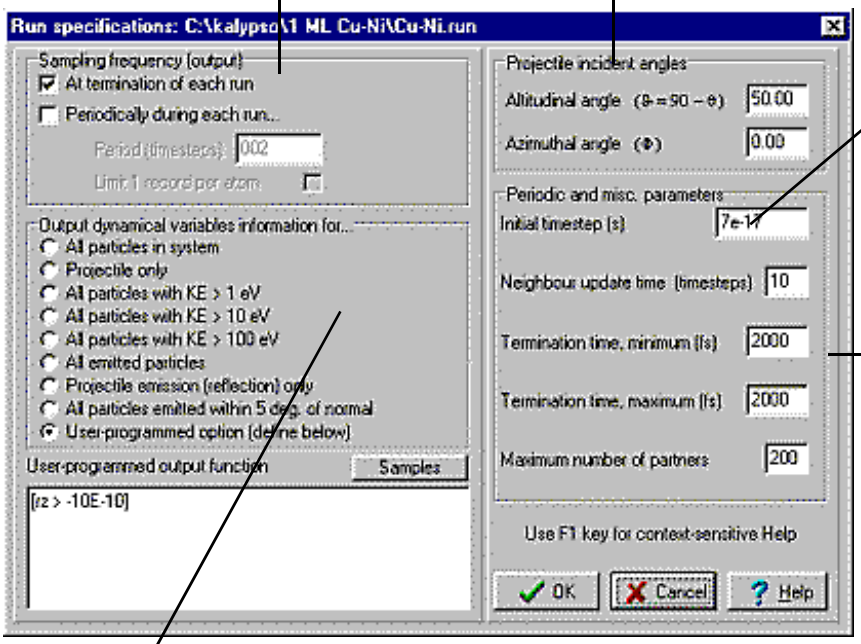
The Run file defines the kind of output which is written to disk, the projectile incident angles relative to the target coordinate system, and some miscellaneous parameters, including the integration timestep (see documentation for more details). If the timestep is too small, or the 'maximum number of partners' is too low, the simulation can abort with an error message to this effect. If the timestep is slightly too large, you will see excessive energy leakage in the simulation, but it may not abort - so err on the cautious side when setting the timestep.

The azimuthal angle (ϕ) represents anticlockwise rotation away from the x-axis. The altitudinal angle (φ) is measured relative to the surface, as shown here.



1. Specify how often you want output data to be written. Typically (as shown) this is at the termination of each run only.

3. It is best to leave the azimuthal angle at 0.0, and rotate the target if necessary. Normal projectile incidence corresponds to an altitudinal angle of 90.0.



4. Use the Utilities|Velocity Reckoner gadget to estimate the timestep. Don't set it too large, or it will affect energy conservation. If in doubt, check the effect of timestep variations on ΔE.

5. The neighbour update time is not critical, and a value of 10 can always be used. The termination time values reflect the timescale of your process. The 'maximum number of partners' parameter is used to compute memory needs. If you set it too low you will get a warning during the simulation. A value of 100+ should be adequate.

2. The options here determine what kind of output is written. Normally you will only be interested in a small fraction of atoms in the system. You can select standard options, or define a condition yourself. Excessive output can always be filtered later, but may take up a lot of space on your hard drive.

