

# KALYPSO 2 TUTORIAL

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## 1. Introduction

This document will briefly guide the reader through the steps required to construct, execute and analyse a standard sputtering simulation using the *Kalypso* 2 package. The system studied will involve the sputtering of 1 ML Cu/Ni(100) at 300 K by 2 keV Ar projectiles that are incident from the normal direction. The goal of the simulation is to predict: (a) the sputter yields of Cu and Ni; (b) the energy distribution of sputtered Cu atoms; (c) the yields of the dimer species Cu<sub>2</sub>, CuNi and Ni<sub>2</sub>. This document should be read in conjunction with the *Kalypso* User Guide which explains the meanings of options and commands in more detail.

## 2. Input files

### 2.1. Introductory remarks

Begin by choosing a name for the project: Ar-CuNi, and by creating a directory with this chosen name in which the input files will be stored. It is not a good idea to store more than one project in each directory. In this tutorial, the project input file stems will be named according to the same convention: Ar-CuNi.trg, Ar-CuNi.prj, Ar-CuNi.run, Ar-CuNi.mdl, Ar-CuNi.imp, Ar-CuNi.inl. (These files are also supplied in the \tutorial directory of the *Kalypso* distribution.) However, you can choose different names for each file if you prefer.

Start the program *Spider*, which will be used to create the input files. The input files will be created in the order (left to right) that they appear on the menu bar of *Spider*. For this project, we have to create 6 input files, starting with the Target file.

In this tutorial (and in the *Kalypso* documentation generally), the locations of menu items are indicated by a notation of the following kind: Model|New which means ‘the menu item *New* that is found under the *Model* menu item’.

### 2.2. Target file

1. Select Target|New target|Face-centred cubic|[100] surface from the *Spider* menu. In the dialog box that comes up, enter the values shown in Fig. 1. Then save the file as Ni100.trg. These inputs will create a target file that contains the

coordinates of a Ni(100) lattice. It will consist of 5625 atoms arranged into 9 atomic layers.

- Optional: if you wish, you can examine this target file as a graphical display (Target|Visualiser). In the Visualiser, you will see that the surface <011> rows are aligned with the  $x$  and  $y$  axes. The azimuthal orientation of the target is not important for this project, which involves projectile bombardment from the normal direction. For oblique projectile bombardment, you would normally have to rotate the Target so that the azimuth ( $\phi$ ) of interest is aligned with the direction of projectile incidence (by default, the  $x$ -axis, although this can be modified by selecting another value for  $\phi$  in the Run file).

The dialog box is titled 'Elemental data' and contains the following fields:

- Symbol:
- Lattice const. (Å):
- Atomic No. (Z):
- Atomic mass (amu):

Below this are two panels:

- Lattice dimensions (atoms):**
  - X-width =  \* 2 + 1
  - Y-width =  \* 2 + 1
  - Z-depth =
  - 5625 atoms
- Lattice origin (Å):**
  - X-origin:
  - Y-origin:
  - Z-origin:

At the bottom is a panel titled 'Relaxations (Å)' with three layers:

- Layer 1:
- Layer 2:
- Layer 3:

Fig. 1. Target file input data dialog box.

- Open the Target file in a text editor (or use the Utilities|Editor command), and examine the data:

```
0.00000 0.00000 0.00000 28 58.71000 0 Ni fcc
29.90213 29.90213 0.00000 28 58.71000 0 Ni fcc
29.90213 27.41029 0.00000 28 58.71000 0 Ni fcc
29.90213 24.91844 0.00000 28 58.71000 0 Ni fcc
```

- Carry out a global search and replace operation on this file:

```
Replace: "0.00000 28 58.71000 0 Ni fcc"
By:      "0.00000 29 63.54600 0 Cu ads"
```

- The first three columns of the Target file represent the atomic coordinates, so this operation will replace surface Ni atoms ( $z = 0.000$ ) with (adsorbed) Cu atoms. The atomic labels ("Ni fcc" and "Cu ads") do not affect the simulation in any way, and are included purely to make the file more readable. Save the edited file as CuNi.trg. This Target file represents an unrelaxed Cu/Ni(100) target in which Cu

atoms substitute for Ni atoms in the surface layer. Unless you are concerned about relaxation effects, the Target file coordinates are now ready for use. However, we will make one final modification that will simplify later data analysis. (Appendix 1 discusses how to determine and apply appropriate layer relaxations, but most simulations published in the literature ignore relaxation because its effects on predicted properties are too small to be of concern.)

- Now examine this target file as a graphical display (Target|Visualiser). A greyscale image is shown in Fig. 2. Note that the surface layer on the left hand side has an overhanging atom. It is possible to trim this off using the Visualiser, but in this project we will instead label it as an edge atom using another Visualiser feature.

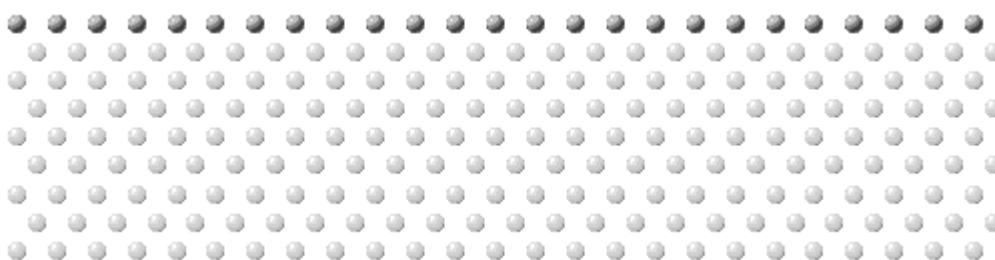


Fig. 2. Target file Ar-CuNi.trg as viewed from side (xz plane). Dark grey symbols represent Cu atoms, light grey symbols represent Ni atoms.

