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Handling material in **TRACER** for groups and individuals

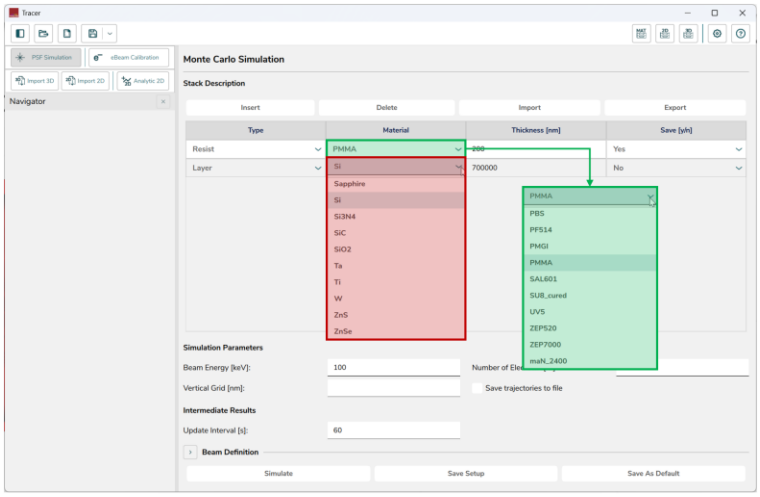
TRACER is a front-end graphical user interface (GUI) for managing and creating point spread functions (PSFs) for electron scattering.

The point spread function (PSF) describes the energy deposited into a resist layer as a function of distance from the beam incident position. This energy spread is largely dependent on the substrate material and beam energy. The primary function of **TRACER** is to compute the PSF for a given stack of materials and beam conditions using the Monte Carlo simulation method. Describing the beam conditions and running a Monte Carlo simulation is straightforward.

In this Application Note, we will concentrate on the stack definition, material archive generation, and how to handle materials for groups and individual usages.

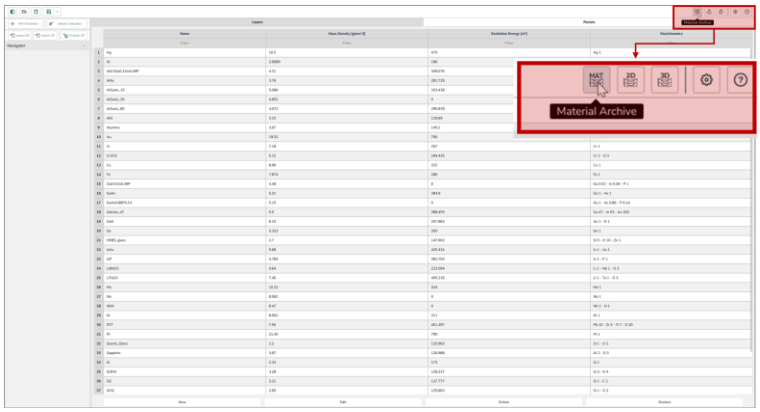
Stack description

The Stack Description defines the layer type, material and the corresponding thickness. The layer type can be either resist (Resist) or non-resist (Layer). A list of Resist / Layer is available in the drop-down menu in the Material window. The contents of the lists can be edited by opening the Material Archive. As shown in the figure below, PMMA has been selected as the Resist and Si as Layer (see figure below).