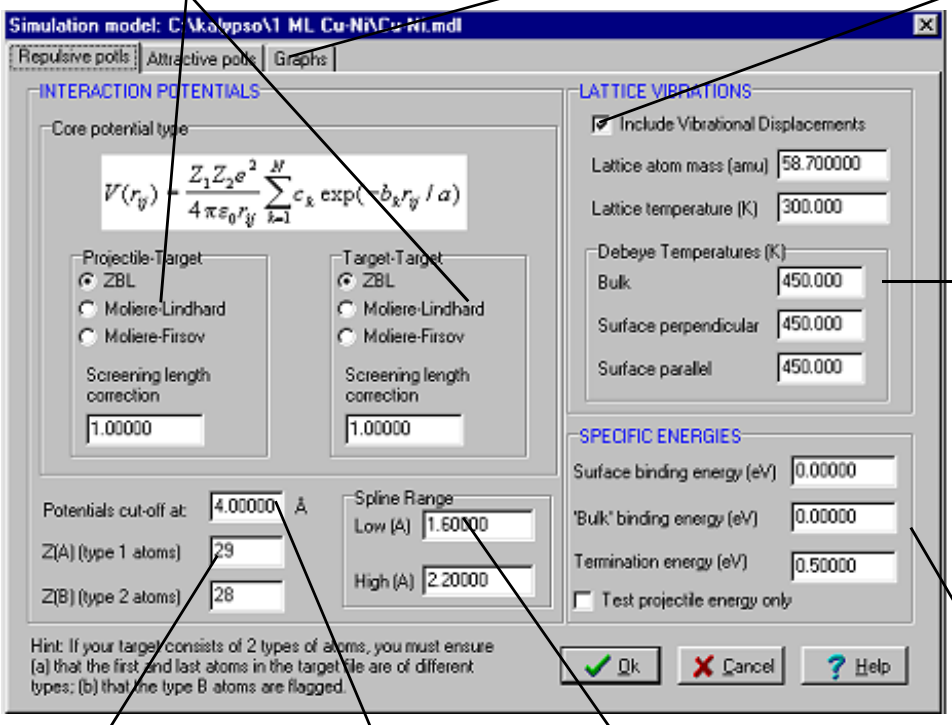
MODEL FILE DIALOG BOX

Before you begin, you will have to know the parameters of the attractive potential(s) for your systems. Probably you will use a tight-binding potential. For an element, one parameter set is required (AA); for a binary compound, three sets (AA, AB, BB). The simulation potential is a composite potential. A spline function joins a screened Coulombic potential to an attractive potential in a region which you will have to determine by trial and error. Before you can fit the spline, both attractive and repulsive potentials must be fully specified, as well as the atomic number(s), Z(A) [and Z(B) for a compound target] of the target atom(s). You may also need to access the relevant target file in order to compute the lattice sum S_n which is required for each set of potential parameters. [Use the graphing feature provided to inspect your potentials. Note that what is displayed in the attractive potential region is the 'effective' two-body potential. Read the documentation for an explanation of this.]

2. Specify the type of screened Coulomb potential to use for the short range interaction. The ZBL form with screening length correction 1.0 is recommended by the author.

1. This dialog box has 3 tabs. The Graphs tab is for viewing the potential and force field. The other 2 tabs are for parameter input. Some fields can be ignored if you are using an elemental target, or a simplified model.

6. Check here only if you want to add vibrational displacements to lattice atoms. If not, ignore other parameters in this box.



7. Get Debeye temperatures (DTs) for elements from the Spider Help. For a binary target you can either use mean values of masses and DTs, or edit the MDL file by hand for a more exact model (see the documentation).

8. The BEs are usually set to 0.0. The TE may optionally be used to stop the simulation when the energies of lattice atoms (or the projectile) fall below the specified value.