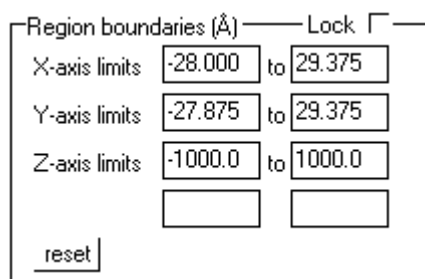
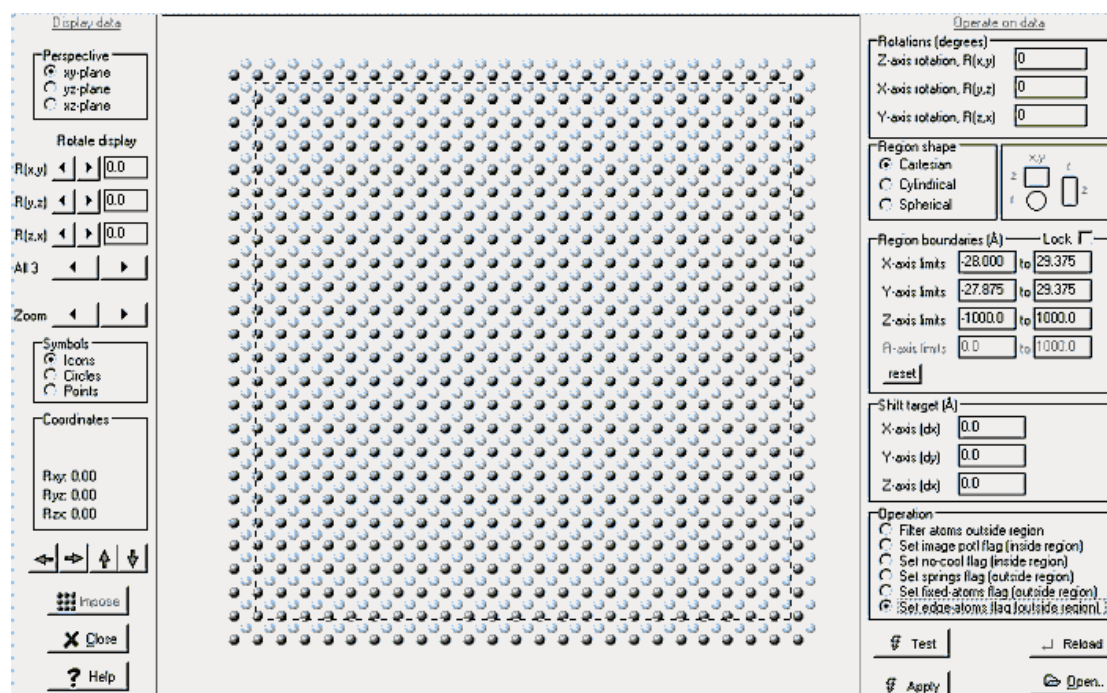


Fig.3. Top: Visualiser window showing how the edge atom flag is set for the Target file in this project. Left: Region boundaries data that are used to flag edge atoms for the Target file. (If you look carefully, you may be able to see the selected region, as a dashed line, on the graphic that corresponds to the boundaries.)

7. Now view the target in the  $xy$  plane, as shown in Fig. 3 (reduce the zoom if necessary in order to fit the target into the viewing area). Use the mouse cursor to select the region boundaries shown (or enter them by hand). In the boxed labelled **Operation** select the item labelled **Set edge-atoms flag**. Click **Test** followed by **Reload** to see which atoms will be affected. Then Click **Apply** to save a modified version of your Target file to disk as `Ar-CuNi.trg`. This is the file that will be used for the simulation project.
8. This operation has labelled atoms at the edges of the target as edge-atoms by modifying their flags. Examine the file `Ar-CuNi.trg` created in step 7 in a text editor. You will find that the flags field has been modified to 16 (or 10000 in binary) for the edge atoms (this will have no effect on the simulation, but will make the output data easier to process):

27.41029	29.90213	0.00000	29 63.54600	16 Cu ads
27.41029	27.41029	0.00000	29 63.54600	0 Cu ads
27.41029	24.91844	0.00000	29 63.54600	0 Cu ads
27.41029	22.42660	0.00000	29 63.54600	0 Cu ads

### 2.3. Projectile file

Select Projectile|New from the *Spider* menu. In the dialog box that comes up, enter the values shown in Fig. 4. Then save the file as `Ar-CuNi.prj`.

Specifications

Elemental symbol	Energy (keV)
Ar	2.0
Atomic number	Atomic mass (amu)
18	39.948
No. of atoms	
1	

Fig. 4. Projectile file input data dialog box.

### 2.4. Run file

Select Run|New from the *Spider* menu. In the dialog box that comes up, enter the values shown in Fig. 5 (you can ignore input items that are blanked out in Fig. 5). Then save the file as `Ar-CuNi.run`. This Run file specifies that each run in the simulation will continue for 2000 fs, at which time data will be recorded for all particles in the system.

The timestep is estimated with the help of the Velocity Calculator tool (Utilities menu) based on input data for 2 keV Ar projectiles. Vibrational displacements calculated for Cu (type 0 atoms, upper box) and Ni (type 1 atoms, lower box) will be added for an assumed temperature of 300 K (the calculations require a knowledge of Debye temperatures; the atom types refer to the order specified in the Model file).

You can refer to the User guide (Chapter 4) for further information on the meaning of the Run file parameters and options.

