

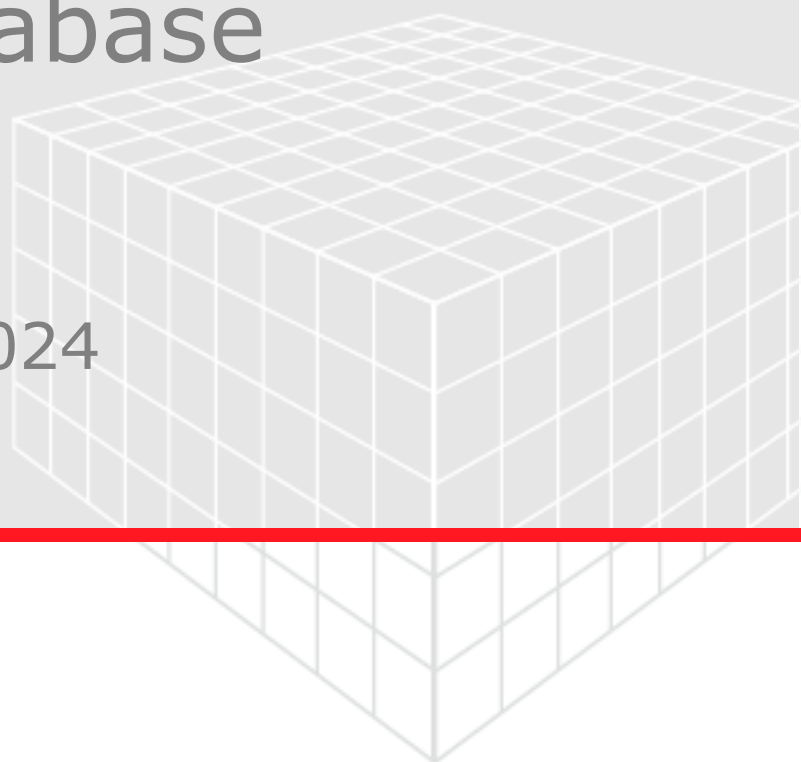
GEO DICT

Material database

User Guide

GeoDict release 2024

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GEO DICT

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The handbooks in the User Guide series of Math2Market GmbH can be obtained from:

Math2Market GmbH
Richard-Wagner-Strasse 1
67655 Kaiserslautern
Germany

Phone: +49 631 205 605 0
Fax: +49 631 205 605 99
Email: info@math2market.de
Web: www.math2market.de

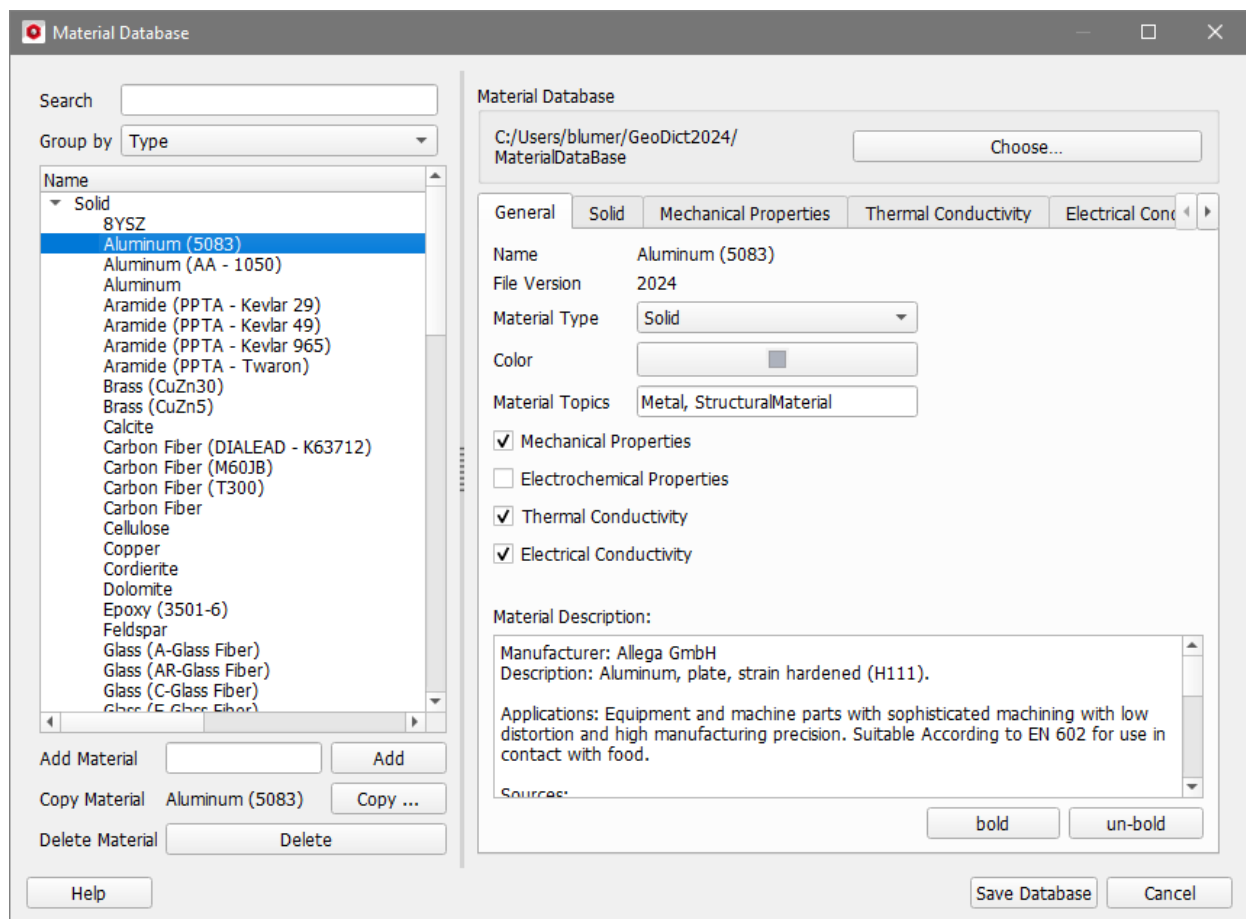
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THE GEODict MATERIAL DATABASE

Structures in **GeoDict** are 3D voxel images where each voxel has one of 256 possible material IDs. To each of these material IDs, a material can be assigned. This means that a structure in **GeoDict** can contain up to 256 different materials. Materials in **GeoDict** can contain all material properties that are needed for simulations in **GeoDict**.

The **GeoDict** material database is the place to store material data. A selection of standard materials is already predefined, but the true strength of the database is that it allows the user to define additional materials to be used in **GeoDict** simulations.