3. Atomic nos. are used for spline calculation. Ignore Z(B) for an elemental target.

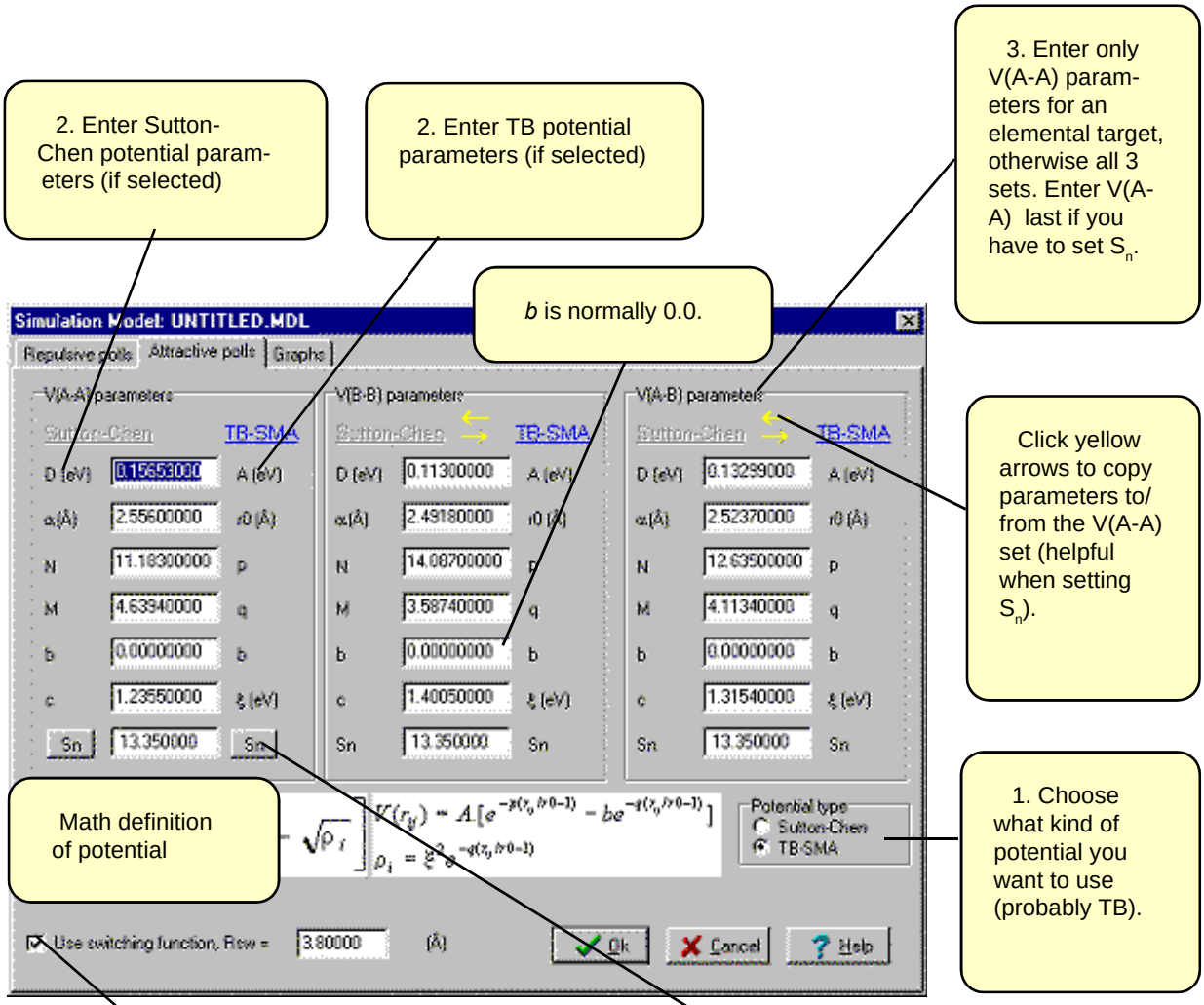
4. The cut-off refers to the attractive potential. Do not choose arbitrarily - it affects material properties, e.g. cohesive energies.

5. The spline range is guessed iteratively. Refer to the plots of V(r) and F(r) on the Graphs tab. The High value should be below the 1st NN distance, to ensure that all lattice sites lie in the attractive potential region.

If you use the potential parameters provided in the Simuation Primer, the only difficult part is knowing how to calculate S_n for the heteronuclear potential, V(A-B) [S_n is provided for the elemental cases V(A-A) and V(B-B)]. This isn't a critical parameter, so if in doubt, use a mean value of V(A-A) and V(B-B) for V(A-B). This is what I recommend.

