

TLA2L
Calculation Tool for Estimation of Depth Profile
for Thin Layer Activation
(TLA)

Sándor Takács
Institute of Nuclear Research of the
Hungarian Academy of Sciences
stakacs@atomki.hu
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Application of TLA technique is divided into two main steps i.e. *activation* and *measurement* of activity. A calculation tool TLA2L.xls was developed to help planning of irradiation and calculating the amount of wear from the measured activity. The calculation tool requires MS Excel XP or higher version to run. The user can select items from lists and need to type in the required input parameters while the results are presented in the corresponding result cells and figures.

TLA2L is intended to replace the calculation package: TLAPrfl, described in documentation series of IAEA, IAEA-NDS-192, September 1999.

Planning irradiation in 6 steps

Step 1: *Selection of nuclear reaction*

The list of possible nuclear reactions is determined by the composition of the matrix and the type and energy of the available bombarding beams. Generally one of the available reactions on the main component of the matrix should be selected. The reaction can be selected from a list.

Step 2: *Selection of irradiation mode*

Irradiation mode can be selected from a two-component list according to the desired activity distribution for producing quasi constant or quasi linearly decreasing activity depth profile.

Step 3: *Introducing the parameters of matrix*

The built in routines calculates the stopping power not only for pure chemical elements but for a complex matrix material with combination of maximum 10 components. From the given composition of the matrix its density is approximated. There is an option to introduce the value of known density and replace the calculated one when they disagree.

Step 4: *Selection of bombarding energy*

Default bombarding energies are built into the calculation tool for both irradiation types. The proposed energy can be changed according to the requirements. The resulting activity depth profile is presented in the corresponding figure. The depth

profile calculation routine uses the built in stopping power calculator and cross section data of the selected nuclear reaction.

Step 5: *Selection of other irradiation parameters*, beam intensity, irradiation time and irradiation angle.

Adjusting the irradiation time, beam intensity and irradiation angle one can change the value of specific activity on the surface as well as the total activity of the chosen radioisotope.

Step 6: *Checking the calculated depth profile* of the produced isotope

After setting all the parameters the calculated depth profile can be seen in a figure and if necessary can be modified by repeating the above steps 1 - 5. The activity distribution of other possible longer lived radioisotopes produced simultaneously in the matrix also shown in the figure for comparison. Their ratio to the main isotope can be adjusted by changing the applied cooling time.

Application of TLA technique requires a good control and reproduction of irradiation conditions. Errors may arise from instability of bombarding energy and uncertain irradiation geometry.

Activity measurements

The wear rate of friction surfaces can be determined via the change of the activity caused by loss of material. It is essential to separate and trap the removed activity at a shielded place in order to avoid the influence of the measurement of the remaining activity. When the circumstances allow one can measure both part of the activity, the activity of removed and collected wear debris and the remaining activity of the investigated parts. This way the uncertainty of the measurement can be decreased.

Reference measurement

As the first step it is necessary to perform a reference measurement in order to determine the reference activity of the investigated part in the given geometry at the beginning of the wear study. The calculation tool provides help to determine the activity from the primary spectrometry data (peak area, measuring time, detector efficiency and decay data of the radionuclide).

Activity measurements for wear rate

The calculation tool provides help to determine the wear rate via the measured activity by introducing the primary spectrometry data (peak area, measuring time, detector efficiency and decay data of the radionuclide). The measure of the wear can be calculated from both parts of the measured activities, activity of the removed particles and activity of the remaining part.

Step-by-step help on the use of the calculation tool

The calculation tool is prepared in MS Excel, therefore the user should have basic knowledge about how to work in Excel.

The TLA2L tool was created in a single Excel workbook with several sheets in it. The sheets containing data and formulas for calculations are hidden and password protected. Only two sheets can be reached by the users these are named as "Input" and "Figs".

The Input sheet is divided into three sections: irradiations, reference activity measurements and wear determination. This sheet contains cells for input parameters as well as cells for the calculated results.

The Figs sheet contains figures with the calculated depth profiles at EOB and after cooling time. The changes of activities of radionuclides produced in the main and secondary nuclear reactions are compared in time and presented on figures.

A short description is given below for each selectable parameter and result cells and figures of the TLA2L calculation tool. Both sheets are protected, therefore only contents of certain cells can be selected and modified. The selectable white background cells are to introduce data and cells with colored background are for the results of the calculation or giving information.

The figures show the calculated results, depth profile, activity, ratio of activity according to the actual selected parameters in the *Irradiation* part.

