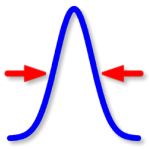

RESOLNRA User's Guide

Matej Mayer

Max-Planck-Institut für Plasmaphysik
Boltzmannstr. 2
85748 Garching
Germany

matej.mayer@ipp.mpg.de
Tel.: +49 89 32 99 16 39
Fax.: +49 89 32 99 22 79
www.simnra.com
home.mpcdf.mpg.de/~mam

This manual describes RESOLNRA version 1.10

Publications

Additional publications about RESOLNRA. The first should be used as general reference for the program:

- M. Mayer. "RESOLNRA: A new program for optimizing the achievable depth resolution of ion beam analysis methods". In: *Nucl. Instr. Meth. B* 266 (2008), p. 1852. DOI: 10.1016/j.nimb.2007.11.071. eDoc: http://edoc.mpg.de/319936. URL: http://home.mpcdf.mpg.de/~mam/Mayer-Nuclear-Instruments-Methods-B-266-(2008)-1852.pdf

DOI: Link to the original version of the publication at the journal pages. You may need institutional access in order to view the full text.

eDoc: Link to the full text of the publication at the eDoc server of the Max Planck Society. The text is available within the open access initiative of the Max Planck Society. Text and figures are identical to the original publication, but has been reformatted due to copyright reasons.

URL: Link to the full text of the publication at the SIMNRA home page. The text is freely available. The text is identical to the eDoc version.

Contents

1. Overview

RESOLNRA is a program for calculating the depth resolution of ion beam analysis methods. It allows to find the optimum experimental conditions in order to achieve the best depth resolution. This enables optimized measurements and is indispensable for the design of new experimental set-up's. RESOLNRA is based on the spectrum simulation code SIMNRA [4–6]. RESOLNRA can be used for Rutherford backscattering (RBS), elastic recoil detection analysis (ERDA) and nuclear reaction analysis (NRA). The energy broadening contributions due to electronic energy loss straggling, geometrical straggling, multiple scattering, absorber foils and detector resolution can be included. Additional constraints, such as minimum or maximum beam energies or tilt angles, can be taken into account.

1.1. Organization of this manual

This manual is organized in the following way:

- System requirements and the installation of the program are described in chapter 2.
- The use of the program is described in chapter 3. A quick overview about the necessary steps to display data is given in section 3.1. More details are found in the rest of chapter 3.
- Some examples for depth resolution optimizations are given in chapter 6.

1.2. Conventions in this manual

Links to sections, figures, pages, references, Internet web sites and additional text files are highlighted in blue. A click with the mouse will bring you to the link destination.

2. Installation

System requirements, the installation process of the program, and the uninstallation process are describes in this chapter.

2.1. System requirements

- RESOLNRA requires Windows 7 or higher.
- A screen resolution of 1024×768 pixels or higher is required.
- User's Guide and help system require Adobe Acrobat or Adobe Reader. Adobe Reader can be downloaded freely from the Adobe web site.
- RESOLNRA 1.7 requires SIMNRA 6.98 or higher. SIMNRA can be downloaded from http://www.simnra.com.

2.2. Installation

RESOLNRA is distributed together with the SIMNRA package and a setup program. Simply run the SIMNRA setup program and follow the instructions.

2.3. Uninstalling RESOLNRA

RESOLNRA cannot be uninstalled separately. It can be uninstalled together with the SIMNRA package, which is shipped with an automatic uninstall program. Refer to your Microsoft Windows documentation on how to uninstall programs.

3. Using RESOLNRA

This section describes the use of RESOLNRA. A quick overview about the necessary steps to display data is given in section 3.1. More details are found in the rest of chapter 3.

3.1. Basic steps

This section gives a quick overview about the basic steps necessary to perform depth resolution calculations.

1. Use SIMNRA to define your experiment: Incident ion species, target composition, detector position etc. Click *Calculate:Calculate Spectrum* in order to be sure that a spectrum can be calculated. Save your experiment and the spectrum in a nra-file.

2. Run RESOLNRA. By starting RESOLNRA the RESOLNRA program and one (hidden) instance of SIMNRA are started.

3. Click *File:Open...* in RESOLNRA and open the nra-file you just created with SIMNRA. RESOLNRA will open the file and run SIMNRA to perform the necessary calculations. The depth resolution as function of depth is then displayed by RESOLNRA for each isotope present in the target.

4. Click *Calculate* in RESOLNRA in order to calculate the depth resolution as function of varying incident energy, incident angle, or both. Each calculation will open a new window.

5. Click *Plot:Select Data* in order to remove data from the plot, or to add additional information, such as the individual straggling contributions. You will get a window as shown in Figure 3.1. Available data are visible on the left hand side in the *Available data* tree. Available data are ordered by reaction. The right hand side *Selected data* shows the data which are selected for plotting in the graph. Select the *Available data* you want to see, and click . The data are now placed in the *Selected data* tree. To delete data from the plot select the data in the *Selected data* tree and click  .

3.2. Principle of operation

RESOLNRA does not perform any calculations by itself, but uses the SIMNRA program. Both programs are connected through the OLE automation objects exported by SIMNRA. SIMNRA writes details of calculations into the file SIMNRA.LOG, if *Logfile* is checked in the *Options* tab of *Setup:Calculation...*. RESOLNRA sets this switch, performs a calculation using SIMNRA, reads

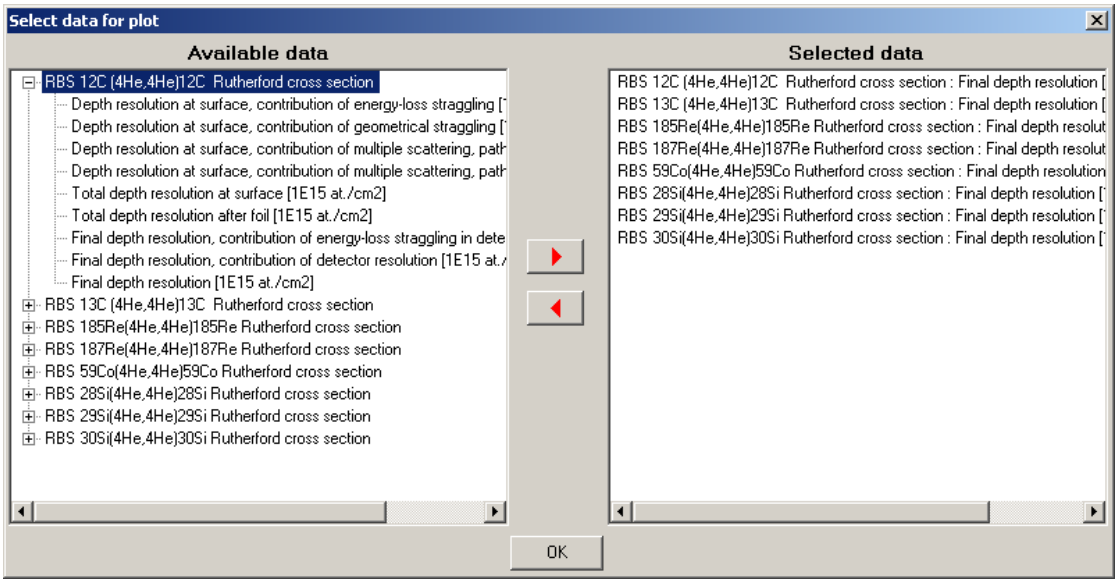

Figure 3.1.: The *Select Data* window allows to select the data for the plot. Usually the depth resolution for each isotope (and each reaction) and the different depth resolution contributions (energy loss straggling, geometrical straggling etc.) are available.

the SIMNRA.LOG file, calculates the depth resolution from the data, and displays it. In order to obtain the depth resolution as a function of incident energy or incident angle several SIMNRA calculations are performed. From a technical point of view, RESOLNRA is a post-processor for the SIMNRA log file.