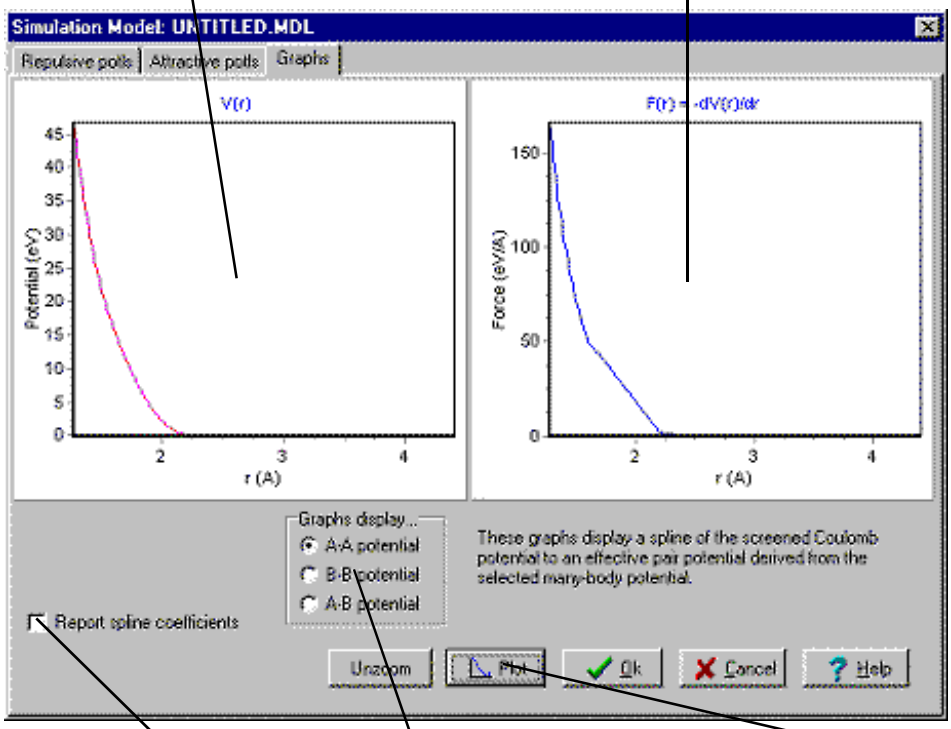
Otherwise, some serious attention to detail is required. S_n is not well-defined for a random alloy system. S_n is a lattice sum - a sum of interactions experienced at a representative lattice site (see Simulation Primer for details). Choose a lattice site which is representative of the environment in which heteronuclear interactions occur. For a metal overlayer, this might be a site in the surface layer.

The lattice sum is only used to fit a spline potential which is used for the region between the repulsive and attractive potentials. This is a necessary approximation, because a two body potential cannot be fitted exactly to a many-body potential. Ultimately, the quality of the approximation will be justified by the energy conservation in your simulation.



Shows the effective potential, based on the parameters you entered.

Shows the force field associated with the effective potential. Typically, the gradient of the force will show a discontinuity at one or both nodes of the spline function (as seen here at 1.6 and 2.2 Angstroms). However, you should try to eliminate unphysical maxima or minima in the force curve by varying the the spline range parameters iteratively.



If checked, the current spline parameters will be reported when you refresh the graphs.

Select which set of potential parameters to graph. You can zoom graphs by selecting a region with the mouse right button, or drag them using the mouse left button. Hit 'Unzoom'button to display default graph.

Refresh/update the graphs.

When you are satisfied with the appearance of your spline function, you may click the OK button and save the MDL file to disk. You can also save the file at any intermediate step, and continue editing it later.

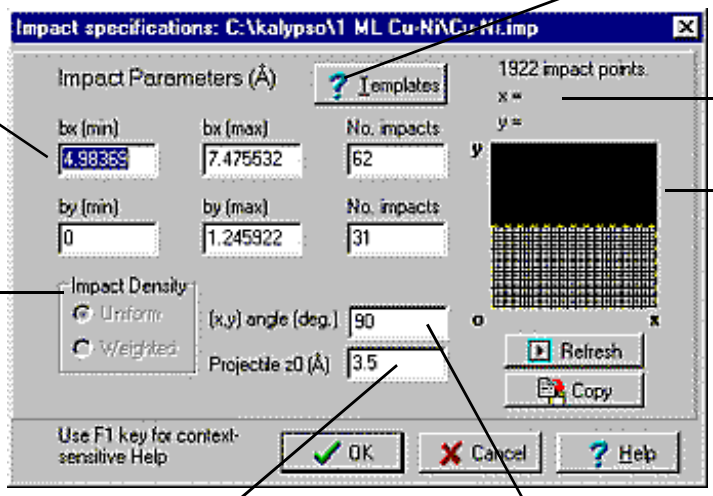
IMPACT FILE DIALOG BOX

The impact file is probably the most difficult input file to prepare. A number of common cases are discussed in the User Guide.