The information for each material in the **GeoDict** material database is saved as a *.txt file in the material database folder. Therefore, materials can either be edited in the material database editor or by editing the corresponding *.txt file. Materials can be exchanged by copying these *.txt files.

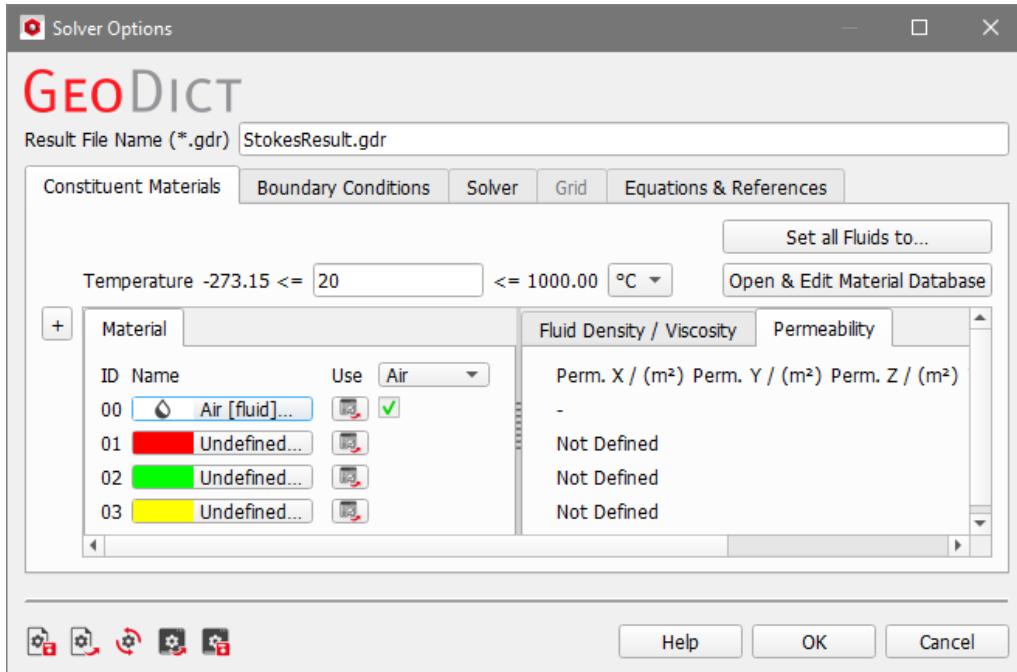


Materials can be assigned to **GeoDict** structures during the creation with **GeoDict** structure generation modules (e.g., **FiberGeo**, **GrainGeo**, **WeaveGeo**...) or during the import from e.g., μ CT-scans. Additionally, they can be set for the structure currently in memory. When saving a structure in a **GeoDict** format (as *.gdt or *.gad file), its constituent materials and their properties are saved in that file, too.

This allows for directly simulating on a structure loaded from its file, there is no necessity to select the materials and their properties for the simulation run. However, it is always possible to change the materials and their properties prior to simulation.

MATERIALS IN GEODICT

A material in GeoDict can either be a specific material, which is selected from the GeoDict material database, or set to be **Manual**. In some cases, the material for a given material ID might be unclear. Then, the material is **Undefined**.



Manual materials allow to quickly set the needed parameters, whereas using materials from the material database allows to reuse them for further simulations.

Materials can be defined during the creation of a microstructure using the GeoDict structure generation modules or prior to simulation with one of the GeoDict predictor modules. For a structure in memory, the materials can also be changed independently of any module.

Different parameters from various application fields can be entered and saved for all materials, except for undefined materials. Depending on the material type, different parameters of the material must be entered.

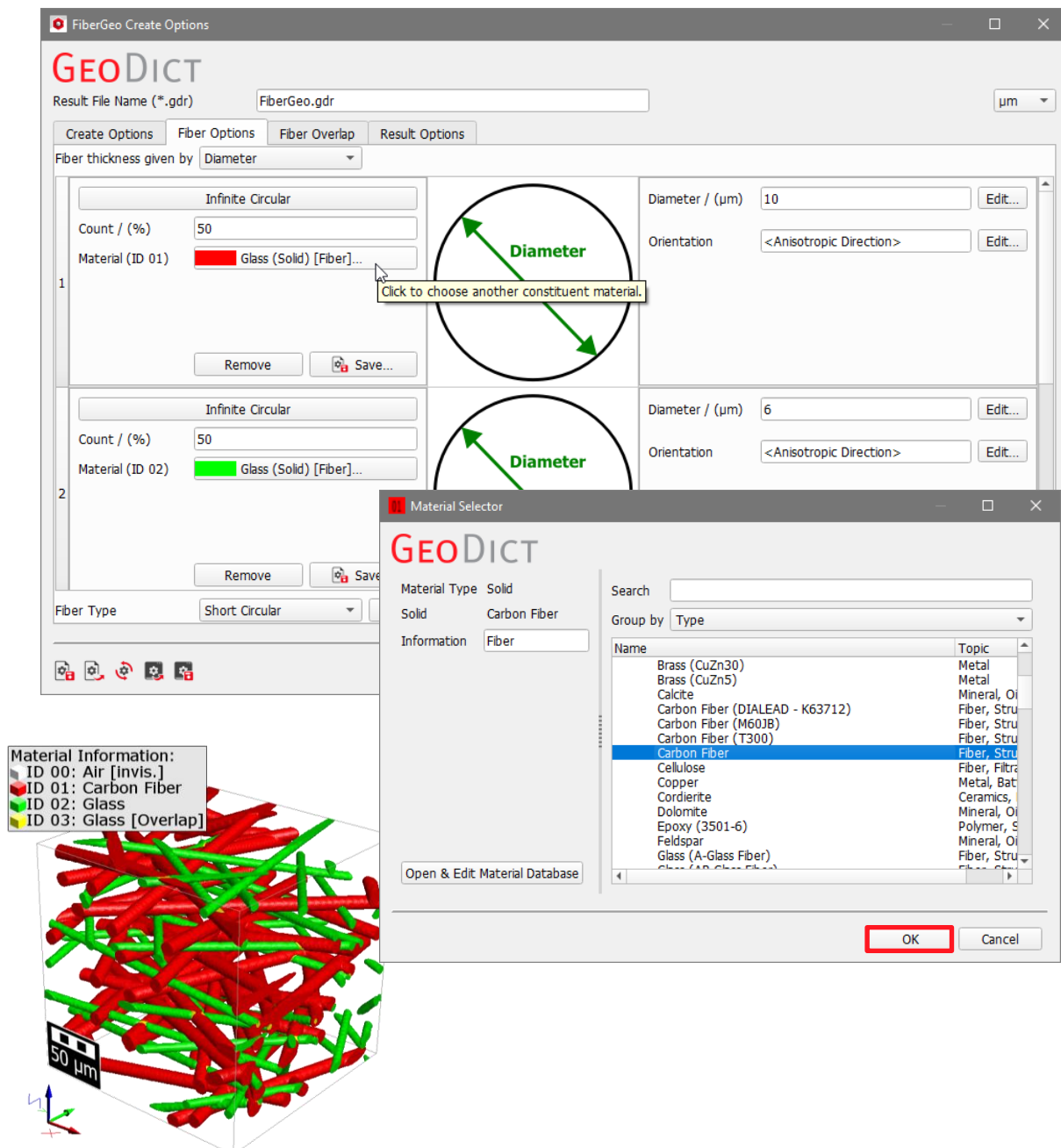
SETTING THE CONSTITUENT MATERIALS IN GEODICT

The constituent materials are selected during the generation of a structure or during the import from 3D image data. Afterwards, the constituent materials can be changed if needed.