3.3. *File* menu

In the *File* menu all necessary commands for reading and writing files and data, and terminating the program are located.

- *New*: Closes all windows and deletes all data from memory.
- *Open...*: Opens a nra-file. RESOLNRA opens the file and starts SIMNRA to perform the calculations. This may take a few seconds, depending on your computer hardware.
- *Write Data...*: The data from the active window are written to file. The file is in ASCII format and can be imported into graphics programs, such as Microsoft Excel or Microcal Origin. The data format depends on the active window content. For line graphs (*resolution as function of depth, resolution as function of angle, resolution as function of energy*) it is as follows:

  x_1 Data_1 x_2 Data_2 ...
  x_1 Data_1 x_2 Data_2 ...
  x_1 Data_1 x_2 Data_2 ...

x_1 is the x-scale for column Data_1, x_2 the x-scale for column Data_2, and so on. The x-scale depends on the active window and may be either depth (in 10^{15} Atoms/cm^2), or angle of incidence (in °), or incident energy (in keV).

For contour graphs (*resolution as function of energy and angle*) the data are in matrix format:

z_{11} z_{12} z_{13} ...
z_{21} z_{22} z_{23} ...
z_{31} z_{32} z_{33} ...

z_{12} is the resolution for the first energy and second angle value. The file created by *Write Data...* can be read into a Microcal Origin Matrix.

- *Exit*: Terminates RESOLNRA and the linked instance of SIMNRA.

3.4. *Edit* menu

- *Copy data*: Copies all data from the active window to the clipboard. These data can be pasted into any spreadsheet program such as Microsoft Excel or Microcal Origin. The data format depends on the active window content. For line graphs (*resolution as function of depth, resolution as function of angle, resolution as function of energy*) it is as follows:

  x_1 Data_1 x_2 Data_2 ...
  x_1 Data_1 x_2 Data_2 ...
  x_1 Data_1 x_2 Data_2 ...

  x_1 is the x-scale for column Data_1, x_2 the x-scale for column Data_2, and so on. The x-scale depends on the active window and may be either depth (in 10^{15} Atoms/cm^2), or angle of incidence (in °), or incident energy (in keV).

  For contour graphs (*resolution as function of energy and angle*) the data are in matrix format:

  z_{11} z_{12} z_{13} ...
  z_{21} z_{22} z_{23} ...
  z_{31} z_{32} z_{33} ...

  z_{12} is the resolution for the first energy and second angle value. These matrix data can be pasted into a Microcal Origin Matrix.

- *Copy page*: Copies the graph from the active window to the clipboard. From there it can be pasted into other programs, such as Microsoft Word or Microsoft PowerPoint.

3.5. *Calculate* menu

All depth-resolution calculations are performed through the *Calculate* menu. Calculations are always performed for all isotopes in the target, and the final depth resolution is displayed. The individual straggling contributions (energy loss straggling, geometrical straggling, multiple scattering etc.) can be displayed by selecting them in the *Plot:Select Data...* menu, see section 3.6.

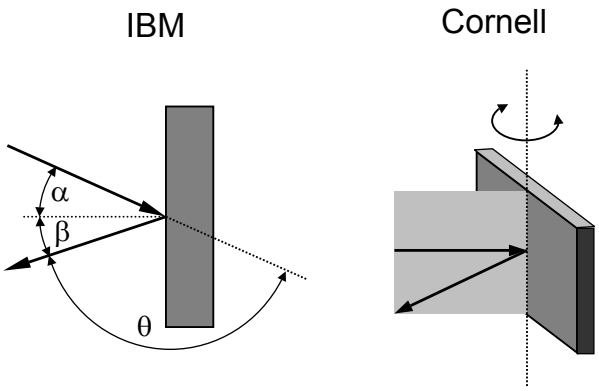

Figure 3.2.: IBM and Cornell geometries.

For most calculations you have to provide the scattering geometry, which may be either *IBM*, *Cornell* or *General* geometry. In *IBM geometry* the incident beam, exit beam and the surface normal are in the same plane, see Figure 3.2, and the exit angle β is simply given by

$$\beta = |180^\circ - \alpha - \theta|.$$

In *Cornell geometry* incident beam, exit beam and the sample rotation axis are in the same plane, and β is given by

$$\cos\beta = -\cos\theta\cos\alpha.$$

In *General geometry* there can be any relation between the three angles. Geometrical straggling cannot be calculated in general geometry.

- *Resolution as Function of Depth...*: Calculates the depth resolution as a function of depth for a specific incident energy and incident/exit angle combination.
- *Resolution as Function of Angle...*: Calculates the depth resolution at a specific depth and for a specific incident energy as function of incident angle. The geometry must be either IBM or Cornell.
- *Resolution as Function of Energy...*: Calculates the depth resolution at a specific depth and for a specific incident/exit angle combination as function of incident energy.
- *Resolution as Function of Energy and Angle...*: Calculates the depth resolution at a specific depth as function of incident energy and incident angle. The geometry must be either IBM or Cornell. The result is displayed as a 2-dimensional contour plot. A separate window is opened for each isotope.
- *Abort Calculation*: Aborts the current calculation.

3.6. *Plot* menu

The plot menu allows to select data for the plot and to change the appearance of the plot. Some plot-related commands are not accessible via menus. These commands are also described in this section.

- *Select Data*: The *Select Data* item allows to change the data content of the active window. The *Select Data* menu shows all available data and the data already selected for the active window.

  An example of the data window is shown in Figure 3.1. Available data are visible on the left hand side in the *Available data* tree. Available data are ordered by reaction. The right hand side *Selected data* shows the data which are selected for plotting in the graph. Select the *Available data* you want to see, and click  . The data are now placed in the *Selected data* tree. To delete data from the plot select the data in the *Selected data* tree and click  .

  You can select more than one data set by holding the CTRL or SHIFT keys while selecting: CTRL selects the clicked data set in addition to already selected data, while SHIFT selects all data sets between the last selected data and the currently selected.

  By selecting a node (a node contains sub-data and can be recognized by the ⊞ or ⊟ sign preceding it), all data belonging to the node will be selected automatically.

  The available data are described in chapter 4.

- *Rescale x-Axis*: Rescales the x-axis to maximum and minimum values.
- *Rescale y-Axis*: Rescales the y-axis to maximum and minimum values.
- *Rescale z-Axis*: This menu item is only meaningful for contour plots. It rescales the z-axis to maximum and minimum values.
- *x-Axis*: Allows to set the x-axis scale and axis format (linear or logarithmic axis, grid lines etc.). Same as a double-click with the left mouse button on the x-axis.
- *y-Axis*: Allows to set the y-axis scale and axis format (linear or logarithmic axis, grid lines etc.). Same as a double-click with the left mouse button on the y-axis.
- *z-Axis*: This menu item is only meaningful for contour plots. Allows to set the z-axis scale and axis format (linear or logarithmic axis, grid lines etc.).
- *Zooming into the plot:* To zoom into the plot click with the left mouse button into the upper left corner of the range you want to zoom in. Keep the mouse button down and tear a rectangle to the lower right corner of the zooming range.
- *Panning:* Click with the right mouse button into the plot, keep the mouse button down and move the mouse.
- *Zooming out:* Click with the left mouse button into the plot. Keep the mouse button down and move the mouse towards the upper left corner.

- *Information about a specific curve:* Double-click on any curve or contour line to get additional information about that curve.

3.7. *Window* menu

The *Window* menu allows to manipulate data windows.