The impact file defines a mesh of points into which the projectile is directed. The shape and dimensions of the mesh, or 'reduced impact zone', are dictated by surface structure and the experimental geometry (projectile azimuthal and altitudinal incident angles). It might help to examine a 3D model of the problem.

bx(min) and bx(max) define the length of the impact zone along the x-direction, while 'No. impacts' determines the spacing of impact points along the same dimension.

Help for common cases.



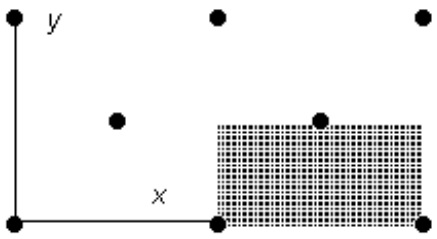
Displays the impact zone produced by the current parameter set. Use the mouse cursor to get coordinates in Angstroms.

Ignore (this feature is obsolete)

This initialises the projectile height above the anchor atom. Normally 3 A or greater. For some non-standard types of simulation, you might want to put the 'projectile' inside or below the target (negative value).

Trims the impact zone mesh at the specified angle. Used for creating triangular zone shapes.

It may be necessary to edit (trim, rotate) an impact file created by this method. To do this, the Impact|Display/Orient utility is used. Functionally this utility is similar to the corresponding target file utility (see preceding). Use the Display|Link File menu option provided therein to compare the impact file mesh with the target file coordinates. The example shown here is for a (100) fcc surface, which the projectile approaches along the -x direction.



INELASTIC FILE DIALOG BOX

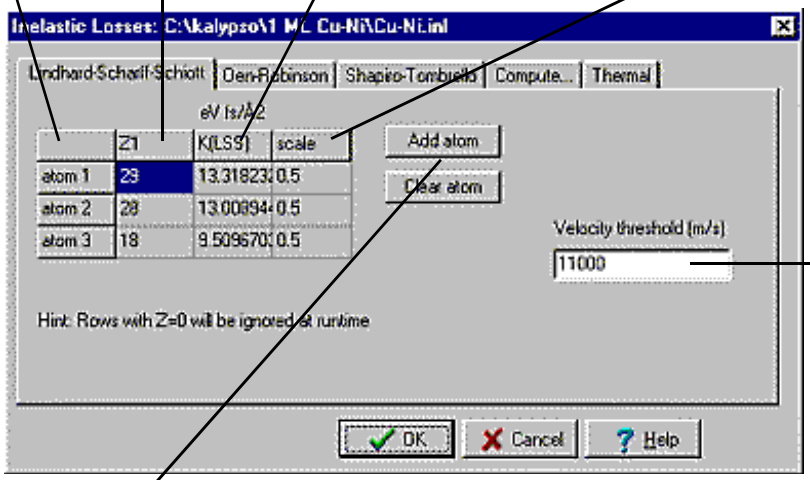
The inelastic file defines the parameters used by models of inelastic energy loss processes. This file is optional: if you don't want to include such effects in your simulation, you do not have to create the file. [In order to incorporate inelastic effects in your simulation, you must also enable the relevant option in Kalypso/Snook.] Before you attempt to create or use an inelastic file, you should read up on the theory and formalism in the Simulation Primer. The LSS and OR models are the only models you will need to use. Typically one uses the LSS model, or combines the LSS and OR models. The ST model is only used for specialised problems that require the modelling of discrete inelastic loss processes. The inelastic file also defines the parameters used for implementing temperature changes (normally cooling) in the target. Again, this is an optional and rarely used feature.

You must define parameters for each atom type in the system. In this case (Cu/Ni bombarded by Ar) the system has 3 types of atoms, therefore 3 sets of parameters.

The LSS parameter, K(LSS), can be calculated on the 'Compute' tab of this dialog box (see below).