<p>General specifications</p> <p>Random number seed <input type="text" value="1723983"/></p> <p><input type="checkbox"/> Ignore interactions between target atoms</p> <p><input type="checkbox"/> Multiple-impact simulation</p> <p>No. of replica atoms <input type="text" value=""/></p>	<p>Output</p> <p>When to write output</p> <p><input type="checkbox"/> At start of each run (t = 0)</p> <p><input checked="" type="checkbox"/> At end of each run</p> <p><input type="checkbox"/> Periodically during each run... <input type="text" value=""/></p> <p><input type="checkbox"/> Do not write more than one record per run for any atom</p> <p><input type="checkbox"/> Output log of inelastic events</p>
<p>Periodic boundaries</p> <p><input type="checkbox"/> Use periodic (x, y) boundaries</p> <p>Period, Lx (Å) <input type="text" value=""/></p> <p>Period, Ly (Å) <input type="text" value=""/></p>	<p>Which atoms to write output for</p> <p><input checked="" type="radio"/> All atoms in system</p> <p><input type="radio"/> Projectile atom #1 only</p> <p><input type="radio"/> All particles with KE &gt; 10 eV</p> <p><input type="radio"/> All ejected atoms with rz &gt; 5 Å</p> <p><input type="radio"/> Ejected projectile atom #1 with rz &gt; 5 Å</p> <p><input type="radio"/> Atoms that satisfy the output condition specified below</p>
<p>Projectile initialisation</p> <p>Altitudinal angle (°) (<math>\phi</math>) <input type="text" value="90.0"/></p> <p>Azimuthal angle (°) (<math>\phi</math>) <input type="text" value="0.00"/></p> <p>Projectile mode</p> <p><input checked="" type="radio"/> Impinging atom(s)</p> <p><input type="radio"/> Recoiling atom(s)</p> <p><input type="radio"/> Mixed</p> <p><input type="checkbox"/> Randomly rotate projectile (for clusters only)</p>	<p>Meaning of tag fields in output records (advanced option)</p> <p><input checked="" type="radio"/> Normal (proj: alt, phi; target: bx, by)</p> <p><input type="radio"/> Inverted (proj: bx, by; target: alt, phi)</p> <p><input type="radio"/> Caloric data [bx = T, by = U(T)]</p>
<p>Termination criteria</p> <p>Termination time, minimum (fs) <input type="text" value="0.00"/></p> <p>Termination time, maximum (fs) <input type="text" value="2000.0"/></p> <p>Termination energy (eV) <input type="text" value="0.00"/></p> <p><input type="checkbox"/> Perform energy tests on projectile only</p> <p>Projectile z(min), z(max) (Å) [no effect if = 0] <input type="text" value="0.0"/> <input type="text" value="0.0"/></p>	<p>Neighbour lists and timestep</p> <p>Range search</p> <p><input type="radio"/> Brute force (faster for very small targets)</p> <p><input checked="" type="radio"/> Cell-index (normal choice)</p> <p>Cell-index search cell size (Å) <input type="text" value="5.0"/></p> <p>Range test constant <input type="text" value="1.0"/></p> <p>Maximum number of partners <input type="text" value="100"/></p> <p>Neighbour update period (timesteps) <input type="text" value="10"/></p> <p>Time to start timestep updates (fs) <input type="text" value="10.0"/></p> <p><input type="checkbox"/> Fixed timestep</p> <p>Initial timestep (fs) <input type="text" value="0.06"/></p>
<p>Thermal vibrations</p> <p><input checked="" type="checkbox"/> Apply vibrational displacements</p> <p><input type="checkbox"/> Apply thermal velocities</p> <p>Lattice vibrational temperature (K) <input type="text" value="300.0"/></p> <p>Location of surface/bulk boundary (on z-axis) (Å) <input type="text" value="0.00"/></p> <p><input type="checkbox"/> Do not apply y-axis vibrational displacements (e.g. for 2D simulations)</p> <p>Mean square vibrational displacements, &lt;x<sup>2</sup>&gt; (type 0 atoms)</p> <p>Bulk (Å<sup>2</sup>) <input type="text" value="0.00605"/></p> <p>Surface perpendicular (Å<sup>2</sup>) <input type="text" value="0.01885"/></p> <p>Surface parallel (Å<sup>2</sup>) <input type="text" value="0.0083"/></p> <p><input type="button" value="Calculate"/></p> <p>Mean square vibrational displacements, &lt;x<sup>2</sup>&gt; (type 1 atoms)</p> <p>Bulk (Å<sup>2</sup>) <input type="text" value="0.00390"/></p> <p>Surface perpendicular (Å<sup>2</sup>) <input type="text" value="0.01492"/></p> <p>Surface parallel (Å<sup>2</sup>) <input type="text" value="0.0064"/></p> <p><input type="button" value="Calculate"/></p>	

Fig. 5. Run file input data dialog box.

Screened Coulombic potential: I = inert atom, M(0), M(1) = metallic atoms

Set system type [disables unneeded items]

- ☐ Mono-metallic with inert atom(s)
- ☐ Mono-metallic without inert atom(s)
- ☒ Bi-metallic with inert atom(s)
- ☐ Bi-metallic without inert atoms

Constants (b, c) for I-M and M-M potential

	Inert - Metal	Metal - Metal
c1	<input type="text" value="0.028171"/>	<input type="text" value="0.028171"/>
c2	<input type="text" value="0.28022"/>	<input type="text" value="0.28022"/>
c3	<input type="text" value="0.50986"/>	<input type="text" value="0.50986"/>
c4	<input type="text" value="0.18175"/>	<input type="text" value="0.18175"/>
b1	<input type="text" value="0.20162"/>	<input type="text" value="0.20162"/>
b2	<input type="text" value="0.40290"/>	<input type="text" value="0.40290"/>
b3	<input type="text" value="0.94229"/>	<input type="text" value="0.94229"/>
b4	<input type="text" value="3.1998"/>	<input type="text" value="3.1998"/>

Set

- ☒ ZBL
- ☐ Molière
- ☐ (no action)

Set

- ☒ ZBL
- ☐ Molière
- ☐ (no action)

$$V(r_{ij}) = (Z_i Z_j e^2 / 4\pi\epsilon_0 r_{ij}) \sum_{k=1}^4 c_k \exp(-b_k r_{ij}/a)$$

