# Handling materials in TRACER for group and individuals

## Introduction

**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 description of materials.

## 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* (Fig. 1).

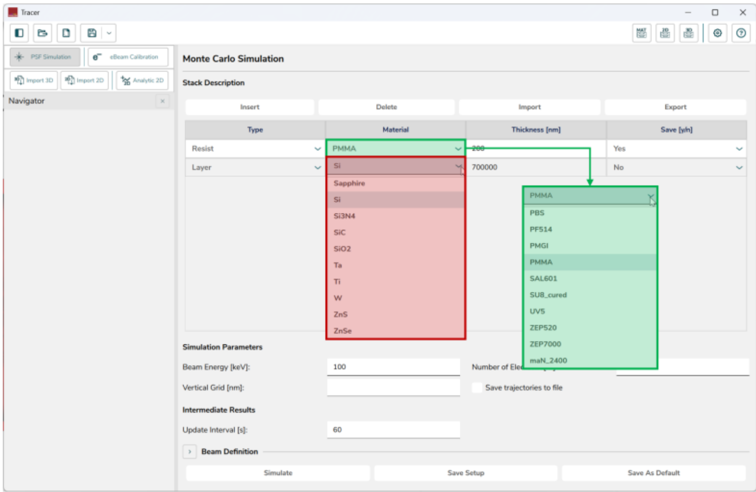


*Figure 1. Stack description for Monte Carlo Simulation*

## Material Archive

The *Resist / Layer* are described in the *Material Archive* (Fig.2). By left-click the *MAT* (*Material Archive*) icon on the top right corner of the **TRACER** GUI, the *Material Archive* can be opened as shown below (Fig. 2). 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 and 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.

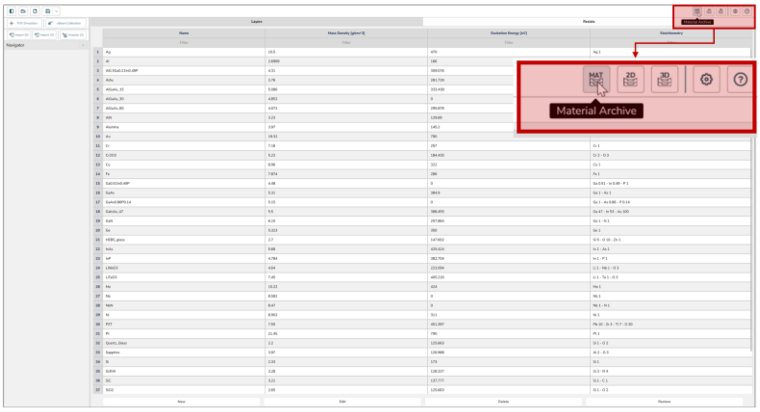


*Figure 2. Content of Material Archive*

## 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*) (Fig.3).

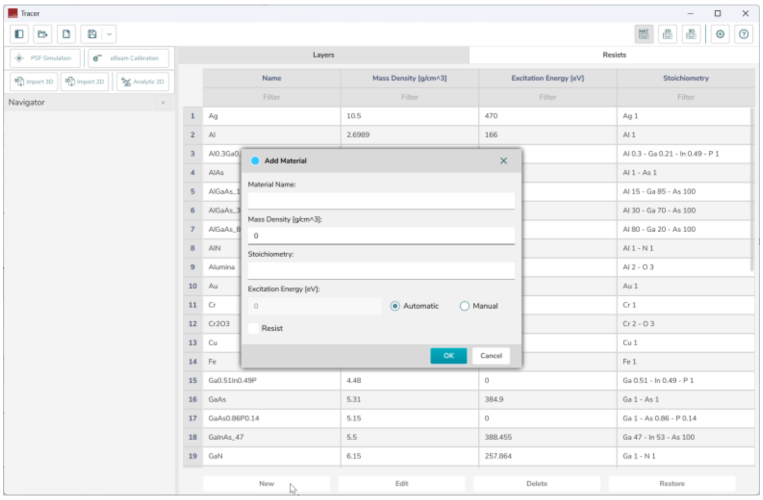


*Figure 3. Add new entry to Material Archive*

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/cm3]*
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, Resists box is not activated (Fig.4).