For quick help there are comments attached to certain cells that can be made visible by placing the pointer over the cell.

Input Sheet

Section: Irradiation

Main reaction: By clicking on the cell it provides a list of reaction from which one can be selected by clicking on it. Selecting a reaction the type of bombarding particle, the produced radionuclide and the main matrix component are also selected.

Mode: By clicking on the cell “Constant” or “Linear” can be selected from a list according to the desired activity depth profile. By selecting the activation mode a default bombarding energy is also suggested that can be override by typing other value into the energy input cell.

Irradiation time: Input for irradiation time in unit of hour.

Beam current on target: The beam intensity reaches the target after collimation in unit of micro Amperes.

Geometry factor: This factor applies for any correction arising from the irradiation geometry, target enrichment or other parameters. Value can be in the interval (0,1).

Tolerance: Measure of allowed deviation of the linear fit approximation from the actual calculated depth distribution in percentage.

Irradiation angle: Direction of the bombarding beam to the irradiated surface in unit of degree.

Selected bombarding energy: One can select bombarding energy different from the suggested one. In this case this selected energy is applied in the calculations. Leaving this cell empty or typing zero result in the use of suggested bombarding energy. The unit of the energy is MeV.

Matrix density: In the first position the density of the matrix calculated as weighted average of the density of the individual matrix components is given. The calculated density can be different from the actual one because of the structure of the matrix. In that case value of the actual density should be given in the second cell in unit of g/cm^3 , otherwise that cell should be empty.

Matrix components: Up to 10 different matrix components can be introduce by typing the chemical symbol of the element and its weight proportion in percentage. As default the first component of the matrix is selected by selecting the nuclear reaction. If necessary its weight proportion can be adjusted.

Produced isotope: The value is selected by selecting the main reaction.

Activity values are calculated at EOB (end of bombardment) and at a given cooling time. The actual calculated values are listed under “EOB” and “Cooling” respectively.

Cooling time: Can be any positive value in unit of day. The selected cooling time is applied for the activity calculation of the main radioisotope as well as for the other

possible radionuclide. Its effect can be seen in the corresponding result cells and also in the figure. Obviously zero cooling time gives the activity values at EOB.

Total activity: Gives the total activity of the main radionuclide produced with the actual irradiation parameters in unit of kBq. Activity of other radionuclide produced in side reactions is not included.

Activity of the constant/linear layer: Gives the activity of that part of the activated zone that can be approximated by a linear fit within the given tolerance as constant or linear (according to the selected activation mode) starting from the surface. Unit is kBq. Description of the cell is changing according to the selected irradiation mode

Specific activity on the surface: Gives the specific activity in kBq/microns unit calculated from the fit of the depth profile. The fit is described by an $A=ax+b$ type linear equation.

Thickness of the constant/linear activity layer: Gives the thickness of the surface layer in unit of microns in which the depth profile can be approximated by an $A=ax+b$ function.

Free level activity: Information about the amount of activity (upper limit in kBq units) of the produced radioisotope that can be handled freely.

Half life: The half life of the produced radionuclide in unit of day.

Gamma line energy: The energy of the most intense gamma line of the produced isotope.

Gamma abundance: The branching ratio of the most intense gamma line used by default in the calculations.

Range of particle: Distance in which the bombarding particle stops in the matrix measured along the path of the particles in units of microns.

Activation depth: Gives the depth in which the activation takes place measured perpendicular to the irradiated surface in units of microns.

Fitting parameter a : Parameter of the $A=ax+b$ fit.

Fitting parameter b : Parameter of the $A=ax+b$ fit.

Figure: The figure shows the depth profile generated with the actual selected irradiation parameters. The solid thick red line indicates the activity depth profile of the produced main radionuclide. The solid thick blue line corresponds to the linear fit. The dashed lines indicate the validity of the fit. The thin solid lines indicate the activity distribution of other radionuclide produced simultaneously. The values of the fitting parameters are also shown in the figure. Data presented in the figure always represent the values calculated for the applied cooling time.

Section: Reference activity measurement

Main reaction: Value is set in the *Irradiation* section

Stop of irradiation: Date and time information of the end of bombardment (EOB) in format: mm/dd/yy hh:mm:ss. This data is optional, if not given (empty cell) no EOB activity is calculated.

Start of reference measurement: Date and time information of start of reference activity measurement in format: mm/dd/yy hh:mm:ss.