Screening lengths (a) for I-M and M-M interactions

Atomic numbers

I:  M(0):  M(1):

Set screening length

- ☒ ZBL
- ☐ Molière-Lindhard
- ☐ Molière-Firsov
- ☐ (no action)

	Screening length (Å)	Correction
I - I	<input type="text" value="0.1204948666"/>	<input type="text" value="1.0"/>
I - M(0)	<input type="text" value="0.1138927914"/>	<input type="text" value="1.0"/>
I - M(1)	<input type="text" value="0.1143776935"/>	<input type="text" value="1.0"/>
M(0) - M(0)	<input type="text" value="0.1079766084"/>	<input type="text" value="1.0"/>
M(0) - M(1)	<input type="text" value="0.1084123458"/>	<input type="text" value="1.0"/>
M(1) - M(1)	<input type="text" value="0.1088516143"/>	<input type="text" value="1.0"/>

Parameters

(i - j) pair	(0 - 0)	(0 - 1)	(1 - 0)	(1 - 1)
2A (eV)	<input type="text" value="0.156525"/>	<input type="text" value="0.134760"/>	= <input type="text" value=""/>	<input type="text" value="0.112995"/>
r0 (Å)	<input type="text" value="2.5560"/>	<input type="text" value="2.5239"/>	= <input type="text" value=""/>	<input type="text" value="2.4918"/>
p	<input type="text" value="11.18320"/>	<input type="text" value="12.63493"/>	= <input type="text" value=""/>	<input type="text" value="14.08666"/>
2q	<input type="text" value="4.63941"/>	<input type="text" value="3.92837"/>	<input type="text" value="3.92837"/>	<input type="text" value="3.21733"/>
ξ (eV)	<input type="text" value="1.23552"/>	<input type="text" value="1.31789"/>	<input type="text" value="1.31789"/>	<input type="text" value="1.40054"/>
b	<input type="text" value="0.0"/>	<input type="text" value="0.0"/>	= <input type="text" value="0.0"/>	<input type="text" value="0.0"/>

Figs. 6a (top) and 6(b) (bottom). Model file input data dialog box.

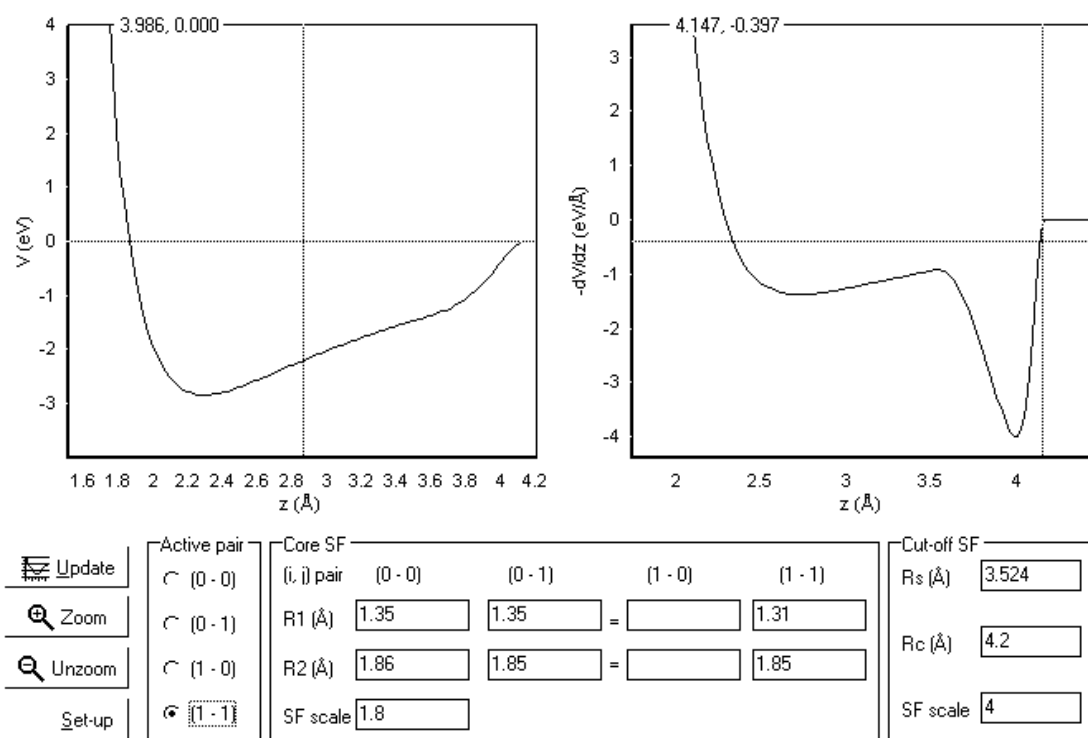


Fig. 6(c). Model file input data dialog box. The charts show the Ni-Ni potential and forces (type 1-1 interaction) .

## 2.5. Model file

Select Model|New from the *Spider* menu. In the dialog box that comes up, enter the values shown in Figs. 6(a)-6(c) (the values entered in Figs. 6(a) and 6(b) are the default values; blanked out input values can be ignored).

The atomic numbers of the inert atom and the metallic atom types (0 = Cu and 1 = Ni) are specified in Fig. 6(a) as  $I$ ,  $M(0)$  and  $M(1)$  respectively. If the order of Cu and Ni were reversed, you would have to change the order of the vibrational corrections specified in the Run file. Other files in the project would not be affected.

The potentials are fitted to the second neighbour distances of Cu and Ni, and therefore are cut off at 4.2 Å or just before the 3<sup>rd</sup> neighbour distance in Ni (4.316 Å). A switching function is applied between the 2<sup>nd</sup> neighbour distance (3.524 Å) and the cut-off distance. As a result of the short switching function distance, the magnitude of the Ni-Ni force increases very rapidly just below the cut-off distance (see Fig. 6(c)). The **switching function (SF) scale** (the parameter  $a$  in Eq. 2.13 of the User Guide) is chosen in order to reduce the force near the cut-off so that atoms in the 3<sup>rd</sup> shell are not strongly affected by this large force if they are only slightly displaced, but to a large extent this parameter is subjective and large forces in this region are an unavoidable feature of any truncated potential.