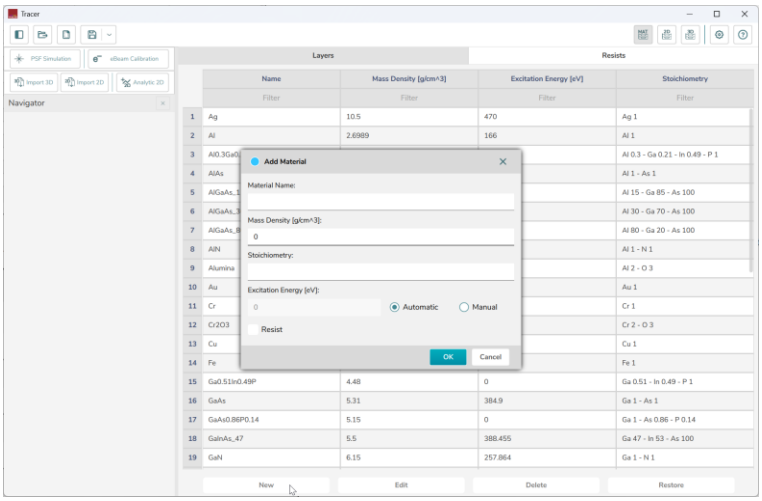
Material archive

The Resist / Layer are described in the Material Archive (see figure below). By left-clicking the MAT (Material Archive) icon on the top right corner of the **TRACER** GUI, the Material Archive can be opened as shown below. Selecting Material Archive will toggle the list of material stored in **TRACER**. There are two tabs in the Material Archive: Layers and Resists. Layers are metals or oxides, Resists are self-explanatory. Here, you can select material by clicking a row in the table and apply any of the two operations by clicking of the buttons (Edit or Delete) below the table.



How to create new material in material archive

To create new entries in the material table, left click the New button below the table will open a dialog window (Add Material – see figure below).



In this dialog, you should enter the required parameters. Excitation Energy [eV] can be either calculated automatically or entered manually. Distinguish between Non-Resist Materials and Resists can be done by activating the Resist box shown above.

Material Name

When adding a new entry, use a suitable name to describe the material.

Mass Density [g/cm^3]

Density of the material.

Excitation Energy [eV]

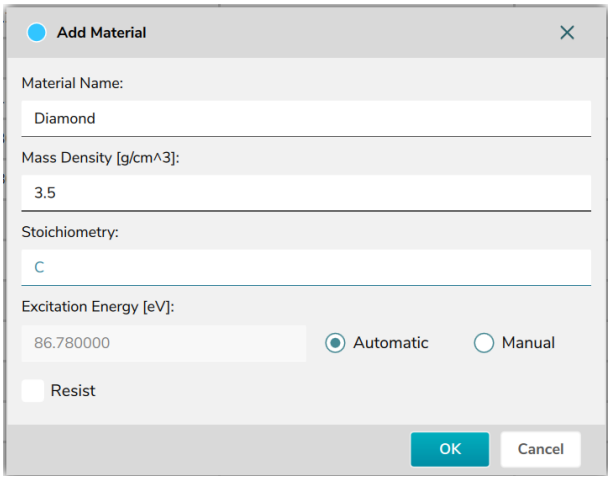
Excitation energy (mean) is the amount of energy needed to put electrons into a higher energy state. The excitation energy values for standard elements and compounds are stored in a databank and are assigned when *Automatic* is selected for a standard stoichiometry. For an unknown stoichiometry a warning is issued.

Resist

Activate if the material is a resist.

Examples

For example, to add diamond substrate as a new entry, enter a name as Diamond for *Material Name*. The *Mass Density* of diamond is 3.5g/cm^3. In this case diamonds are composed of carbon and thus the *Stoichiometry* is C. Finally, the *Excitation Energy [eV]* can be calculated automatically by selecting *Automatic*. Since diamond is non-resist material, Resist box is not activated (see figure below).



For another case, if you want to add a III-V compound semiconductor $Al_xGa_{1-x-y}In_yP$ into the *Material Archive*, it will be a bit more complicated. In this case, the x and y describe the mole fractions (compositional ratios) of the elements in the crystal lattice.

