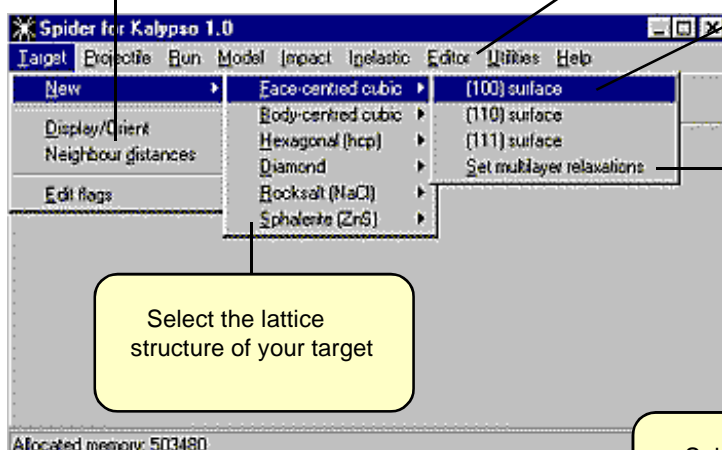# TARGET FILE DIALOG BOX

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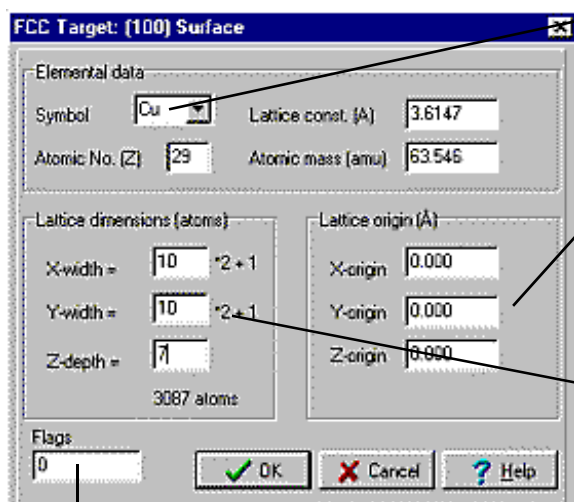
Editor menu offers a simple editor for viewing/changing input filesas text. The Utilities menu contains tools which perform useful calculations related to ion scattering.

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).

Spider for Kalypso 1.0

Target Projectie Run Model Impact Inelastic Editor Utilities Help

New
Face-centred cubic ▶ (100) surface
Body-centred cubic ▶ (110) surface
Hexagonal (hcp) ▶ (111) surface
Diamond ▶ Set multilayer relaxations
Display/Orient
Neighbour distances
Rocksalt (NaCl) ▶
Edit flags
Sphalerite (ZnS) ▶

Allocated memory: 503480

FCC Target: (100) Surface

Elemental data

Symbol Cu   Lattice const. (A) 3.6147
Atomic No. (Z) 29   Atomic mass (amu) 63.546

Lattice dimensions (atoms)

X-width = 10 *2 + 1
Y-width = 10 *2 + 1
Z-depth = 7

3087 atoms

Lattice origin (A)

X-origin 0.000
Y-origin 0.000
Z-origin 0.000

Flags
0

✓ OK   ✗ Cancel   ? Help

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.

Orient Target Lattice: C:\mk\apps\cu100.TRG (486 atoms)

Display   Edit

Orient Parameters

Rotations (degrees)
Z-axis rotation, R(x,y)   0
X-axis rotation, R(y,z)   0
Y-axis rotation, R(z,x)   0

Type (symmetry) of cut.
○ Cartesian
○ Cylindrical
○ Spherical

Boundaries of cut (Å)
X-axis limits   -100.0   to   100.0
Y-axis limits   -100.0   to   100.0
Z-axis limits   -100.0   to   100.0
R-axis limits   0.0   to   100.0

Position of new origin (R - dr, in Å)
X-axis (dx)   0.0
Y-axis (dy)   0.0
Z-axis (dz)   0.0

[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.

Test   Reload   Exit
Apply   Impose   Help

Orientation involves (a) rotation, (b) cut, (c) move to new origin. The Apply operation acts on disk, not on the display.

Display Parameters

Perspective
○ xy-plane
○ yz-plane
○ xz-plane

Rotate display
R(x,y)   ◄ ►   0.0
R(y,z)   ◄ ►   0.0
R(z,x)   ◄ ►   0.0

Apply Rotation

Zoom   ◄   ►

Symbols
○ Icons
○ Circles
○ Points

Information
x: 1.50
y: 14.50
Rxy: 0.00
Ryz: 0.00
Rzx: 0.00

Move display

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 information.

PROJECTILE FILE DIALOG BOX

Projectile: UNTITLED.PRJ

Projectile Data

Elemental symbol   Energy (keV)
A▼   1.0

Atomic number
18

Atomic mass (amu)
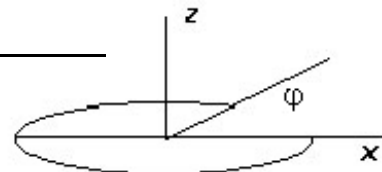39.948

Flags
0

OK   Cancel   Help

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 Simulation 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.