## 2.6. Impact file

1. Select Impact|New from the *Spider* menu. In the dialog box that comes up, enter the values shown in Fig. 7, then click the **Refresh** button. The input parameters define a triangular grid that consists of 325 impact points. These points represent the coordinates (expressed relative to those of the anchor atom) towards which the

impinging projectile will travel when each run is initialised. Save these data to disk in a file named `Ar-CuNi.imp`.

Impact parameters

bx (min) (Å)	bx (max) (Å)	No. impacts
0.0	1.246	25
by (min) (Å)	by (max) (Å)	No. impacts
0.0	1.246	25
(x,y) angle (deg.)		45
Projectile-anchor $\Delta z$ (Å)		4.5

325 impact points.  
x = 0.69776  
y = 0.04984

o x y

Refresh

Fig. 7. Impact file input data dialog box.

2. Select Impact|Visualiser, and load the Impact file that you have just created.
3. On the commands menu, select New Imposition file, and load the Target file that you created in section 2.2. This shows the coordinates in the Impact file superimposed on the Target file coordinates (Fig. 8) (useful for checking that the Impact file has the correct dimensions and alignment).

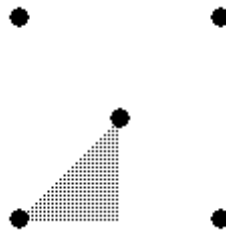


Fig. 8. Impact file coordinates superimposed on the Target file coordinates (detail).

## 2.7. Inelastic file

Select Inelastic|New from the *Spider* menu. In the dialog box that comes up, enter the values shown in Fig. 9. Leave items other than those shown in their default states. Save the Inelastic file as `Ar-CuNi.inl`.

1. This Inelastic file specifies that LSS inelastic losses will be applied to Ar, Ni and Cu atoms that move with velocities  $> 10^4 \text{ m s}^{-1}$  inside the target, or within  $1.5 \text{ Å}$  of the surface plane (which lies at  $z = 0 \text{ Å}$  in this simulation). These values are somewhat arbitrary. The first is chosen to save calculation time for slow atoms that experience negligible losses; the second reflects the fact that electron density spills outside the surface.
2. The scale factors of 1.0 imply no correction to the theoretical LSS expression. The  $K(\text{LSS})$  constants are calculated on the assumption that all atoms move in Ni metal (i.e. stopping atoms = Ni with  $Z = 29, \rho = 8.9$ ).
3. The box labelled **Calculate LSS and OR parameters** can be used to calculate  $K$  for different kinds of atoms (Ar, Cu, Ni) moving in Ni.



What to include in the simulation

- ☒ Include LSS inelastic losses
- ☐ Include OR inelastic losses
- ☐ Include ST inelastic losses
- ☐ Apply temperature control
- ☐ Include image potential effects
- ☐ Include lattice site springs

Lindhard-Scharff-Schiott model

	Z1	eV fs/Å <sup>2</sup>		
		K(LSS)	scale	
atom 1	18	10.1	1	<input type="button" value="Add atom"/>
atom 2	28	13.8	1	<input type="button" value="Clear atom"/>
atom 3	29	14.1	1	Velocity threshold (m/s)
				<input type="text" value="1e4"/>
				Location of surface (on z-axis) (Å)
				<input type="text" value="1.5"/>

Fig. 9. Details from the Inelastic file input data dialog box.

### 3. Running the simulation

After the input files have been created, it is a simple matter to run the simulation.

1. Start *Kalypso*. Click **File|Options** and under **Screen reporting** select **Moderate**. This setting determines the verbosity of the output. **Moderate** or **Minimal** is an appropriate setting (do not use **Verbose** except for debugging because it slows down the simulation excessively).
2. Click **File|Simulation project**. As shown in Fig. 10, locate the input files for the project, and specify the names of the output files, by clicking the appropriate button (note: the **Projectile data** button will auto-complete the other filenames if the named files are found).
3. Click the Run button. The simulation begins.

Input files

Projectile data\*  C:\kalypso package\tutorial\Ar-CuNi.pri ☐ Omit

Target data  C:\kalypso package\tutorial\Ar-CuNi.trg

Run data  C:\kalypso package\tutorial\Ar-CuNi.run

Model data  C:\kalypso package\tutorial\Ar-CuNi.mdl

Impact data\*  C:\kalypso package\tutorial\Ar-CuNi.imp ☐ Omit

Inelastic data\*  C:\kalypso package\tutorial\Ar-CuNi.inl ☐ Omit

Output files

Dynamics  C:\kalypso package\tutorial\dynvars.snk

Log file  C:\kalypso package\tutorial\kalypso.txt

Inelastic events\*  ☒ Omit

Fig. 10. Simulation project files dialog box for *Kalypso*.


When *Kalypso* begins, it writes a summary of the information extracted from the input files to the screen, then proceeds to write information specific to each run (the level of detail in the output for each run depends on the verbosity level chosen in the project options):

```
Run 1 begins...
Energy = -20954.7260422 eV.
  run  step  time(fs)  timestep(fs)  energy(eV)      KE(eV)
    1     0 0.000E+0000  6.000E-0002 -2.0954726E+0004  2.0000000E+0003...
    1  1598 2.001E+0003  3.093E+0000 -2.1229373E+0004  1.2428228E+0003...

Run 1 ends.
Energy = -21229.3730849 eV.
LSS loss = -274.776 eV.
Energy leak = 0.128621 eV (average = 0.1286 eV [ 0.0005424%], max. = 0.1286 eV).
3/15/2004 1:25:30 AM.
Execution time = 90 s.
Status: OK.

...
Run 325 ends.
Energy = -21283.3526975 eV.
LSS loss = -318.482 eV.
Energy leak = 0.0888554 eV (average = 0.3432 eV [ 0.001446%], max. = 1.5 eV).
3/15/2004 8:35:57 AM.
Execution time = 25918 s.
Status: OK.
```

The simulation executes in about  $17/G$  hours, where  $G$  is the CPU clock frequency in GHz. The output shown above indicates that 25918 s (7.2 hours) was required for execution of the 325 runs in the simulation project. The average energy leak was 0.34 eV, and the maximum energy leak (for any of the runs) was 1.5 eV. These values are very good, which suggests that the timestep could be further increased (in order to speed up execution time). Note that the energy of the system is different from run to run, due to the different vibrational displacements that are randomly applied.