- *Duplicate Window*: Duplicates the active window including all associated data. You can subsequently change the content of the window by clicking *Plot: Select data*, see section 3.6.
- *Close All Windows*: Closes all windows and deletes all associated data.

3.8. *Help* menu

- *User's Guide*: Shows the RESONRA User's Guide in pdf format.
- *About*: Information about the program.

4. Available data

The following data are available for each reaction and each isotope, either as function of depth, incident angle or incident energy. A reaction may be backscattering, creation of a recoil, or a nuclear reaction.

The depth resolution is obtained from the energy spread, measured in full width at half maximum (FWHM), and the effective stopping power, see chapter 5. The depth resolution is therefore always in FWHM. See [8, Section 2] for a discussion of this definition.

- *Depth resolution at surface, contribution of energy-loss straggling [1E15 at./cm2]*: Electronic energy-loss straggling of the outgoing particles at the target surface, i.e. after loosing energy in the target, but before penetrating the foil in front of the detector. The energy-loss straggling is converted to depth resolution in 10^{15} atoms/cm^2.

- *Depth resolution at surface, contribution of geometrical straggling [1E15 at./cm2]*: Geometrical straggling of the outgoing particles at the target surface, i.e. after loosing energy in the target, but before penetrating the foil in front of the detector. The geometrical straggling contribution is converted to depth resolution in 10^{15} atoms/cm^2.

- *Depth resolution at surface, contribution of multiple scattering, path in [1E15 at./cm2]*: Straggling due to multiple scattering at the target surface, i.e. after loosing energy in the target, but before penetrating the foil in front of the detector. Contribution of the incident path. The total straggling due to multiple scattering is obtained by quadratic addition of the straggling contributions on the path in and path out.

  Note: *Multiple scattering* in the *Setup:Calculation:Parameter* tab of SIMNRA must be checked in order to calculate multiple scattering. By default multiple scattering is not calculated.

- *Depth resolution at surface, contribution of multiple scattering, path out [1E15 at./cm2]*: Straggling due to multiple scattering at the target surface, i.e. after loosing energy in the target, but before penetrating the foil in front of the detector. Contribution of the outgoing path. The total straggling due to multiple scattering is obtained by quadratic addition of the straggling contributions on the path in and path out.

  Note: *Multiple scattering* in the *Setup:Calculation:Parameter* tab of SIMNRA must be checked in order to calculate multiple scattering. By default multiple scattering is not calculated.

- *Total depth resolution at surface [1E15 at./cm2]*: Total depth resolution at the target surface, i.e. after loosing energy in the target, but before penetrating the foil in front of the detector. The total depth resolution is obtained by quadratic addition of the contributions

by electronic energy-loss straggling, geometrical straggling, multiple scattering path in, and multiple scattering path out.

- *Total depth resolution after foil [1E15 at./cm2]*: Total depth resolution after penetrating the foil in front of the detector. *Total depth resolution after foil* consists of propagation of the *Total depth resolution at surface*, additional electronic energy-loss straggling in the foil, and energy straggling due to multiple scattering in the foil.
- *Final depth resolution, contribution of energy-loss straggling in detector [1E15 at./cm2]*: Electronic energy-loss straggling in the detector. This is zero for most detectors, except for thin solid-state detectors: in these detectors the particles may loose only a fraction of their energy in the detector. This energy loss is always accompanied by energy-loss straggling in the detector.
- *Final depth resolution, contribution of detector resolution [1E15 at./cm2]*: Contribution of the energy resolution of the detector to the final depth resolution.
- *Final depth resolution [1E15 at./cm2]*: Final depth resolution of the whole system, taking the depth resolution at the target surface, influence of absorber foil (if any), straggling in the detector (if any), and detector energy resolution into account. The *final depth resolution* is obtained by quadratic addition of the *total depth resolution after foil*, *contribution of energy-loss straggling in detector*, and *contribution of detector resolution*.

5. Depth resolution calculation

The effective stopping power S_{eff} can be defined by:

$$S_{eff} = \frac{dE}{dx},$$

with E the energy (which may be the particle energy at the surface, after the foil, or the detected energy) and x the depth of origin, i.e. the depth where the backscattering or nuclear reaction occurred. S_{eff} merges the stopping power of incident and outgoing particles (and the change of the initial energy for nuclear reaction products), so it is a book-keeping quantity rather than being directly connected with real physical quantities.

The depth resolution δx is then obtained from

$$\delta x = \frac{\delta E}{S_{eff}},$$

with δE the energy spread due to energy straggling or detector energy resolution. δE is the energy spread in full width at half maximum (FWHM), and correspondingly δx is the depth resolution in FWHM. See [8, Section 2] for a discussion of this definition.

6. Examples

This section gives some examples how RESOLNRA can be used for optimizing measurements by Rutherford backscattering (RBS), elastic recoil detection analysis (ERDA), and nuclear reaction analysis (NRA).

6.1. RBS

A thorough RBS-analysis of Co/Re multi-layers was performed by Barradas et al. in [1, 3], the full set of spectra is shown in [2]. The samples consisted of 16 layers of rhenium with a nominal thickness of 5 Å, separated by cobalt layers with a thickness of 20 Å. A 40–50 Å thick impurity layer of carbon was found at the surface. The samples were analyzed with a 1 MeV ^{4}He beam at a scattering angle of 160° in Cornell geometry at incident angles of 45°, 78°, 80°, 82°, 83° and 84°. The beam spot was 0.6×0.2 mm^2, with a detector aperture of 3 mm diameter at a distance of 70 mm. As was already shown in [1, 3], the layers showed some roughness which prevented to obtain the theoretically possible depth resolution. Nevertheless, the thorough and well designed measurements are an interesting test case for depth resolution optimizations. The surface roughness is neglected in the following.

The depth resolution for the isotope ^{187}Re in the 1st Re-layer is shown in Fig. Figure 6.1 as a function of incident angle and incident energy. The optimum depth resolution of about 6×10^{15} atoms/cm^2 is reached for incident energies of 800–4000 keV and incident angles of 86–87°. For angles above 87° the depth resolution degrades rapidly due to increasing geometrical straggling. The actual measurement was performed at 1000 keV/84° and reaches a theoretical resolution of about 8×10^{15} atoms/cm^2. Keeping the experimental difficulties at grazing angles in mind, this is as close to the theoretical optimum as is practically achievable.

The same as above, but for the 5th Re-layer is shown in Fig. Figure 6.2. The optimum depth resolution has now deteriorated to about 17×10^{15} atoms/cm^2 due to the additional energy broadening contributions by energy loss straggling and multiple scattering, and the optimum depth resolution is now obtained for incident energies of 1400–4000 keV and incident angles of 80–82°. The experiment reaches a theoretical resolution of about 20×10^{15} atoms/cm^2 – this is close to the theoretical optimum, but does not fully reach it. A simultaneous change of incident angle and energy would have provided a better depth resolution than the actually performed change of incident angle at fixed energy, and would have reduced the overlap between the Re and Co signals.