Run specifications: C:\kalypso\1 ML Cu-Ni\Cu-Ni.run

Sampling frequency (output)
- ☑ At termination of each run
- ☐ Periodically during each run...
  - Period (timesteps): 002
  - Limit 1 record per atom ☐

Output dynamical variables information for...
- ○ All particles in system
- ○ Projectile only
- ○ All particles with KE > 1 eV
- ○ All particles with KE > 10 eV
- ○ All particles with KE > 100 eV
- ○ All emitted particles
- ○ Projectile emission (reflection) only
- ○ All particles emitted within 5 deg. of normal
- ⦿ User-programmed option (define below)

User-programmed output function   [Samples]

[rz > -10E-10]

Projectile incident angles
- Altitudinal angle ($\vartheta = 90 - \theta$)   50.00
- Azimuthal angle (Φ)   0.00

Periodic and misc. parameters
- Initial timestep (s)   7e-17
- Neighbour update time (timesteps)   10
- Termination time, minimum (fs)   2000
- Termination time, maximum (fs)   2000
- Maximum number of partners   200

Use F1 key for context-sensitive Help

[✓ OK]   [✗ Cancel]   [? Help]

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.

Simulation model: C:\ka\vpso\1 ML Cu-Ni\Cu-Ni.mdl

Repulsive potls | Attractive potls | Graphs

INTERACTION POTENTIALS

Core potential type

$$V(r_{ij}) = \frac{Z_1 Z_2 e^2}{4\pi\varepsilon_0 r_{ij}} \sum_{k=1}^{N} c_k \exp(-b_k r_{ij}/a)$$

Projectile-Target
- (•) ZBL
- ( ) Moliere-Lindhard
- ( ) Moliere-Firsov

Screening length correction
1.00000

Target-Target
- (•) ZBL
- ( ) Moliere-Lindhard
- ( ) Moliere-Firsov

Screening length correction
1.00000

Potentials cut-off at: 4.00000 Å

Z(A) (type 1 atoms) 29

Z(B) (type 2 atoms) 28

Spline Range
Low (A) 1.60000
High (A) 2.20000

Hint: If your target consists of 2 types of atoms, you must ensure (a) that the first and last atoms in the target file are of different types; (b) that the type B atoms are flagged.

LATTICE VIBRATIONS
[✓] Include Vibrational Displacements

Lattice atom mass (amu) 58.700000
Lattice temperature (K) 300.000

Debeye Temperatures (K)
Bulk 450.000
Surface perpendicular 450.000
Surface parallel 450.000

SPECIFIC ENERGIES
Surface binding energy (eV) 0.00000
'Bulk' binding energy (eV) 0.00000
Termination energy (eV) 0.50000
[ ] Test projectile energy only

✓ Ok   ✗ Cancel   ? Help

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).

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.

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.

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.

3. Enter only V(A-A) parameters for an elemental target, otherwise all 3 sets. Enter V(A-A) last if you have to set S_n.

2. Enter Sutton-Chen potential parameters (if selected)

2. Enter TB potential parameters (if selected)

b is normally 0.0.

Click yellow arrows to copy parameters to/ from the V(A-A) set (helpful when setting S_n).

Simulation Model: UNTITLED.MDL

Repulsive pots | Attractive pots | Graphs

V(A-A) parameters

Sutton-Chen		TB-SMA
D (eV)	0.15553030	A (eV)
α (Å)	2.55600000	r0 (Å)
N	11.18300000	p
M	4.63940000	q
b	0.00000000	b
c	1.23550000	ξ (eV)
Sn	13.350000	Sn

V(B-B) parameters

Sutton-Chen		TB-SMA
D (eV)	0.11300000	A (eV)
α (Å)	2.49180000	r0 (Å)
N	14.08700000	p
M	3.58740000	q
b	0.00000000	b
c	1.40050000	ξ (eV)
Sn	13.350000	Sn

V(A-B) parameters

Sutton-Chen		TB-SMA
D (eV)	0.13299000	A (eV)
α (Å)	2.52370000	r0 (Å)
N	12.63500000	p
M	4.11340000	q
b	0.00000000	b
c	1.31540000	ξ (eV)
Sn	13.350000	Sn

Math definition of potential

$$V(r_{ij}) = A \cdot [e^{-p(r_{ij}/r0-1)} - b e^{-q(r_{ij}/r0-1)}]$$
$$\rho_i = \xi^2 \sum e^{-q(r_{ij}/r0-1)}$$

$\sqrt{\rho_i}$

Potential type
- ○ Sutton-Chen
- ● TB-SMA

1. Choose what kind of potential you want to use (probably TB).

☑ Use switching function. Rsw = 3.80000 (Å)

✓ Ok   ✗ Cancel   ? Help

5. Check this box to use a switching function (recommended in most cases). Set R_{sw} below the cut-off distance, but above the last shell of atoms within the attractive potential range.

4. This button allow you to calculate a lattice sum, S_n, which is needed to compute the effective potential (see documentation). You can also do it by hand. In the dialog box that comes up, enter the name of your target file, and the index of a row in that file which refers to a bulk (non-edge) atom. The value of S_n will be returned.