Use a scale of 1.0 for a pure LSS inelastic loss model, or 0.5 for an equipartition with the OR model (in the latter case you must also enter the applicable OR parameters). If scale is 0.0, the parameters will be ignored by Snook/ Kalypso at runtime.

Enter the atomic number of the atom.

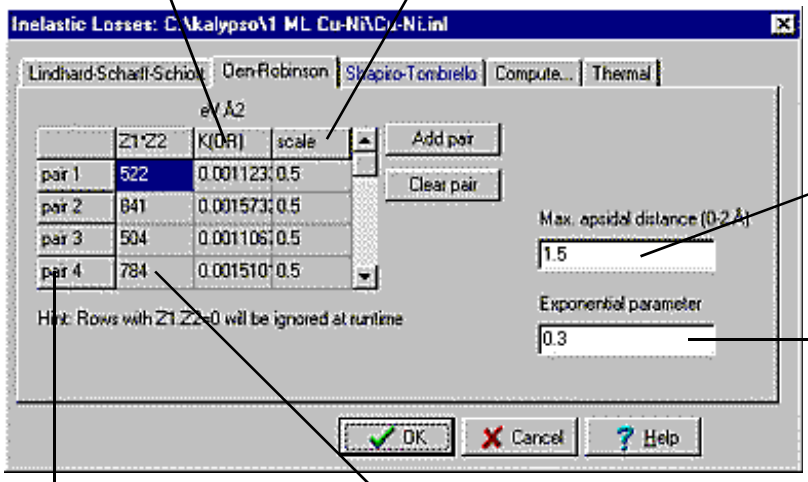


LSS losses are ignored for atoms which have velocities below this threshold. There is no solid guidance from theory. A threshold corresponding to 50-100 eV may speed your simulation.

Click to add/remove a set of atomic parameters.

Calcu-
late the OR
parameter,
K(OR), for
each atomic
pair on the
'Compute'
tab.

The scale
shouldbe 1.0
or 0.5, de-
pending on
your model
(pure OR loss,
or LSS-OR
equipartition).



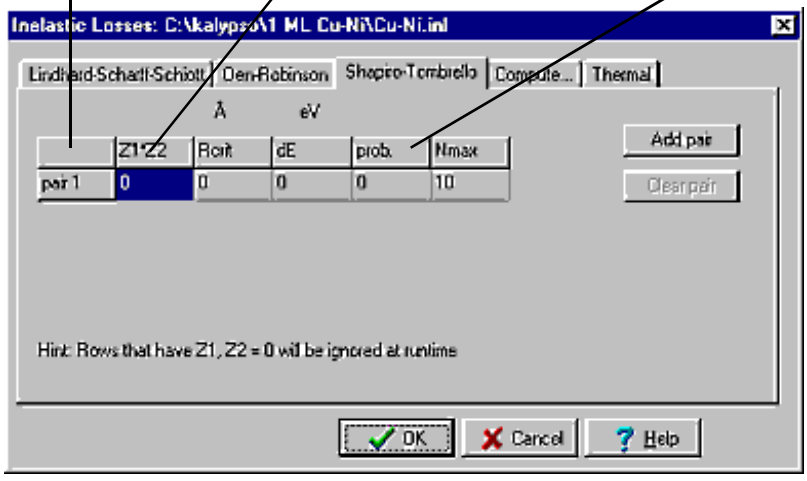
OR losses are not computed if distance of closest approach (apsidal distance) is greater than this amount. Should be set at about 50% of the nearest neighbour distance (possibly less, but not much more).

Parameter used by the OR theory. Not normally modified.

You must define parameters for each pair of colliding atoms. In the system Cu/Ni + Ar projectile this means 5 pairs: Cu-Cu, Cu-Ni, Ni-Ni, Ar-Cu, Ar-Ni. However, Ar-Ar collisions do not arise.

In this column enter the product of atomic numbers, Z1*Z2. For example, Cu-Cu = 29*29=841.