Meaning of x and y

- x = fraction of Aluminum (*Al*) on the cation sublattice
- y = fraction of Indium (*In*) on the cation sublattice
- The remaining fraction is Gallium (*Ga*)

For a specific case: x = 0.30, y = 0.49

- *Al* fraction = 0.30
- *In* fraction = 0.49
- *Ga* fraction = 1 − 0.30 − 0.49 = 0.21

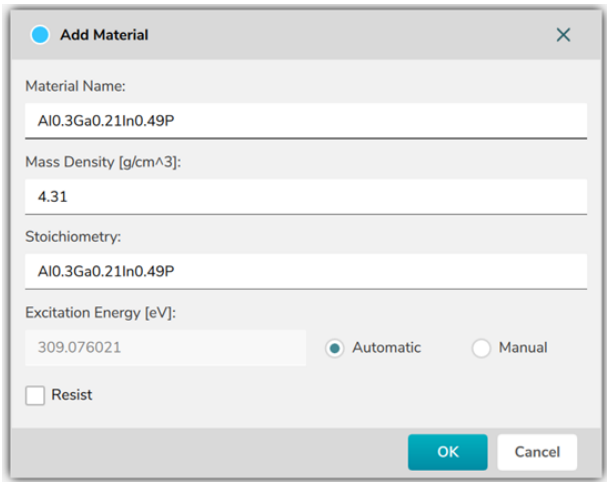
The final composition is $Al_{0.30}Ga_{0.21}In_{0.49}P$. This can be used for *Stoichiometry* in the dialog. About the Mass density, you can find it in the open sources. Otherwise, you can use Vegard's law to interpolate between the binary phosphides:

- $AlP \approx 3.61\ \mathrm{g/cm^3}$
- $GaP \approx 4.14\ \mathrm{g/cm^3}$
- $InP \approx 4.81\ \mathrm{g/cm^3}$

$$\rho = 0.30 * (3.61) + 0.21 * (4.14) + 0.49 * (4.81)$$
$$\rho \approx 4.31\ \mathrm{g/cm^3}$$

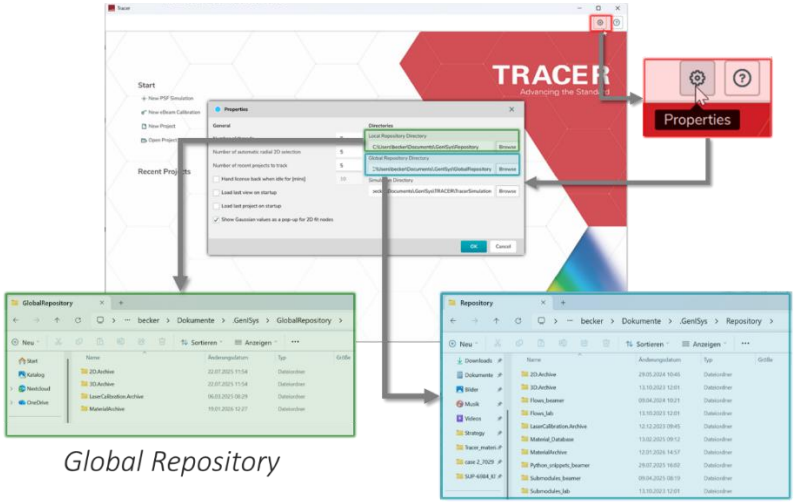
In this case, some small deviations can occur depending on lattice ordering, strain, and growth conditions of the material.

After adding all the information in the dialog (see figure below), new material entry, $Al_{0.30}Ga_{0.21}In_{0.49}P$, is added to the *Material Archive*.



Handling materials in **TRACER** for groups and individuals

TRACER *3.0* supports not only *Global and Local 2D and 3D PSF Archives*, but also *Global and Local Material Archives*. *Local and Global 2D Archives* are defined in the Properties/Directories section (see figure below) in **TRACER**.



Global Repository

Local Repository

Materials can be added, edited or deleted either globally (Global Material Archive), where all users have access, or locally (Local Material Archive), in which case, materials are not shared with all users.

Summary

TRACER provides a flexible approach to defining and managing materials for accurate Monte Carlo simulations of electron scattering and point spread functions (PSFs). By allowing users to add and edit materials based on physical properties such as mass density, chemical composition, and excitation energy, the material archive can be adapted to specific resists, substrates, and compound materials. The use of global and local material archives further enables consistent material definitions across teams while accommodating individual or project-specific requirements, supporting reliable simulations and improved process optimisation.