Live time: The live time of the measurement in seconds.

Real time: The real time of the measurement in seconds.

Peak area of gamma line: The net peak area of the measured gamma line in counts. The gamma line can be the default gamma line given in the irradiation section or any other user selected gamma line can be introduced in this section.

Area error: Statistical error of the net peak area of the gamma line in counts.

Detector efficiency: Detector efficiency of the used gamma line, including geometry.

Uncertainty of detector efficiency: Uncertainty of the detector efficiency for the used gamma line given in percentage.

Beam current and geometry factor uncertainty: Uncertainty of the beam current including uncertainty due to possible collimation ambiguity and beam positioning.

Other gamma line energy: Energy of an optional gamma line in unit of keV that can be used if measurement of the default gamma line is not convenient or some reason is impossible.

Gamma abundance: The branching ratio of the selected optional gamma line used in the calculations instead of the default one.

Measured activity at EOB: Activity of the main radionuclide calculated from the measured peak area in units of kBq. When time information is not given for the stop of irradiation this field has “no data” message.

Measured activity at reference date: Total activity of the main radionuclide calculated at reference date in kBq units.

Activity in the constant (linear) layer at ref. date: Partial activity of the main radionuclide measured in the surface layer that can be approximated as constant (linearly decreasing) given in unit of kBq at the reference date.

Specific activity on the surface at reference date: Specific activity of the main radionuclide determined from the linear fit at the edge of the irradiated volume at reference date given in unit of kBq/microns.

Uncertainty of measured activities: Uncertainty of above activities given in percentages.

Uncertainty of nuclear data: Overall uncertainty of nuclear data including cross section and decay parameter uncertainties.

Uncertainty of stopping power: An average of 10% uncertainty is given on the stopping power.

Section: Wear measurement

Activity measurements of removed wear debris:

Start of measurement, removed: Start of activity measurement of the removed and collected wear debris, in format: mm/dd/yy hh:mm:ss.

Live time: The live time of the measurement in seconds.

Real time: The real time of the measurement in seconds.

Peak area of gamma line: The net peak area of the measured gamma line in counts. The gamma line can be the default gamma line given in the irradiation section or any other user selected gamma line given in “Reference activity measurement” section.

Area error: Statistical error of the net peak area of the gamma line in counts.

Detector efficiency: Detector efficiency of the used gamma line, including geometry.

Uncertainty of detector efficiency: Uncertainty of the detector efficiency for the used gamma line given in percentage.

Activity of the removed layer at ref. date: Activity of the main radionuclide measured in the removed layer in unit of kBq at the reference date.

Thickness of removed layer: Thickness of the removed layer calculated from the measured activity in units of microns using the linear fit of the calibration curve.

Uncertainty: Uncertainty of the thickness given in percentages.

Measurements of remaining activity:

Start of measurement, remaining: Start of activity measurement of the activated machine part, in format: mm/dd/yy hh:mm:ss.

Live time: The live time of the measurement in seconds.

Real time: The real time of the measurement in seconds.

Peak area of gamma line: The net peak area of the measured gamma line in counts. The gamma line can be the default gamma line given in the irradiation section or any other user selected gamma line given in “Reference activity measurement” section.

Area error: Statistical error of the net peak area of the gamma line in counts.

Detector efficiency: Detector efficiency of the used gamma line, including geometry.

Uncertainty of detector efficiency: Uncertainty of the detector efficiency for the used gamma line given in percentage.

Activity of the remaining layer at ref. date: Activity of the main radionuclide measured in the remaining layer in unit of kBq at the reference date.

Thickness of removed layer: Thickness of the removed layer calculated from the measured activity in units of microns.

Uncertainty: Uncertainty of the thickness given in percentages.

Figs Sheet

The sheet **Figs** contains the following four figures:

Figure 1.

Solid red line: Specific activity of the main radionuclides produced in the selected nuclear reaction.

Solid blue line: Linear fit of specific activity

Dashed lines: Validity of the fit

Figure 2.

Solid red line: Specific activity of the main radionuclides produced in the selected nuclear reaction at EOB.

Solid blue line: Linear fit of specific activity

Dashed lines: Validity of the fit

Thin lines: Specific activity of the secondary radionuclides produced in the side nuclear reactions after cooling.

Figure 3.

Changes of relative specific activity in time of the produced radionuclides compared to the activity of the main radionuclide can be measured on the surface.

Figure 4.

Changes of specific activity in time of the produced radionuclides can be measured on the surface.