Fig. 11 shows a graphical snapshot of the atomic positions near the start of a run. This snapshot is taken from the Visualiser window that opens when the speed-button marked by an orange icon:  is clicked. (Close the Visualiser window when not in use, because it slows down the simulation speed.)

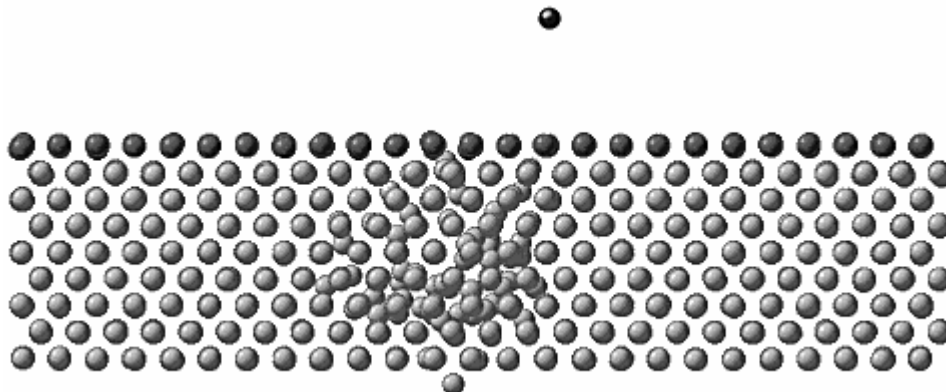


Fig. 11. Snapshot of the running simulation, as viewed in the Visualiser window. The particle above the target is the (receding) projectile. The dark grey symbols represent Cu atoms; the light grey symbols represent Ni atoms.

#### 4. Analysing the simulation data

The simulation data are stored by *Kalypso* in the output dynamics file, named by default `dynvars.snk`. These data can be analysed using the *Winnow* program. Start *Winnow*. The commands needed for data analysis are located on the **Process** menu.

1. **Filter out records that refer to projectile atoms:** The output data include records that refer to the projectile species. These are not needed for sputter yield calculations, so they are filtered out of the data set using the **Filter** command in *Winnow*. The projectile is labelled by a value of 1 for the row number parameter `rw`, which serves as an atomic index. Target atoms have `rw = 2, 3, 4....` Set up the filtering operation as shown in Fig. 12, then click OK.

Source (input) file  
Browse | C:\\_kalypso package\tutorial\dynvars.snk

Destination (output) file ☒ Auto-complete name  
Browse | C:\\_kalypso package\tutorial\sput.snk

Query expression = logical expression [+ [logical operator] + [logical expression]...]  
[rw > 1]

Fig. 12. Filtering out projectile atom records from the simulation output file.

2. The following output is produced in the main window of *Winnow*, showing that 325 projectile records have been removed from `dynvars.snk`, the remainder being stored in `target.snk`:

```
Filter; [rw > 1];
dynvars.snk (1828450 recs.) --> target.snk (1828125 recs. = 99.982%)
```

3. **Inspect the vertical (*z*) distribution of target atoms above the surface.** This is achieved with the **Spectrum** command, using `sput.snk` from item 2 as the input file, and `rz*1E10` as the spectrum variable (with 100 spectrum points in the range 0-100 Å). The resulting plot (Fig. 13) indicates an abrupt transition in the atomic density (i.e. number of hits per unit distance) at  $z = 5$  Å. This represents the interface between the target surface (including adatoms) and the gas phase. From this point onwards, atoms in the region  $z > 5$  Å will be identified as sputtered atoms.
4. **Isolate sputtered atoms by filtering `target.snk`.** A simple filter expression `[rz > 5E-10]` would include contributions from atoms that originate from the edges of the target. However, these sputtered edge atoms should be considered as artefacts of the simulation model, since they represent a failure of lateral containment of the collision cascade. The edge atoms can be excluded by adding a second condition: `[rz > 5E-10] & ![fl ~16]`, resulting in a condition that can be expressed as: “ $z > 5$  Å and edge-atom flag not set” (see Chapter 4 of the User guide for more on flags):

```
Filter; [rz > 5E-10] & ![fl ~16];
target.snk (1828125 recs.) --> sput.snk (1925 recs. = 0.1052%)
```