SETTING MATERIALS FOR STRUCTURE GENERATION

In the structure generation modules (available under **Model** in the menu bar), the materials of the material IDs in the structure can be entered before the structure is created. In most cases, there is the option **Material (ID XX)** and a button with the color and material name on it. Clicking on the material opens the **Material Selector** dialog where another material can be chosen.

An example for the selection of the constituent materials in **FiberGeo** is shown below. For each fiber type, the material can be selected by clicking the corresponding button.



The **Material Selector** dialog opens, and all materials stored in the current material database are available. At the top left, the number and color of the currently selected material ID can be seen.

On the left side, the **Material Type** and the name of the currently selected material are given. Additionally, more information can be entered into the **Information** field, e.g. describing the role of the material in the structure. Below, there is the possibility to **Open & Edit** the **Material Database** to check or change the parameters of this material. The Material Database is described on page 13ff.

On the right side, all available materials can be browsed. Either by directly typing the name in the **Search** bar, or, after grouping by **Type**, **Topic**, or **Property**, scrolling through the list. The currently selected material is highlighted in blue.

The main way to differentiate between materials is the **Material Type**. Available are **Fluid**, **Solid**, and **Porous Solid**, which is a mix between pore and solid. There are two special material types, which are **Pore** and **Undefined**. The type **Pore** can be described as a voxel containing nothing, especially no solid material and has 100% porosity. For **Undefined** materials nothing is known about the material and all parameters are set to **Not Defined**.

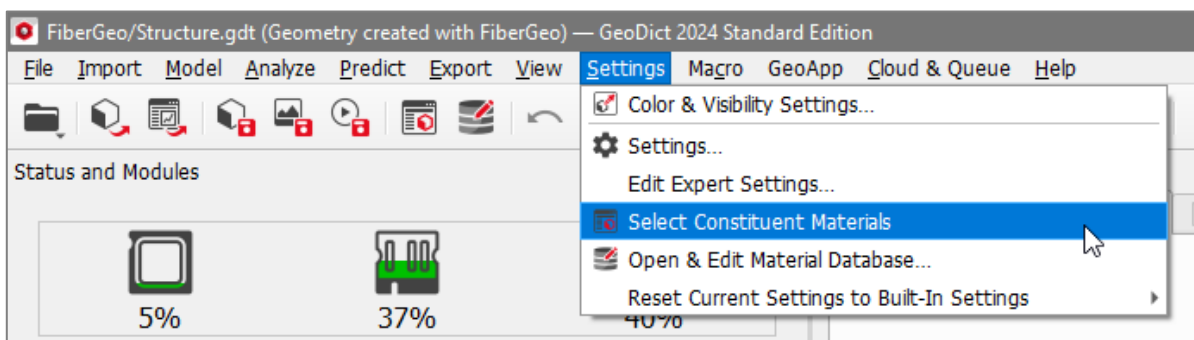
For many materials one or more **Topics** can be entered. This could be an application field or an aggregate state. For example, the predefined material Air has the topics **Gas** and **Filtration**.

When grouping materials by **Property**, a material appears only in those groups where the corresponding properties are defined.

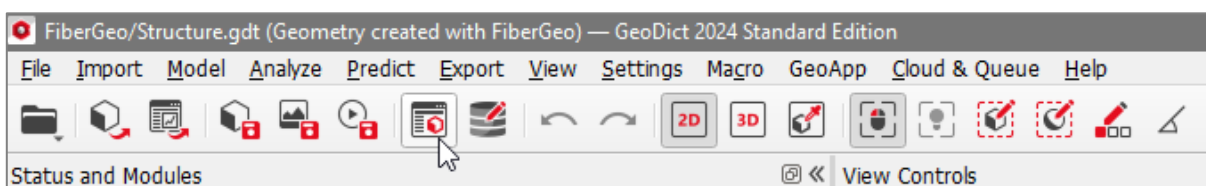
Click **OK** to save the selected material for this material ID and to close the material selector.

SETTING MATERIALS FOR THE CURRENT STRUCTURE

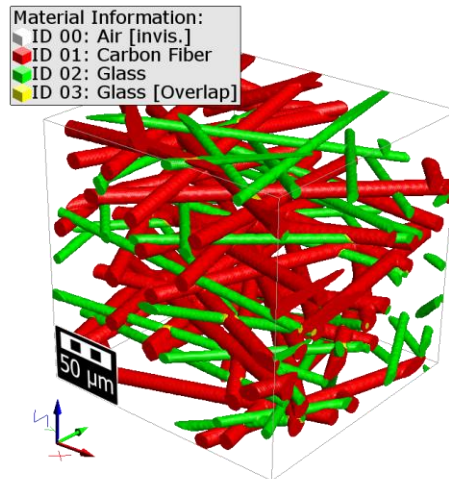
The constituent materials for the structure currently in memory can be changed by selecting **Settings** → **Select Constituent Materials** in the menu bar.



Alternatively, click the corresponding icon in the toolbar.



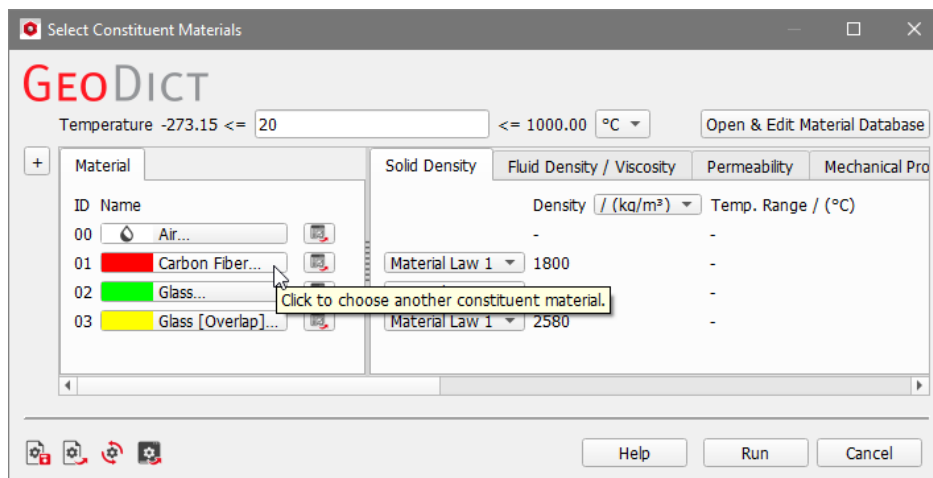
The concept is shown for the structure on the right: The material assigned to material ID 01 is changed from **Carbon Fiber** to **Glass**.