The energy independence of the optimum depth resolution over a larger incident energy range, as shown in Fig. Figure 6.2, may be surprising for many IBA practitioners: An often used rule-of-thumb for determining the incident energy is to set the energy of backscattered particles into the stopping-power maximum. The energy broadening contributions are shown in Fig. Figure 6.3

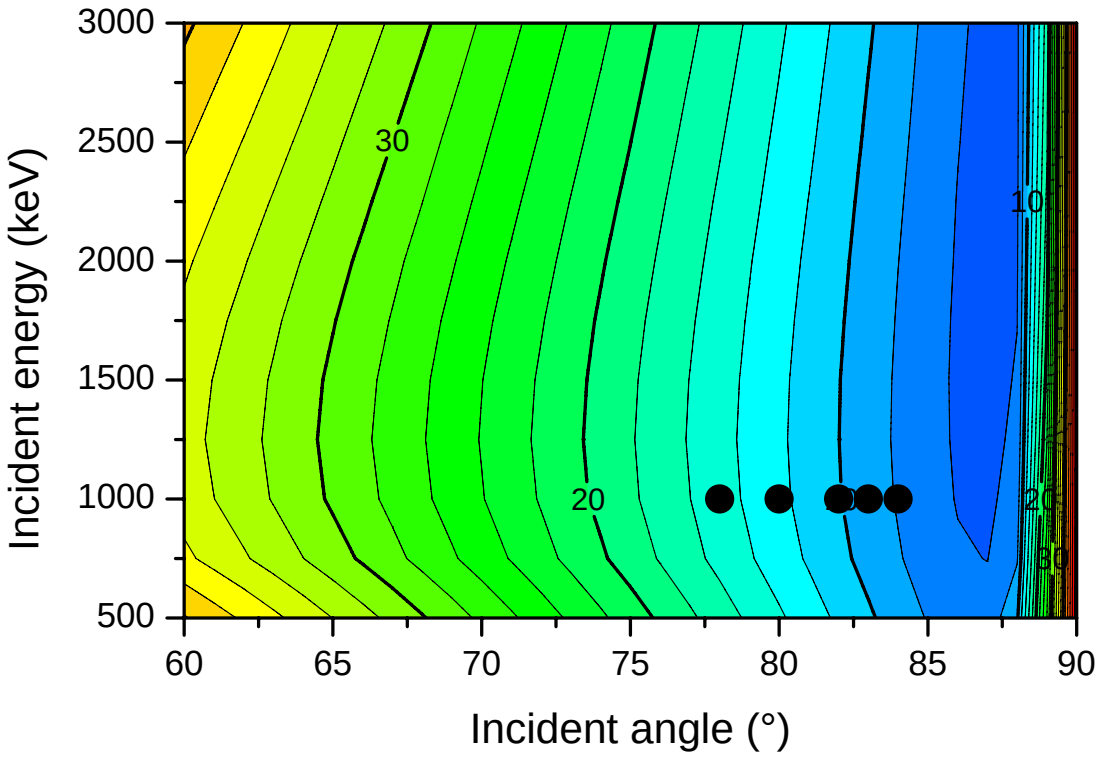

Figure 6.1.: Depth resolution for ^{187}Re (in 10^{15} atoms/cm^2) in the 1st Re-layer as a function of incident angle and incident energy. Black dots indicate angle/energy combinations, at which measurements were performed in [3].

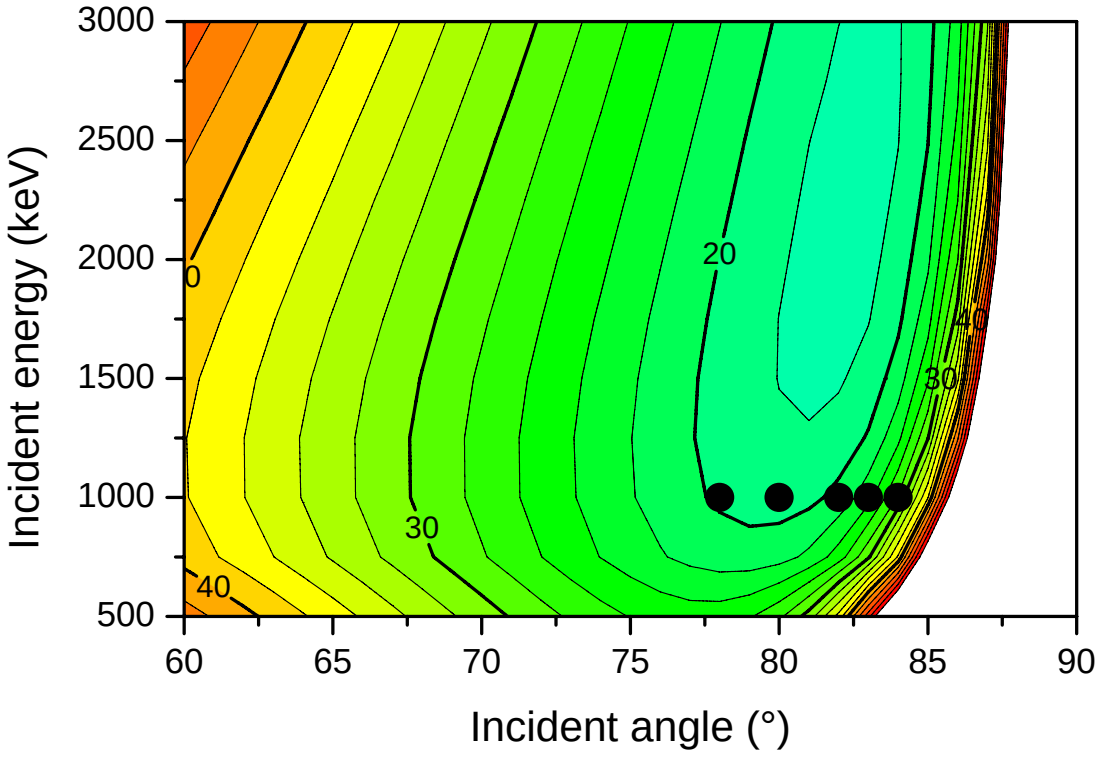

Figure 6.2.: Same as Fig. 6.1, but for the 5th Re-layer.

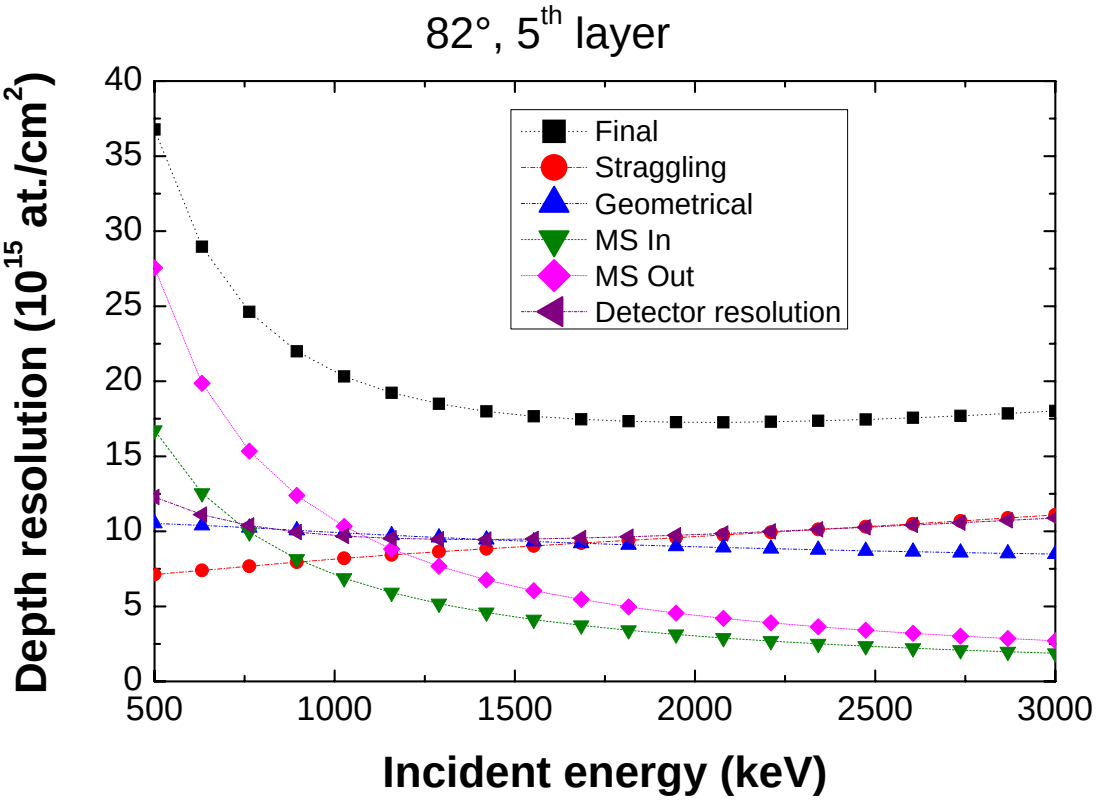

Figure 6.3.: Energy broadening contributions (transformed to depth resolution) for ^{187}Re in the 5th Re-layer at an incident angle of 82° as a function of incident energy. Final: Final depth resolution, taking all contributions into account; Straggling: Electronic energy loss straggling; Geometrical: Geometrical straggling; MS In: Multiple scattering on the incident path; MS Out: Multiple scattering on the outgoing path; Detector resolution: Contribution of detector resolution.