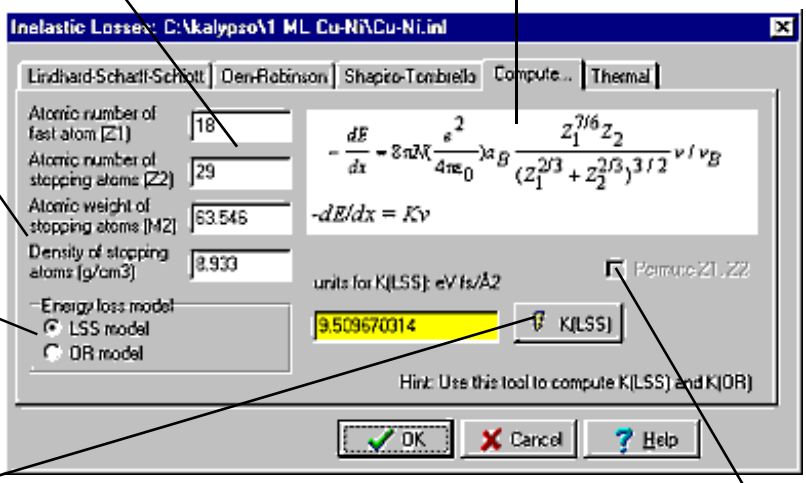
Most users can ignore the ST model, which in essence, is a discretized form of the OR model.Energy losses occur because of excitation transitions occuring between colliding atom pairs. The ST model requires specification of a critical collision radius (Rcrit), a discrete energy loss quantum (dE), an excitation probability (prob) for each transition, and a maximum allowed number of transitions per collision event (Nmax).



The atomic numbers of the fast atom (Z1) and the stopping atom (Z2) are always needed. For the LSS model, Z2 should reflect a target average(if the target is non-elemental). For the OR model, Z2 is the collision partner.

Use this gadget to calculate LSS and OR parameters. The theoretical expression of the currently selected model is shown in the text window.

The atomic weight and density of the target are required for the LSS parameter. Use a molecular weight for a compound.

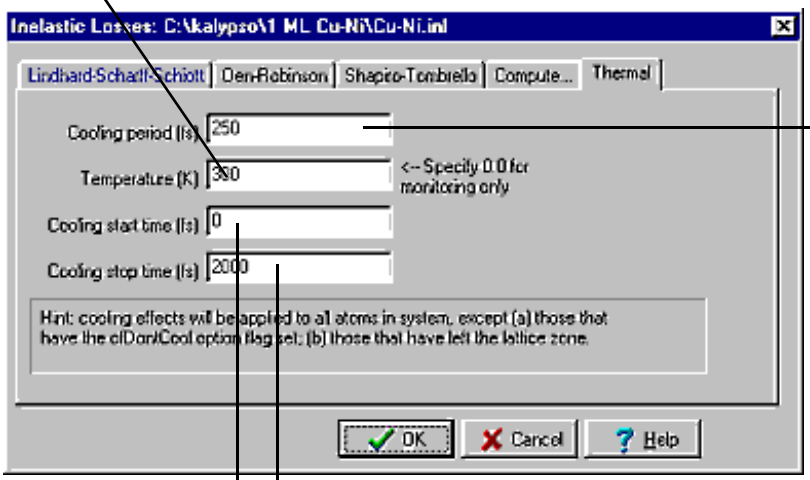


Select the inelastic energy loss model here.

Click the button to calculate. Then copy the result from the yellow box to the relevant field on the LSS or OR tabs. Tip: to copy, you can select the text in the yellow box, then press Ctrl+C. To paste in another place hit Ctrl+V.

Computes an OR parameter which is symmetric with respect to the interchange of Z1 and Z2 (OR model only). Optional: makes theory more self-consistent for compounds, but not necessarily more 'accurate'.

Goal temperature: system moves towards this value (and stays at this temperature once it reaches this value).



The Cooling Period is essentially a time constant which determines the rate of cooling. Typically the system will require twice the cooling period parameter (or more) to move towards the desired target temperature. Set it by trial and error.

These parameters specify the times at which the cooling effects are switched on and off. Don't switch them on too early in a collision system, or you may extract energy unrealistically from fast-moving atoms. The stop time can be set arbitrarily high.