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.

Simulation Model: UNTITLED.MDL

Repulsive potls | Attractive potls | Graphs

V(r)

Potential (eV)
45
40
35
30
25
20
15
10
5
0

r (A)   2   3   4

F(r) = -dV(r)/dr

Force (eV/A)
150
100
50
0

r (A)   2   3   4

Graphs display...
○ A-A potential
○ B-B potential
○ A-B potential

These graphs display a spline of the screened Coulomb potential to an effective pair potential derived from the selected many-body potential.

☐ Report spline coefficients

Unzoom | Plot | ✓ Ok | ✗ Cancel | ? Help

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.
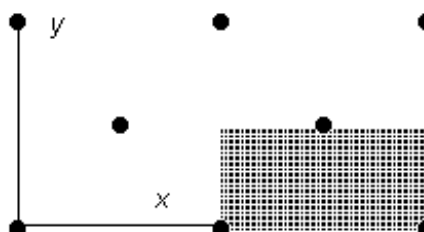
Help for common cases.

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.

Impact specifications: C:\kalypso\1 ML Cu-Ni\CuNi.imp

Impact Parameters (Å)   ? Templates   1922 impact points.
x =
y =

bx (min)   bx (max)   No. impacts
4.98369   7.475532   62

by (min)   by (max)   No. impacts
0   1.245922   31

Impact Density
○ Uniform   (x,y) angle (deg.) 90
○ Weighted   Projectile z0 (Å)   3.5

Use F1 key for context-sensitive Help

✓ OK   ✗ Cancel   ? Help

▶ Refresh
Copy

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.

Inelastic Losses: C:\kalypso\1 M Cu-Ni\Cu-Ni.inl

Lindhard-Scharff-Schiott | Oen-Robinson | Shapiro-Tombrello | Compute... | Thermal

eV fs/Å2

	Z1	K(LSS)	scale
atom 1	29	13.318232	0.5
atom 2	28	13.008940	0.5
atom 3	18	9.509670	0.5

Add atom

Clear atom

Hint: Rows with Z=0 will be ignored at runtime

Velocity threshold (m/s):

11000

✓ OK   ✗ Cancel   ? Help

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.

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

The scale shouldbe 1.0 or 0.5, depending 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.

Inelastic Losses: C:\kalypso\1 ML Cu-Ni\Cu-Ni.inl

Lindhard-Scharff-Schiott | Oen-Robinson | Shapiro-Tombrello | Compute... | Thermal

eV Å2

	Z1*Z2	K(OR)	scale
pair 1	522	0.0011233	0.5
pair 2	841	0.0015733	0.5
pair 3	504	0.0011067	0.5
pair 4	784	0.0015101	0.5

Add pair

Clear pair

Hint: Rows with Z1.Z2=0 will be ignored at runtime

Max. apsidal distance (0-2 Å)

1.5

Exponential parameter

0.3

✓ OK   ✗ Cancel   ? Help

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).

Inelastic Losses: C:\kalypso\1 ML Cu-Ni\Cu-Ni.inl

Lindhard-Scharff-Schiott | Oen-Robinson | Shapiro-Tombrello | Compute... | Thermal

Å   eV

	Z1*Z2	Rcrit	dE	prob.	Nmax
pair 1	0	0	0	0	10

Add pair

Clear pair

Hint: Rows that have Z1, Z2 = 0 will be ignored at runtime

✓ OK   ✗ Cancel   ? Help

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.

Inelastic Losses: C:\kalypso\1 ML Cu-Ni\Cu-Ni.inl

Lindhard-Scharff-Schiott | Oen-Robinson | Shapiro-Tombrello | Compute... | Thermal

Atomic number of fast atom (Z1) `18`

Atomic number of stopping atoms (Z2) `29`

Atomic weight of stopping atoms (M2) `63.546`

Density of stopping atoms (g/cm3) `8.933`

Energy loss model
- ○ LSS model
- ○ OR model

$$-\frac{dE}{dx} = 8nM\frac{e^2}{4\pi\varepsilon_0}a_B\frac{z_1^{7/6}z_2}{(z_1^{2/3}+z_2^{2/3})^{3/2}}\,v/v_B$$

$-dE/dx = Kv$

units for K(LSS): eV fs/Å2

`9.509670314`   ☐ K(LSS)

☐ Permute Z1, Z2

Hint: Use this tool to compute K(LSS) and K(OR)

✓ OK   ✗ Cancel   ? Help

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).

Inelastic Losses: C:\kalypso\1 ML Cu-Ni\Cu-Ni.inl

Lindhard-Scharff-Schiott | Oen-Robinson | Shapiro-Tombrello | Compute... | Thermal

Cooling period (fs) `250`

Temperature (K) `300`   <-- Specify 0.0 for monitoring only

Cooling start time (fs) `0`

Cooling stop time (fs) `2000`

Hint: cooling effects will be applied to all atoms in system, except (a) those that have the clDonlCool option flag set; (b) those that have left the lattice zone.

✓ OK   ✗ Cancel   ? Help

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.