for an incident angle of 82°. The contribution of the detector resolution has a minimum at about 1300 keV due to the stopping power maximum, and increases for higher energies together with the energy-loss straggling contribution. This increase is counterbalanced by the decrease of the multiple-scattering contribution at higher energies together with geometrical straggling, thus resulting in an almost flat energy dependence of the depth resolution for 1300–3000 keV. This example shows, that simple rules-of-thumb are usually insufficient to obtain the optimum experimental conditions, and typically all energy broadening contributions have to be taken into account.

The depth resolution for ^{187}Re in the 5th Re-layer is shown in Fig. Figure 6.4 as a function of incident angle for 1000 keV incident energy. The contributions of detector resolution and energy loss straggling decrease with incident angle, while the contributions of multiple scattering and geometrical straggling increase with angle, resulting in an minimum at about 81°.

A possible optimization strategy for this type of samples would be to use an optimum angle/energy combination for each layer. In case of broad optima lower energies are advantageous

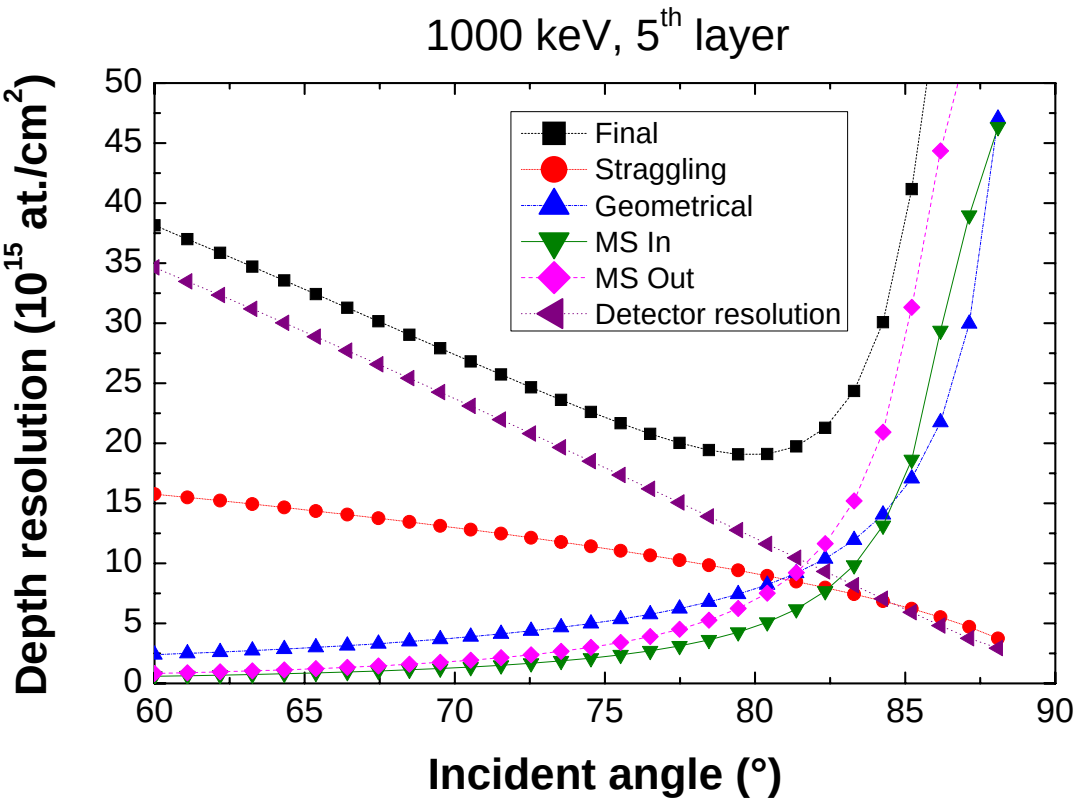

Figure 6.4.: Energy broadening contributions (transformed to depth resolution) for ^{187}Re in the 5th Re-layer at an incident energy of 1000 keV a function of incident angle. The abbreviations are identical to Fig. 6.3.

due to count statistics, and less grazing incident angles due to the possibility to use a wider beam and higher beam currents. It should be also kept in mind that the theoretically possible depth resolution may be not reached in practical applications due to surface roughness. The effects of surface roughness increase with increasing angle, thus favoring less grazing angles of incidence.

6.2. ERDA

ERDA with incident ^{4}He ions and a stopper foil is often used for depth profiling of hydrogen. We consider the example of H in an amorphous hydrocarbon layer with composition $C_{0.7}H_{0.3}$, recoil angle 30°, 0.5×1 mm^2 incident beam, 0.5×2 mm^2 detector aperture at a distance of 50 mm, 5.5 μm thick Ni-foil in front of the detector. This foil is thick enough to fully stop ^{4}He ions up to energies of about 3200 keV.

The depth resolution for a depth of 5×10^{17} at/cm^2 (about 50 nm) is shown in Fig. Figure 6.5. For very grazing incident or exit angles (i.e. close to 90° and 60°) the depth resolution deteriorates