The **Select Constituent Materials** dialog shows the material information of all material IDs that are present in the currently loaded structure. Clicking on the plus icon next to **Material** shows all 256 material IDs. The icon changes from plus to minus to hide the material IDs which are not present in the current structure.

At the top, the current temperature is shown and can be changed. The temperature unit can also be changed, available are **K**, **°C**, and **°F**. This is important if temperature dependent properties are considered.

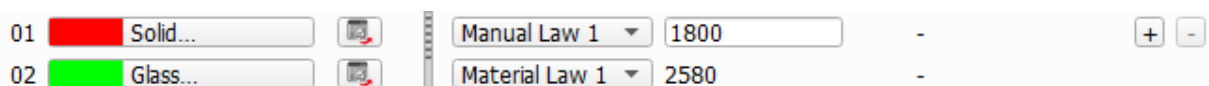
Located at the top right is the button to **Open & Edit Material Database**. The Material Database is explained on page [13ff](#).



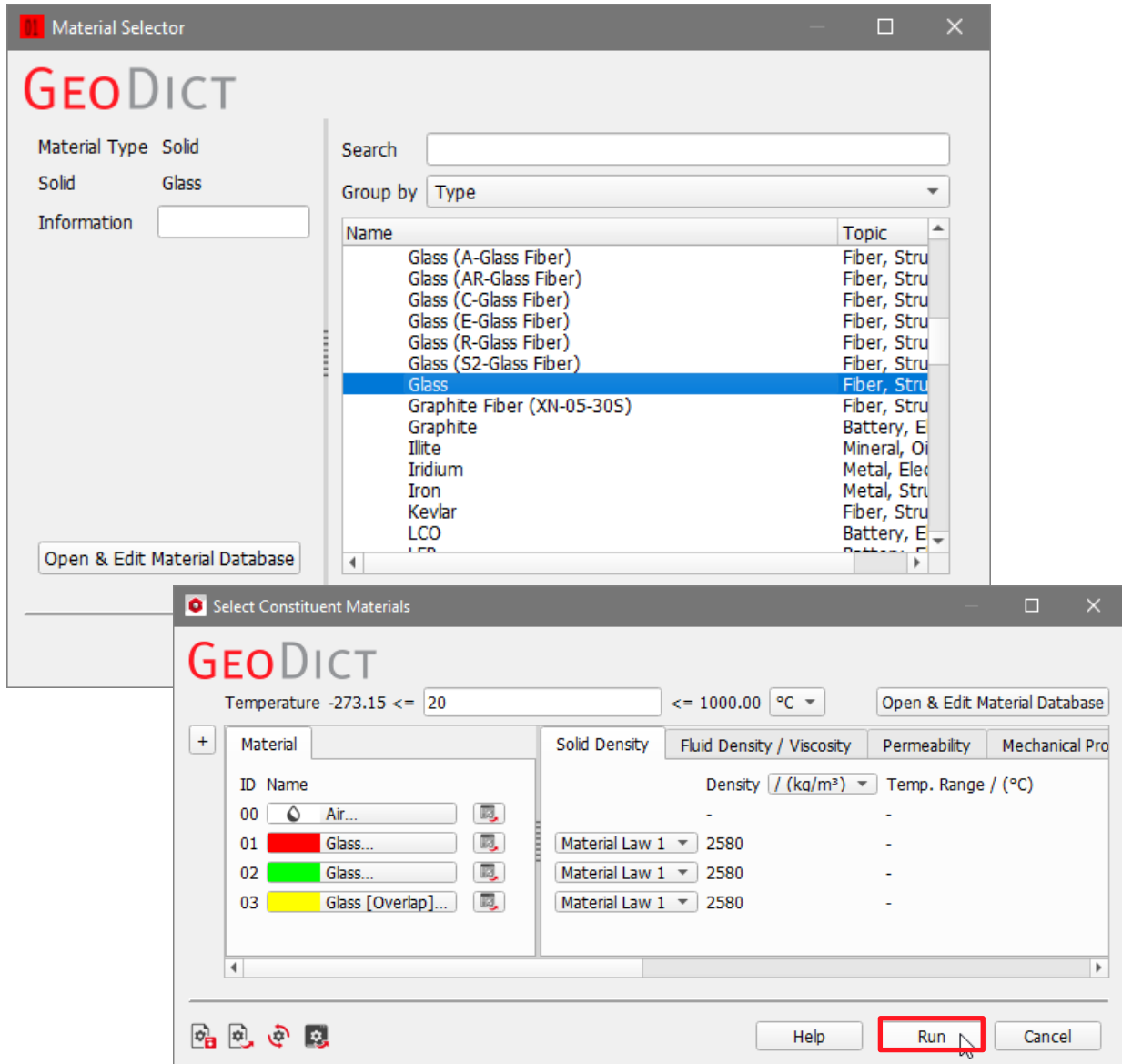
On the left side, the material IDs, their assigned material, and its color (see page [11](#) how to change it) are shown. The button next to it opens a report of the relevant parameters for this material ID.

On the right side, all available parameters are grouped into several tabs. For materials from the Material Database, the user can check the saved parameters. For some of the parameters, multiple material laws can be defined in the Material Database. Then, one can decide in this dialog which material law should be applied.

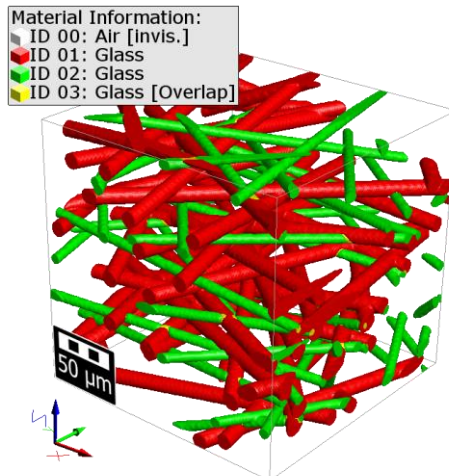
For **Manual** materials, which are not stored in the material database, the user can define the necessary parameters in this dialog. It is also possible to define multiple material laws by clicking on the + icon at the end of a line to add a new material law. Delete additional laws by clicking on the - button.