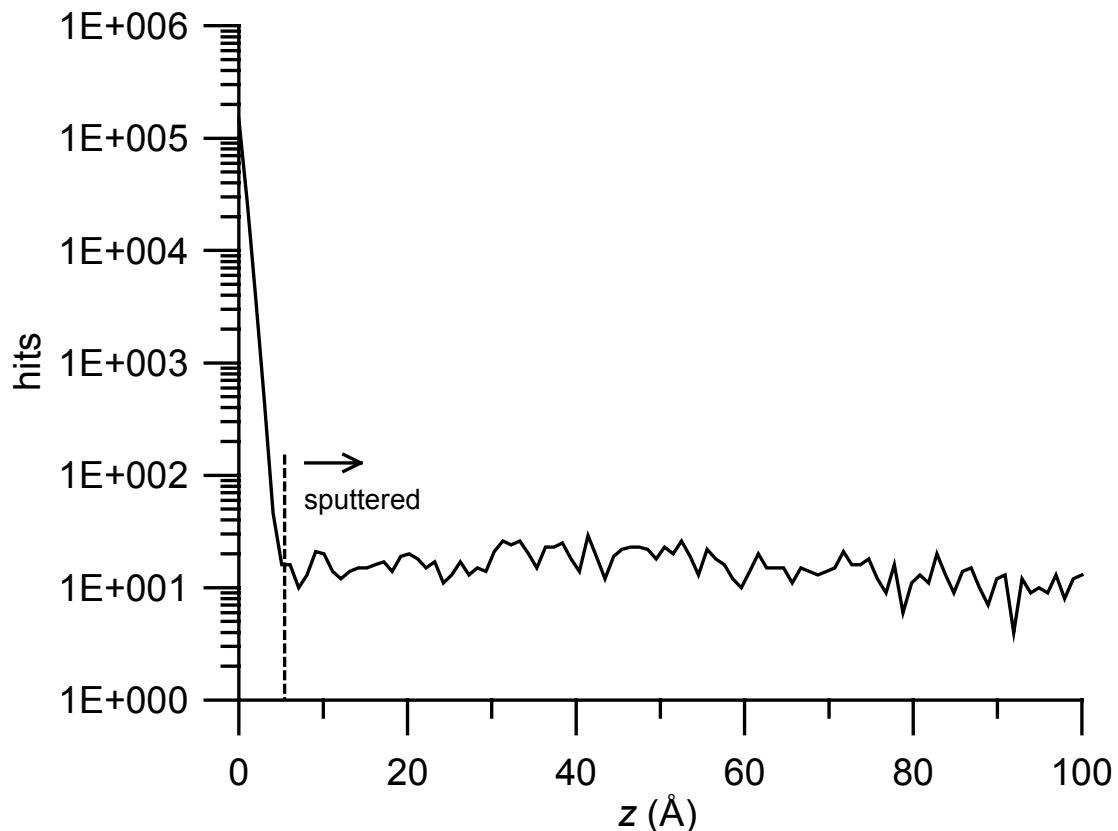


Fig.13. Distribution of sputtered atoms in the  $z$ -dimension.

5. **Sputter yield.** The screen output indicates that 1925 atoms were sputtered in 325 runs, giving a sputter yield ( $Y$ ) of  $1925/325 = 5.9$ . The **sputtering statistics** command supplies the same information (with the associated standard error) , i.e.  $Y=5.9\pm0.3$ :

```
Sputtering statistics for C:\_Kalypso package\tutorial\sput.dat
Total sputtered atoms = 1925
No. of projectile impacts = 325
Mean sputter yield = 5.92308
Standard deviation of sputter yield = 5.61511
Standard error of sputter yield = 0.31147
```

(Further investigation shows that a sputter yield of 6.0 is predicted if the edge atoms are included in the prediction.)

6. **Isolate Cu and Ni atoms in sput.snk.** Visual examination of the Target file in a text editor shows that lines 1-625 refer to Cu atoms in the surface layer. This range corresponds to values of 2-626 of the row number parameter ( $rw$ ). Using a **filter** operation, the Cu and Ni atom records in sput.snk can be separated:

```
Filter; [rw <= 626];
sput.snk (1925 recs.) --> Cu.snk (1848 recs. = 96%)
```

```
Filter; [rw > 626];
sput.snk (1925 recs.) --> Ni.snk (77 recs. = 4%)
```

This operation shows that the sputter yield of Cu is  $1848 / 325 = 5.7$  while that of Ni is  $77 / 325 = 0.24$ . Most sputtered atoms (96%) originate in the surface layer of the target.

7. **Energy distribution of Cu atoms.** The energy distribution is determined by carrying out a **spectrum** operation on Cu.snk (item 5) using the input expression  $k_e$  (particle kinetic energy in eV) over a suitable range (Fig. 14). The number of low-energy particles may be underestimated if the simulation is terminated too soon (this must be determined by trial and error).

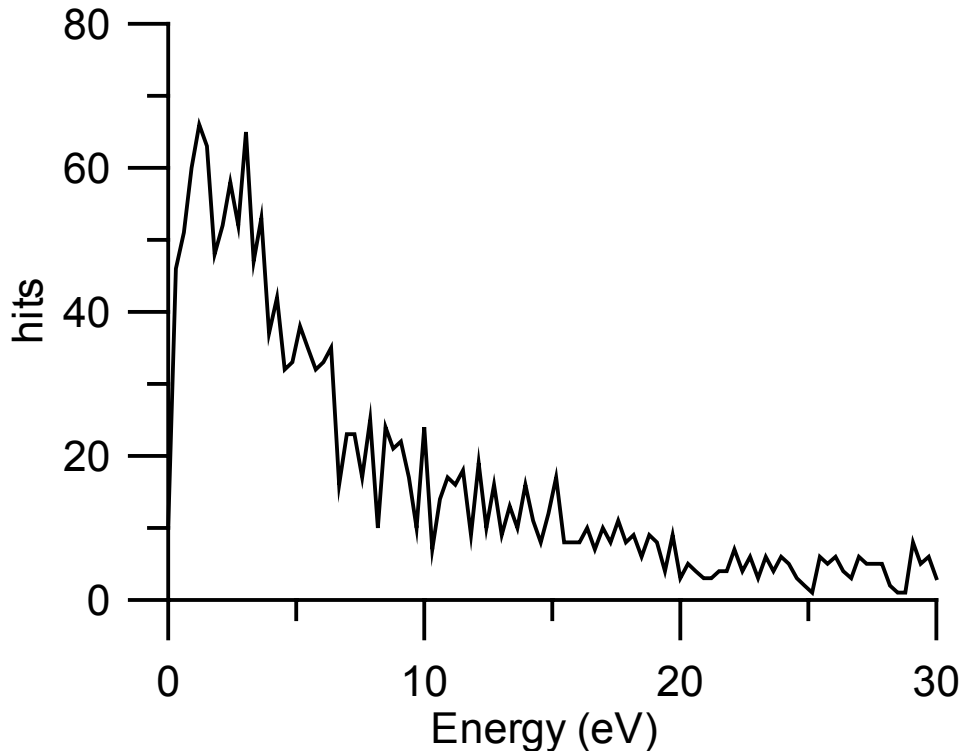


Fig. 14. Energy distribution of sputtered Cu atoms.