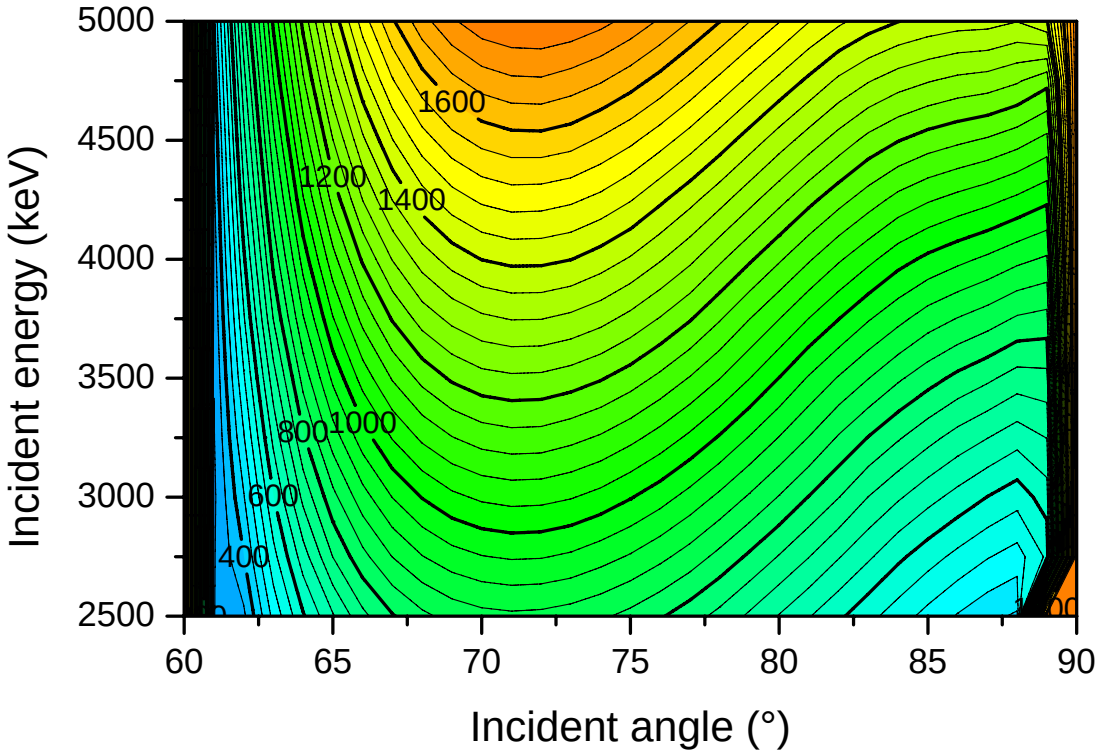

Figure 6.5.: Depth resolution (in 10^{15} atoms/cm^2) for ERDA using ^{1}H(^{4}He,^{1}H)^{4}He in $C_{0.7}H_{0.3}$ in a depth of 5×10^{17} at/cm^2.

quickly due to geometrical straggling and multiple scattering on the incident or exit paths. The optimum depth resolution is reached for an incident angle of 61°. This would result in an exit angle of 89°, which is almost impossible to reach in practical applications. The worst depth resolution is obtained for 72° at all energies: This is very close to the often used symmetric setup with 75° incident and exit angles. Although the shown result is only valid for the given geometry, target and depth, it should be noted that the symmetric experimental setup with identical incident and exit angles is often close to the worst possible solution. A tilt of the sample towards more grazing incidence or exit angles often provides better results.

6.3. NRA

Nuclear reaction analysis (NRA) and backscattering with non-Rutherford cross-sections often has an additional constraint: The incident projectiles should have a specific energy in the depth of interest, usually due to a maximum in the cross-section. For these cases we have to find the optimum energy/angle combination with the additional constraint, that the projectile energy should have a specific value in a given depth.

As example we consider carbon implanted into tungsten in a depth of 5×10^{17} at/cm^2, which is detected using the ^{12}C(^{3}He,p$_1$)^{14}N reaction at 165° scattering angle. This reaction has a

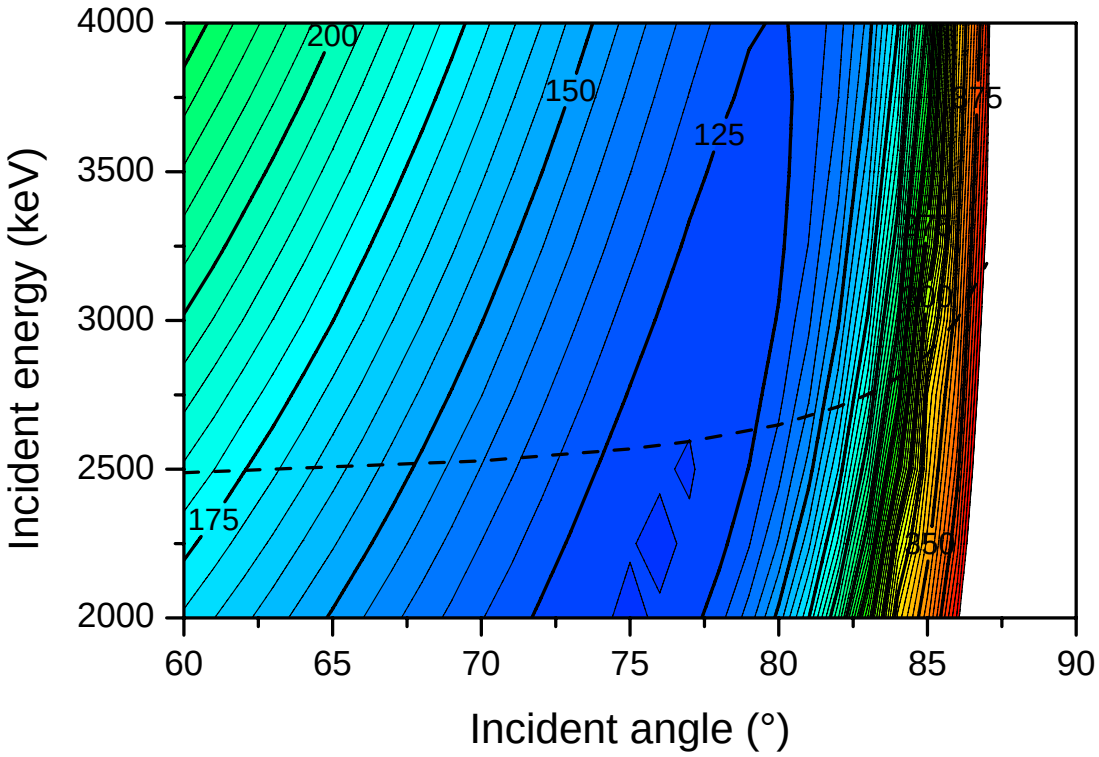

Figure 6.6.: Depth resolution for the $^{12}C(^3He,p_1)^{14}N$ reaction (in 10^{15} atoms/cm^2) as a function of incident angle and incident energy. ^{12}C is implanted in W into a depth of 5×10^{17} at./cm^2. Dashed line: Incident energy as function of incident angle, which gives a projectile energy of 2400 keV in a depth of 5×10^{17} at./cm^2.

maximum in the cross-section at about 2400 keV. The depth resolution as function of incident energy and angle is shown in Fig. Figure 6.6. There is a broad minimum of the depth resolution for incident angles from 72–77° and energies from 2000–3500 keV, providing a resolution of about 1.2×10^{17} at/cm^2. The dashed line is the incident energy, which results in a projectile energy of 2400 keV in a depth of 5×10^{17} at./cm^2, i.e. the incident energy which provides the maximum cross-section in the depth of interest. With the additional constraint of maximum cross-section in the depth of interest the optimum depth resolution is obtained for an incident angle of 76° at an incident energy of 2600 keV.

7. Acknowledgments

Helpful discussions with E. Szilágyi about the different straggling contributions and with N.P. Barradas about the experimental difficulties at grazing angles are gratefully acknowledged. The OLE automation methods were introduced as result of various discussions with K. Schmid (Max-Planck-Institut für Plasmaphysik, Garching, Germany).

Valuable bug reports were obtained from Martin Oberkofler (Max-Planck-Institut für Plasmaphysik, Garching, Germany).

A. OLE automation reference

This section describes OLE 2.0 automation support in RESOLNRA. RESOLNRA is an OLE automation server, which allows other applications to control RESOLNRA. This is useful for example for developing new applications, which need information about the depth resolution. A short overview of the OLE objects and methods is given below, for a complete description of the parameters associated with OLE automation methods see Appendix A.

A.1. Programming overview

RESOLNRA does not perform any calculations by itself. All calculations are performed by a (usually hidden) instance of SIMNRA, which is controlled by RESOLNRA using the OLE automation objects exported by SIMNRA. SIMNRA writes its calculation results to the file SIMNRA.LOG, which is subsequently read and interpreted by RESOLNRA. All depth resolutions are extracted from the data contained in this file.

The *Resolnra.App* object allows to control RESOLNRA (hiding, maximizing, minimizing, etc.), and allows to open data files and perform depth resolution calculations.