The material of a material ID can be changed by clicking on the material name. Then, the **Material Selector** dialog (see above on page 4) opens and the desired material can be selected.



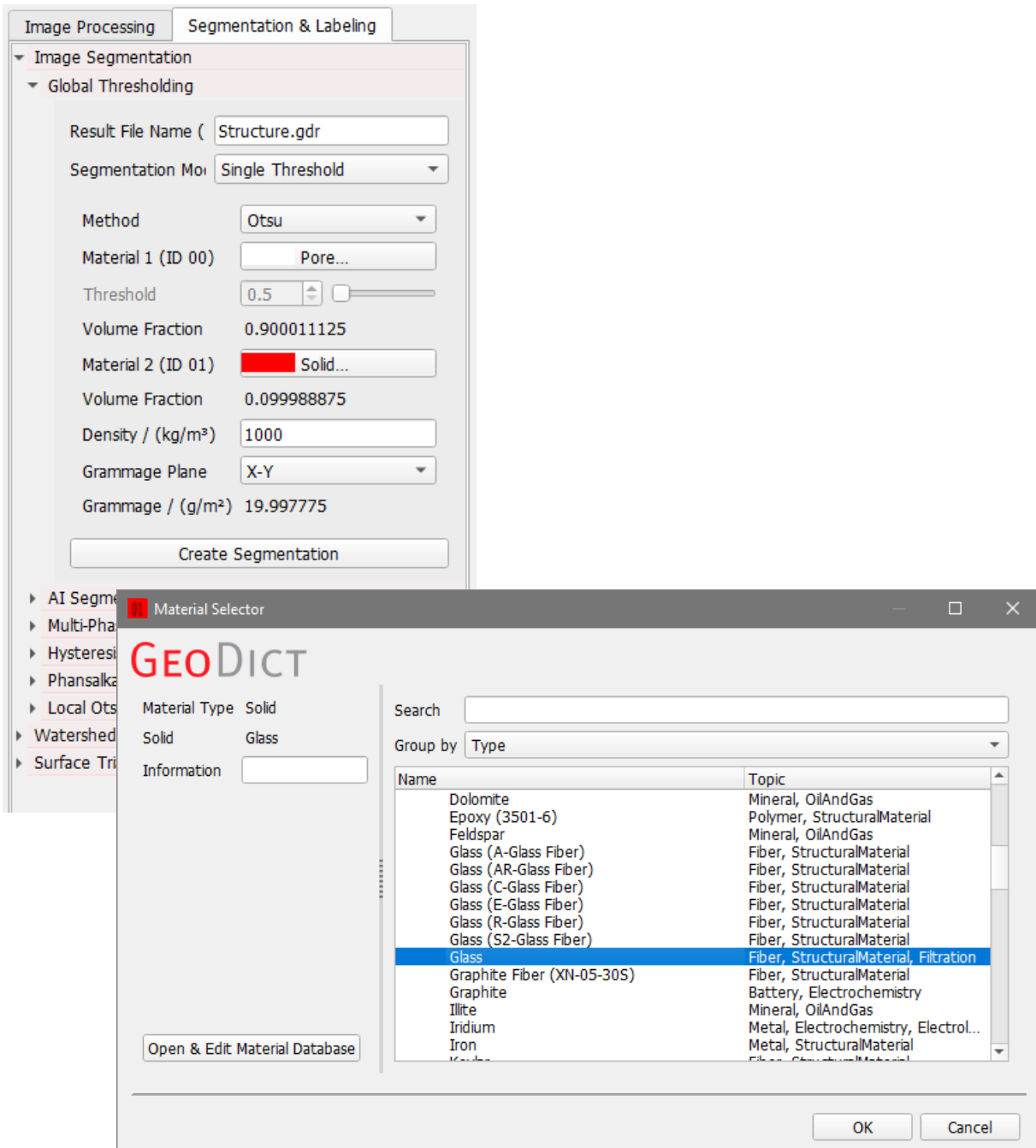
Click on **Run** to save and apply the selected materials and their properties.



SETTING MATERIALS DURING IMPORT

When a structure is imported in GeoDict (e.g., from a μ CT-scan), its constituent materials can be set during the import.

By default, the material with material ID 00 is set to **Pore (Fluid)**, whereas all other material IDs are set to **Manual (Solid)**.