8. **Sputtered dimer yields.** Sputtered dimers can be identified using the command **Find sputtered clusters**, using sput.snk as the input file, with a clustering radius of 4.2 Å (same as the potential cut-off). A **sorting value** (index) of 626 is used to distinguish Cu atoms from Ni atoms, as in item 5 above. The **No. of atoms in cluster** parameter is set to 2 (for dimers). At the bottom of the output file, the results are summarised like this:

```
No of clusters with 2 atoms: 265
No of *atoms* (not clusters) with rw <= sorting index: 511
No of *atoms* (not clusters) with rw > sort index: 19
Largest cluster in this file has 6 atoms
```

9. This statement means that there are 511 Cu atoms sputtered in dimers (as Cu<sub>2</sub> or CuNi) and 19 Ni atoms sputtered in dimers (as Ni<sub>2</sub> or NiCu). The easiest way to count the number of Ni<sub>2</sub> dimers is (the old-fashioned way) to load the output file list of clusters into a spreadsheet and sort the *rw* columns.
10. On inspection, one finds that **no** Ni<sub>2</sub> clusters are produced (i.e. no columns where both indexes have values > 626), which implies that there are 19 NiCu clusters.

The number of  $\text{Cu}_2$  clusters (2 Cu atoms per cluster) is therefore  $(511-19)/2 = 255$  (or about 0.8  $\text{Cu}_2$  dimers per incident projectile). The CuNi yield is  $19/325 = 0.06$ . Clearly, an accurate prediction of the CuNi and  $\text{Ni}_2$  yields would require a greater number of simulation runs than the 325 that were used in this tutorial.

## APPENDIX 1: Computing target layer relaxations

In this appendix, the computation of layer relaxations using *Spider* is briefly explained.

1. In *Spider* click the **Target|Layer relaxations** menu command. A dialog box comes up, as shown in Fig. A1. Enter the data as shown (specify the Target and Model files of your project using the Browse buttons).

Target file that defines the lattice    
 C:\\_kalypso package\tutorial\Ar-CuNi.trg

Model file that defines the potentials   
 C:\\_kalypso package\tutorial\Ar-CuNi.mdl

$\Delta z(\text{start})$    $\Delta z(\text{end})$   Step  (Å)  
 From target file row... to row...  
 Layer 1    
 Layer 2    
 Layer 3

☒ Number of layers to relax  
☒ One layer  
☐ Two layers  
☐ Three layers

☐ Periodic (x, y) boundaries: Lx  Ly  (Å)

One-layer scan begins...  
 One-layer scan (target atoms 1..625): U(0) = -23356.81221229 eV  
 U(0)-U(min) = -3.58076523 eV, dz(min) = 0.04500000(±0.00250) Å.  
 Log file is C:\mk\projects\d7\Spider\temp\\_logfile.dat  
 Scan data written to file C:\mk\projects\d7\Spider\temp\\_relax.dat

Fig. A1. Layer relaxations dialog box.

2. Click the **Run** button, which will initiate a scan of the system energy for the specified Target file as the surface layer (consisting of rows 1-625 in the Target file) is displaced (scanned) vertically in steps of 0.005 Å between the limits specified (-0.1 to +0.1 Å). The value of  $\Delta z$  for which the energy is found to be a minimum is reported.
3. In this case,  $\Delta z$  is reported as  $0.0450 \pm 0.0025$  Å, which means that an outward relaxation of the surface layer is predicted. This can be explained by the larger atomic radius of Cu than Ni. The predicted relaxation is, in fact, identical to the difference of the Cu(100) and Ni(100) interlayer distances (by chance).
4. The reported relaxation refers to the potential specified in the Model file, **including any interactions in the switching function region**. The results may be sensitive to the positioning of the potential cut-off (when the surface layer relaxes inwards, the 3<sup>rd</sup> coordination shell can move into the switching function region). If you want to restrict the calculation to the pure tight-binding potential, place the cut-off between the 2<sup>nd</sup> and 3<sup>rd</sup> coordination shells (instead of just below the 3<sup>rd</sup> coordination shell).
5. Due to edge effects, the results will be sensitive to the size of the surface layer slab, but will converge eventually for very wide targets. The best method for obtaining a prediction for slabs of infinite width is to set up a periodic target (and select the appropriate option in Fig. A1).

6. Multiple layer relaxations can also be computed, but these can be quite time consuming if carried out in a brute force fashion. The most efficient way to proceed is: (a) compute the relaxation for layer 1, then create a new Target file in which this relaxation is applied; (b) using this new Target file, compute the layer relaxations for layers 1 and 2, over a restricted  $\Delta z$  range (e.g.  $\pm 0.03$  Å instead of  $\pm 0.1$  Å). This method is based on the idea that layer relaxations diminish in magnitude as the bulk of the target is approached.
7. For a single layer scan, a file `_relax.dat` is produced that contains a listing of the energy vs.  $\Delta z$  data. If an error occurs, you should examine the log file named in the output window (Fig. A1) for error messages.

A check on the accuracy of this procedure is to compute the lattice energy directly for a Target file with the optimised relaxation, and for Target files with slightly larger and small relaxations (the lattice energy should most negative for the optimised relaxation). Use the menu command Target|Lattice energy in *Spider* for this purpose, or examine the screen output produced by *Kalypso* when the Target file is employed in a simulation project.