All depth resolutions are available through the *Resolnra.DepthResolutions* object. The number of available depth resolution data sets is contained in the *Count* property, the *Reaction* and *Title* methods provide textual information about each depth resolution data set. A depth resolution data set consists of nodes, i.e. x-y values, with the depth as x-value and the corresponding depth resolution as y-value. The number of nodes is available by the *NodeCount* method, node values are accessible with the *NodeDepth* and *NodeResolution* methods. RESOLNRA uses linear interpolation between the node values. There are, however, some complications: The depth resolution is a discontinuous function, with discontinuities at layer boundaries. At a layer boundary the depth resolution may have two values, and if an element or isotope is not present in a layer, then depth resolution information is not available for that layer (and linear interpolation based on adjacent layers has to be definitely avoided). The presence of discontinuities between individual nodes is indicated by the *Break* method. The *Resolution* method takes discontinuities into account and offers the easiest way to access the depth resolution.

A.2. Objects

RESOLNRA exports the following OLE automation objects:

- *Resolnra.App* — The application itself.
- *Resolnra.DepthResolutions* — Depth resolutions for all reactions of all isotopes contained in the target.

A.3. Properties and methods

RESOLNRA exports the following OLE automation properties and methods, grouped by object:

A.3.1. Resolnra.App

- *BringToFront* — Brings RESOLNRA to the front above all other applications.
- *BringToRear* — Brings RESOLNRA behind all other applications.
- *FileName* — Name of the currently used nra- or xnra-file.
- *Hide* — Hides RESOLNRA.
- *Maximize* — Maximizes RESOLNRA to fill the whole screen.
- *Minimize* — Minimizes RESOLNRA to the Windows task bar.
- *OLEUser* — Specifies which program controls the current RESOLNRA instance.
- *Open* — Opens a nra- or xnra-file and calculates all depth resolutions.
- *Restore* — Restores the minimized application to its normal size.
- *Show* — Shows RESOLNRA, if it was hidden.

A.3.2. Resolnra.DepthResolutions

- *Count* — Number of available depth resolutions. Usually one depth resolution is available for each reaction of each isotope.
- *NodeBreak* — Indicates if a break (i.e. a discontinuity in the depth resolution) appears at a specif node. Breaks appear for example at all layer boundaries.
- *NodeCount* — Number of nodes for a specific depth resolution data set.
- *NodeDepth* — Depth value of a specific node.
- *NodeResolution* — Depth resolution value of a specific node.
- *Reaction* — Name of the reaction of a specific depth resolution data set, for example 'RBS 12C(1H,1H)12C Rutherford cross section'.
- *Resolution* — Depth resolution for a specif reaction in a specific depth.
- *Title* — Title of a specific depth resolution data set, for example 'RBS 12C(1H,1H)12C Rutherford cross section : Final depth resolution [1E15 at./cm2]'.

A.4. Data types

RESOLNRA is written in Borland Delphi and uses only automation compatible data types. The data types used by Delphi, the corresponding types in Microsoft's Interface Definition Language IDL, and the corresponding types used in Variants are summarized below.

Delphi type	**I**DL type	**V**ariant type	**D**escription
Boolean	VARIANT_BOOL	VT_BOOL	True = -1, False = 0
Double	double	VT_R8	8-byte real
Integer	long	VT_I4	4-byte signed integer
WideString	BSTR	VT_BSTR	binary string

A.5. Resolnra.App

The *Resolnra.App* object represents the application itself.

A.5.1. Properties

FileName

[Get] Property FileName : WideString;

Description

Name of the currently used nra- or xnra-file including full path. *FileName* is readonly. If you want to change *FileName*, you have to open a file.

Related Properties and Methods

App.Open 26

OLEUser

[Get/Set] Property OLEUser : WideString;

Default Value

"

Description

Calling *CreateOLEObject('Resolnra.App')* will return a pointer to an already running instance of RESOLNRA, if one or more instances of RESOLNRA are already active: This may result in problems, if RESOLNRA is controlled by two (or more) OLE clients simultaneously. *OLEUser* allows to determine if RESOLNRA is already controlled by a user or by a different OLE client.

OLEUser returns

User	RESOLNRA was invoked by a user
ProgramName	Name of the program controlling RESOLNRA
”	The RESOLNRA instance is not controlled by a user or by a different program

The following code creates a new instance of RESOLNRA:

```
var
  RESOLNRA : Variant;
begin
  repeat
    RESOLNRA := CreateOLEObject(Resolnra.App');
  until RESOLNRA.OLEUser = ”;
  RESOLNRA.OLEUser := 'MyProgramName';
end;
```

It has to be noted that RESOLNRA is not able to detect by itself if it is controlled by an OLE client or not. If your program controls RESOLNRA then you should set *OLEUser* to the name of your program as shown in the code fragment above.

A.5.2. Methods

BringToFront

Procedure BringToFront;

Description

Brings RESOLNRA to the front above all other applications.

Parameters

None

Return Value

None

Related Properties and Methods

App.BringToRear 24
App.Minimize 25

BringToRear

Procedure BringToRear;

Description

Brings RESOLNRA to the rear behind all other applications.

Parameters

None

Return Value

None

Related Properties and Methods

App.BringToFront 23
App.Minimize 25

Hide

Procedure Hide;

Description

Hides RESOLNRA. The program is still running, but not visible.

Parameters

None

Return Value

None

Related Properties and Methods

App.Minimize 25
App.Show 26

Maximize

Procedure Maximize;

Description

Maximizes RESOLNRA to fill the whole screen. RESOLNRA must be visible, i.e. not minimized or hidden, otherwise *Maximize* has no effect.

Parameters

None

Return Value

None

Related Properties and Methods

App.Minimize 25

Minimize

Procedure Minimize;

Description

Minimizes RESOLNRA to the Windows task bar.

Parameters

None

Return Value

None

Related Properties and Methods

App.Maximize 25
App.Restore 26
App.BringToFront 23

Open

Function Open(FileName : WideString) : Boolean;

Description

Opens an XNRA, NRA or IDF-file and calculates all depth resolutions. RESOLNRA will try to determine the format of the file automatically from the file extension.

Parameters

FileName The name of the file including path. Allowed file extensions are:

nra	NRA file format, as used by SIMNRA 6 and earlier.
xnra	XNRA file format, as used by SIMNRA 7 and later.
idf, xml	IBA data format (IDF).

Return Value

Returns *true* if the file was opened successfully and the depth resolution calculation succeeded.

Restore

Procedure Restore;

Description

Restores the minimized application to its normal size.

Parameters

None

Return Value

None

Related Properties and Methods

App.BringToFront 23
App.Minimize 25

Show

Procedure Show;

Description

Shows RESOLNRA, if it was hidden.

Parameters

None

Return Value

None

Related Properties and Methods

App.Hide 24

A.6. ResolnraDepthResolutions

The *ResolnraDepthResolutions* object allows access to all calculated depth resolutions. See section A.1 for a short overview of the data structures and methods.

A.6.1. Properties

Count

[Get] Property Count : Integer;

Description

Number of available depth resolution data sets. Usually one depth resolution is available for each reaction of each isotope in the target. *Count* is readonly.

A.6.2. Methods

NodeBreak

Function NodeBreak(Index, NodeIndex : Integer) : Boolean;

Description

Indicates if a break (i.e. a discontinuity in the depth resolution) appears between the nodes with indexes *NodeIndex* and *NodeIndex + 1*. Breaks appear for example at all layer boundaries.

Parameters

Index Index number of the depth resolution data set. 1 ≤ Index ≤ Count.

NodeIndex Index number of the node. 1 ≤ NodeIndex ≤ NodeCount.

Return Value

True, if a break appears between the nodes with indexes *NodeIndex* and *NodeIndex + 1*.

Related Properties and Methods

DepthResolutions.Count 27
DepthResolutions.NodeCount 28
DepthResolutions.NodeDepth 28
DepthResolutions.NodeResolution 29

NodeCount

Function NodeCount(Index : Integer) : Double;

Description

Number of nodes in the depth resolution data set with index *Index*.