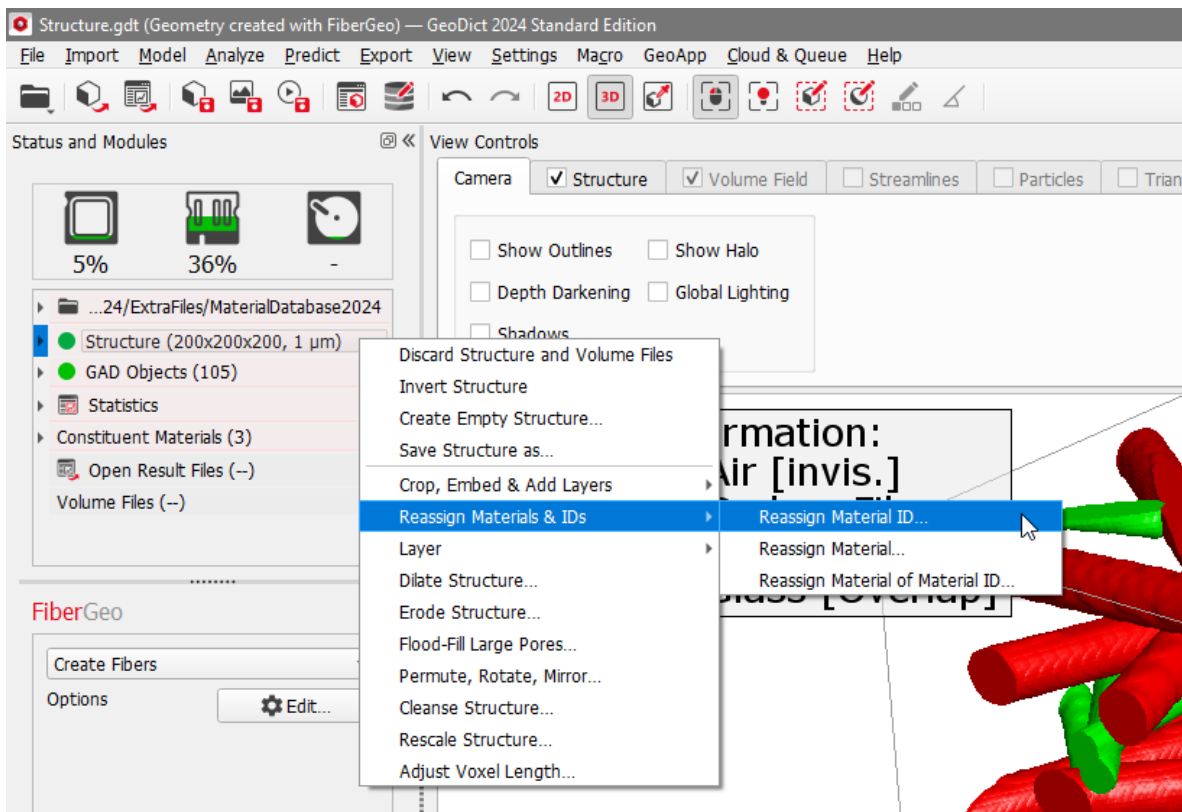


REASSIGNING MATERIALS AND MATERIALS IDS

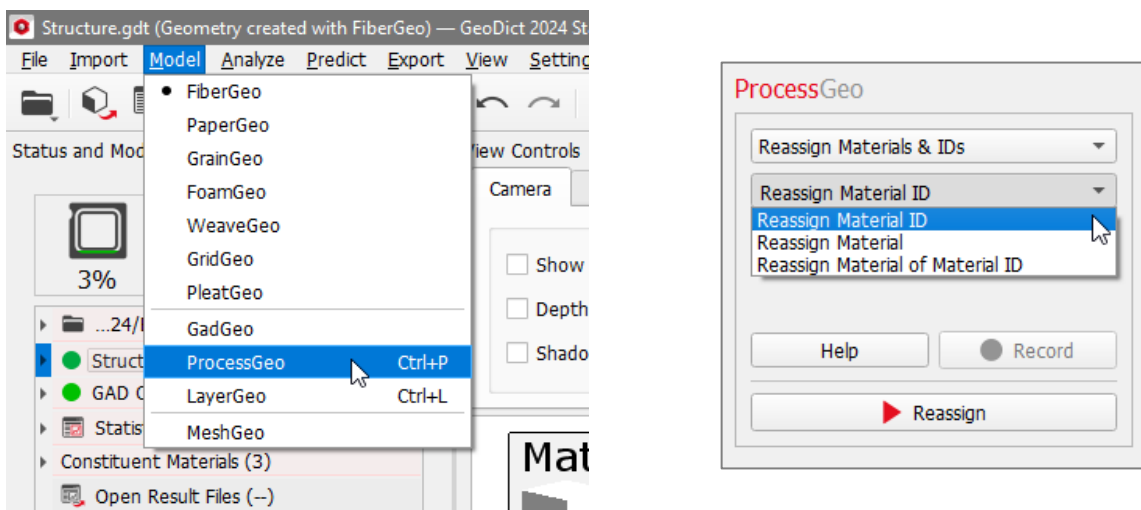
One option to change materials in the structure is the **Select Constituent Materials** dialog, as described above on page 4. Depending on the use case, there are other options available through the **ProcessGeo** module.

It is possible to **Reassign Material IDs**, to **Reassign Materials** and to **Reassign the Material of a Material ID** (this corresponds to the option in the **Select Constituent Materials** dialog). These options are shortly described here but more information is available in the **ProcessGeo** User Guide.

To access the options for reassigning quickly through a shortcut, right-click on **Structure** in the **Project Status** section on the left side of the **GeoDict** GUI.

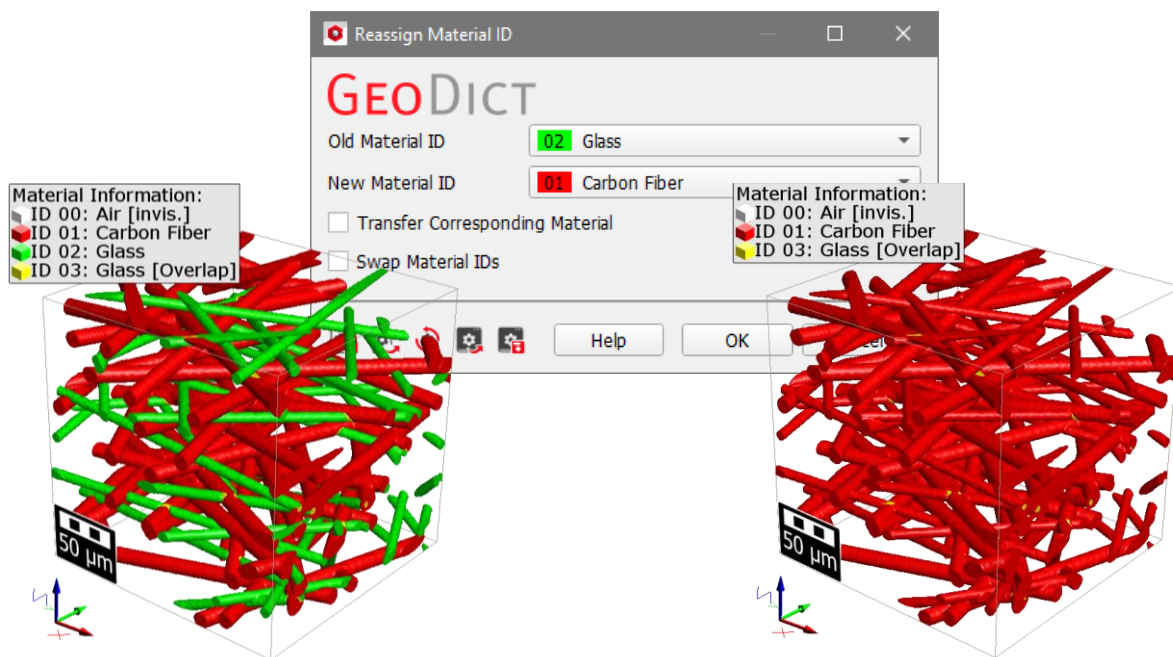


Alternatively, these options are also available from the menu bar by selecting **Model** → **ProcessGeo** → **Reassign Materials & IDs**.