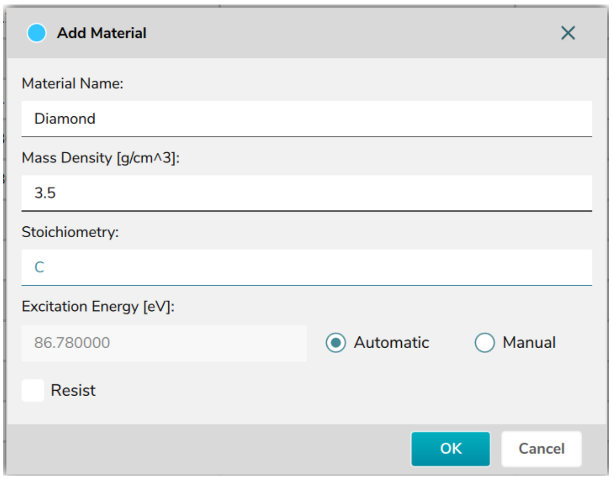


*Figure 4. Add diamond as new entry*

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:

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

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

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, new material entry, $Al_{0.30}Ga_{0.21}In_{0.49}P$, is added to the *Material Archive*.

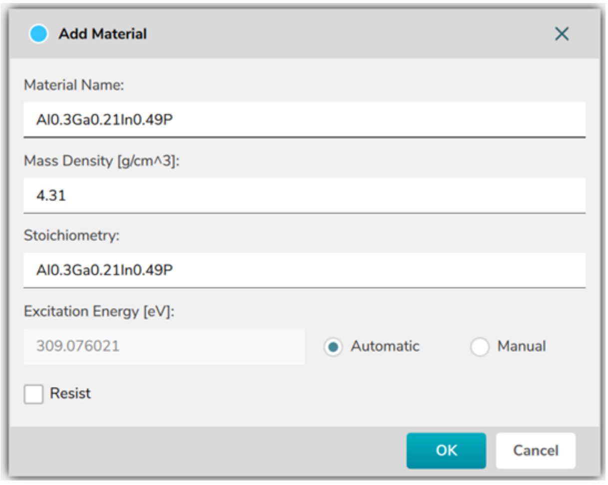


*Figure 5. Add III-V compound semiconductor $Al_{0.30}Ga_{0.21}In_{0.49}P$ as new entry*

## Handling materials in TRACER for group 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 (Fig. 6) in ***TRACER***.

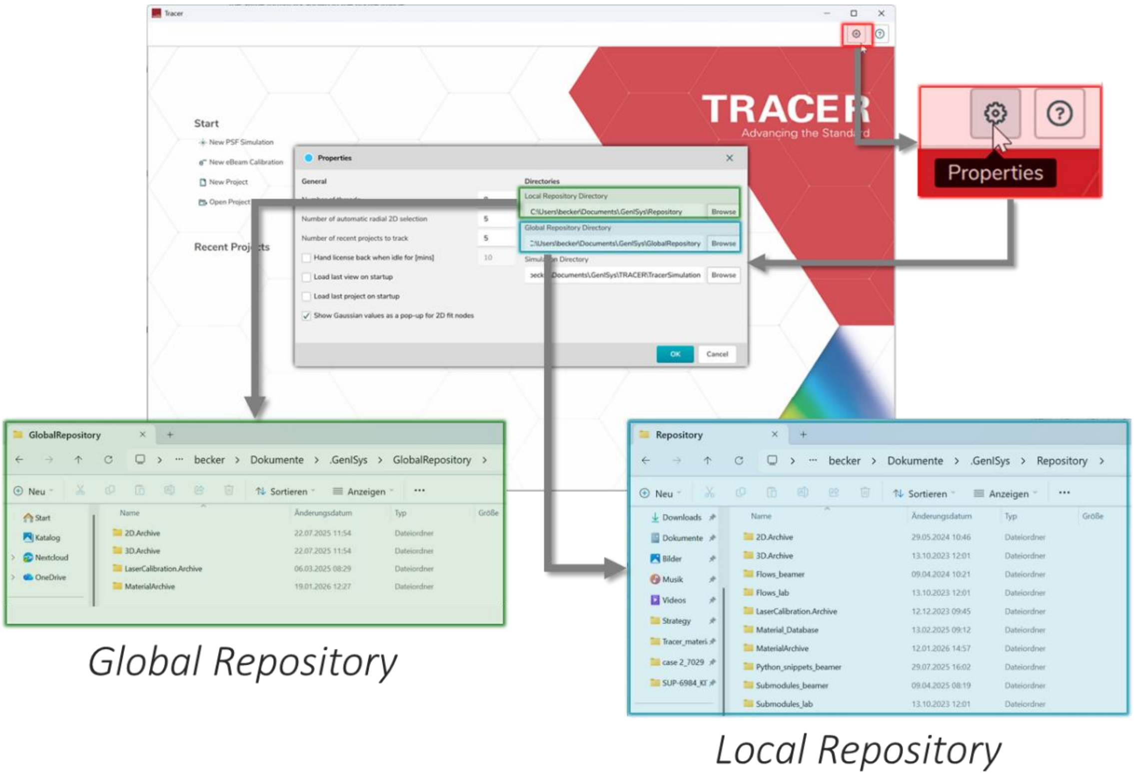


*Figure 6. Global and Local Repository*

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