Parameters

Index Index number of the depth resolution data set. 1 ≤ Index ≤ Count.

Return Value

Number of nodes in the depth resolution data set with index *Index*.

Related Properties and Methods

DepthResolutions.Count 27
DepthResolutions.NodeCount 28
DepthResolutions.NodeDepth 28
DepthResolutions.NodeResolution 29

NodeDepth

Function NodeDepth(Index, NodeIndex : Integer) : Double;

Description

Depth value of node with index *NodeIndex*.

Parameters

Index	Index number of the depth resolution data set. 1 ≤ Index ≤ Count.
NodeIndex	Index number of the node. 1 ≤ NodeIndex ≤ NodeCount.

Return Value

Depth value of the node with node index *NodeIndex*. In 10^{15} atoms/cm^2.

Related Properties and Methods

DepthResolutions.Count 27
DepthResolutions.NodeCount 28
DepthResolutions.NodeDepth 28
DepthResolutions.NodeResolution 29

NodeResolution

Function NodeResolution(Index, NodeIndex : Integer) : Double;

Description

Depth resolution value of node with index *NodeIndex*.

Parameters

Index	Index number of the depth resolution data set. 1 ≤ Index ≤ Count.
NodeIndex	Index number of the node. 1 ≤ NodeIndex ≤ NodeCount.

Return Value

Depth resolution value of node with node index *NodeIndex*. In 10^{15} atoms/cm^2 FWHM.

Related Properties and Methods

DepthResolutions.Count 27
DepthResolutions.NodeCount 28
DepthResolutions.NodeDepth 28
DepthResolutions.NodeResolution 29

Reaction

Function Reaction(Index : Integer) : WideString;

Description

Name of the reaction of depth resolution data set with index *Index*, for example 'RBS 12C(1H,1H)12C Rutherford cross section'.

Parameters

Index Index number of the depth resolution data set. $1 \leq \text{Index} \leq \text{Count}$.

Return Value

Name of the reaction of depth resolution data set with index *Index*.

Related Properties and Methods

DepthResolutions.Count 27
DepthResolutions.Title 31

Resolution

Function Resolution(Index : Integer; Depth : Double) : Double;

Description

Depth resolution in depth *Depth* of the depth resolution data set with index *Index*.

Parameters

Index Index number of the depth resolution data set. $1 \leq \text{Index} \leq \text{Count}$.

Depth Depth of the requested depth resolution. In 10^{15} atoms/cm^2.

Return Value

Depth resolution in the depth *Depth*. In 10^{15} atoms/cm^2 FWHM.
The result is zero, if *Index* < 1, if *Index* > *Count*, or if the reaction *Index* does not occur in depth *Depth* (because the isotope is not present in that depth, or because its concentration is zero). At layer boundaries the depth resolution is discontinuous and may have two values, if an element or isotope is present in both layers: In that case there is one depth resolution value in the first layer, and another depth resolution value in the adjacent layer. In that case *Resolution* returns the average of both values.

Related Properties and Methods

DepthResolutions.Count 27

Title

Function Title(Index : Integer) : WideString;

Description

Title of the depth resolution data set with index *Index*, for example 'RBS 12C(1H,1H)12C Rutherford cross section : Final depth resolution [1E15 at./cm2]'.

Parameters

Index	Index number of the depth resolution data set. $1 \leq \text{Index} \leq \text{Count}$.

Return Value

Title of the depth resolution data set with index *Index*.

Related Properties and Methods

DepthResolutions.Count 27
DepthResolutions.Reaction 30

A.7. Error handling

If RESOLNRA is run as stand alone application, i.e. not as OLE server, it reports errors by showing message boxes with error messages or warnings, and program execution is stopped until the *OK* button of the message box is pressed by the user. This behaviour is reasonable for an interactive application, but it is not wishful for an OLE server: The server is controlled by another application or script, and the display of a message box to a script is useless. Therefore, if RESOLNRA is running as server, it handles errors in a different way: Message boxes are suppressed and program execution continues, even if an error is encountered. The error is reported by an error flag as return value of the routine which produced it. The text of the last error message can be retrieved with *App.LastMessage*.

This behaviour can be changed by setting *App.ShowMessages = true*: In this case error messages will be shown as message boxes, and program execution is stopped until the *OK* button of the box is pressed. RESOLNRA is able to detect if it is running as stand alone application or as server, and *App.ShowMessages* is set to *false* automatically, if invoked as server.

The following code in Visual Basic Script shows the use of the error handling routines:

```
' Create the application object
Set App = CreateObject("Resolnra.App")

' Wait 1000 ms: May be necessary for the server to start
WScript.Sleep 1000

' Open a XNRA-file
Success = App.Open("c:\temp\test.xnra")

' Some error reported by App.Open: Display last error message and exit
If Not Success Then
WScript.Echo App.LastMessage
Exit
End If
```

Bibliography

[1] N.P. Barradas. "Fitting of RBS Data including Roughness: Application to Co/Re multilayers". In: *Nucl. Instr. Meth. B* 190 (2004), p. 247 (cit. on p. 12).

[2] N.P. Barradas, K. Arstila, G. Battistig, M. Bianconi, N. Dytlewski, et al. "International Atomic Energy Agency intercomparison of ion beam analysis software". In: *Nucl. Instr. Meth. B* 262 (2007), p. 281. DOI: 10.1016/j.nimb.2007.05.018. eDoc: http://edoc.mpg.de/319840. URL: http://home.mpcdf.mpg.de/~mam/Barradas-Nuclear-Instruments-Methods-B-262-(2007)-281.pdf (cit. on p. 12).

[3] N.P. Barradas, J.C. Soares, M.F. da Silva, F. Pászti, and E. Szilágyi. "Study of multilayer substrate surface roughness using RBS with improved depth resolution". In: *Nucl. Instr. Meth. B* 94 (1994), p. 266 (cit. on pp. 12, 13).

[4] M. Mayer. *SIMNRA: Simulation of RBS, ERD and NRA spectra.* http://www.simnra.com (cit. on p. 1).

[5] M. Mayer. *SIMNRA User's Guide.* Tech. rep. IPP 9/113. Garching: Max-Planck-Institut für Plasmaphysik, 1997. URL: http://home.mpcdf.mpg.de/~mam/Report%20IPP%209-113.pdf (cit. on p. 1).

[6] M. Mayer. "SIMNRA, a Simulation Program for the Analysis of NRA, RBS and ERDA". In: *Proceedings of the 15th International Conference on the Application of Accelerators in Research and Industry.* Ed. by J. L. Duggan and I.L. Morgan. Vol. 475. AIP Conference Proceedings. Woodbury, New York: American Institute of Physics, 1999, p. 541. DOI: 10.1063/1.59188. URL: http://home.mpcdf.mpg.de/~mam/Mayer-AIP-Conference-Proceedings-475-(1999)-541.pdf (cit. on p. 1).

[7] M. Mayer. "RESOLNRA: A new program for optimizing the achievable depth resolution of ion beam analysis methods". In: *Nucl. Instr. Meth. B* 266 (2008), p. 1852. DOI: 10.1016/j.nimb.2007.11.071. eDoc: http://edoc.mpg.de/319936. URL: http://home.mpcdf.mpg.de/~mam/Mayer-Nuclear-Instruments-Methods-B-266-(2008)-1852.pdf (cit. on p. iii).

[8] E. Szilágyi, F. Pászti, and G. Amsel. "Theoretical approximations for depth resolution calculations in IBA methods". In: *Nucl. Instr. Meth. B* 100 (1995), p. 103. DOI: 10.1016/0168-583X(95)00186-7 (cit. on pp. 9, 11).