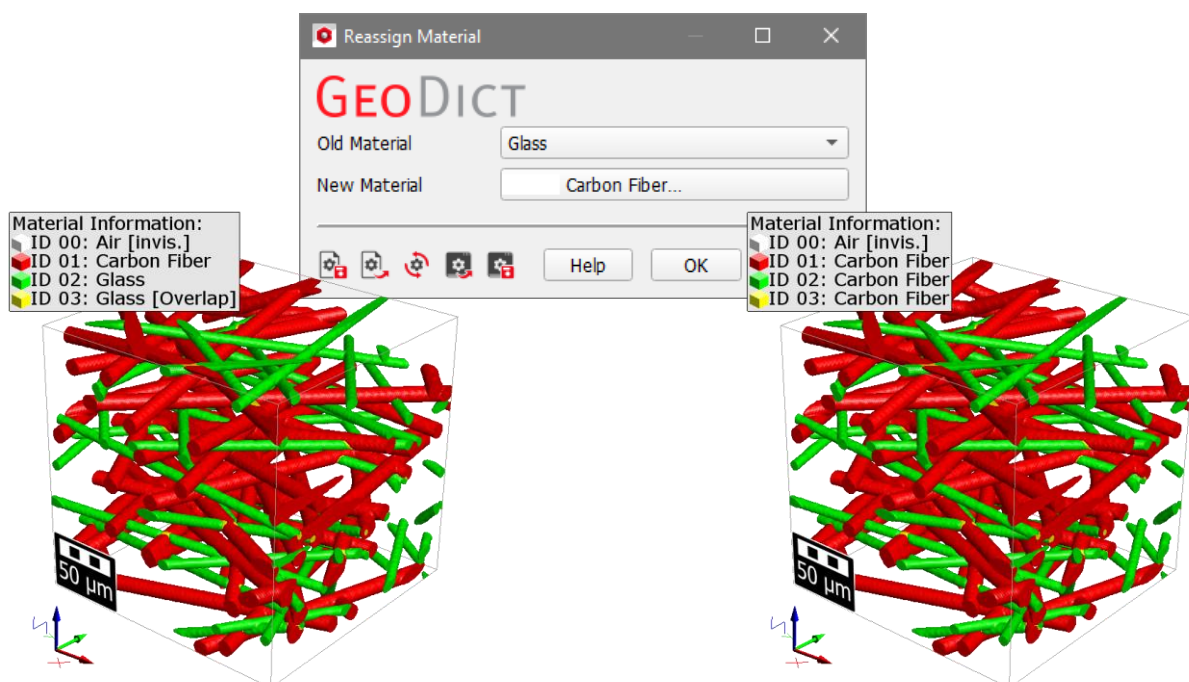
REASSIGN MATERIAL ID

With **Reassign Material ID**, the material ID of the corresponding voxels in the structure is changed. In the example shown below, the material ID 02 is reassigned to the material ID 01. No voxels with material ID 02 remain in the structure, and it is not possible to distinguish which fibers belonged to which ID (01 or 02) after the reassignment. With the additional option **Transfer Corresponding Material** also the material of the new material ID is changed to the material of the old material ID. Using **Swap Material IDs** allows to swap the old and new material ID.



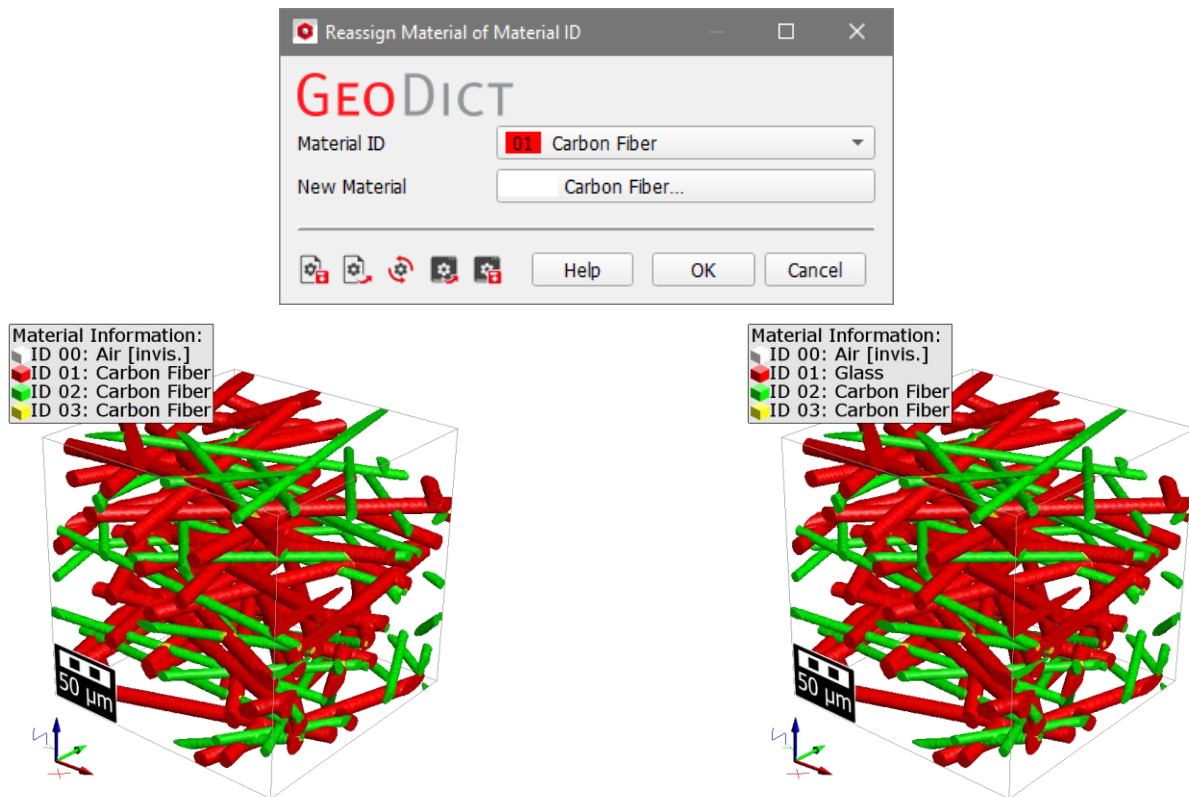
REASSIGN MATERIAL

With **Reassign Material**, a material in the structure is replaced by another material. This means that the material is changed for all material IDs which are set to this material. In the example below, **Glass** is changed to **Carbon Fiber**.



REASSIGN MATERIAL OF MATERIAL ID


Reassign Material of Material ID corresponds to the option available in the **Select Constituent Materials** dialog. As shown in this example, the material is changed for one selected material ID (here: *Carbon Fiber* to *Glass* for Material ID 01).

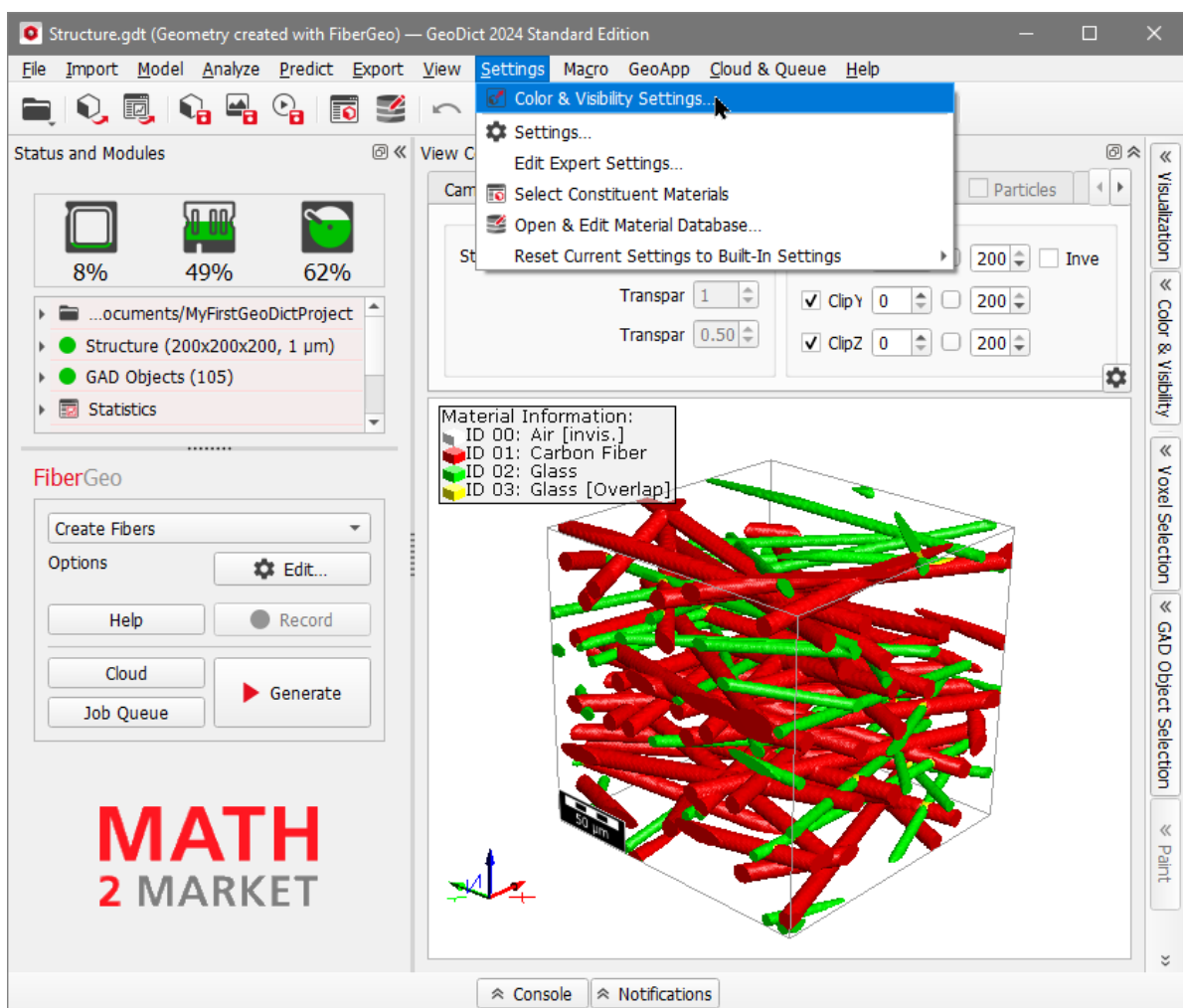


MATERIAL COLORS IN GEODICT

For each material ID in GeoDict, a color can be selected for visualization. These colors are set globally in GeoDict and are not saved in the structure file. For each material in the material database, also a corresponding color is stored (see page [11](#)). In the following, it is described how to use these stored material colors for display.

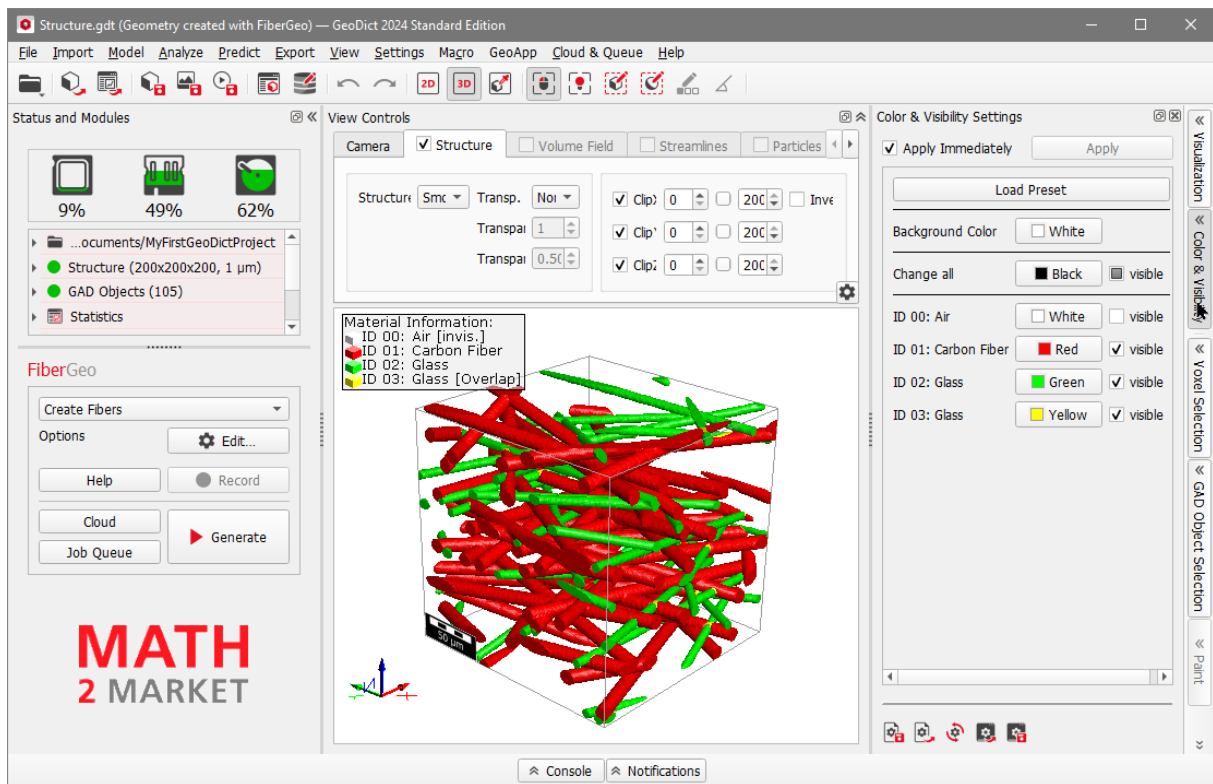
COLOR SELECTION

The color of a material in GeoDict can be changed through the **Color and Visibility Settings** dialog by selecting **Settings** → **Color & Visibility Settings...** in the menu bar, or by clicking the corresponding icon  in the toolbar. This opens the **Color & Visibility Settings** dialog, which can also be accessed directly from the sidebar on the right of the user interface.

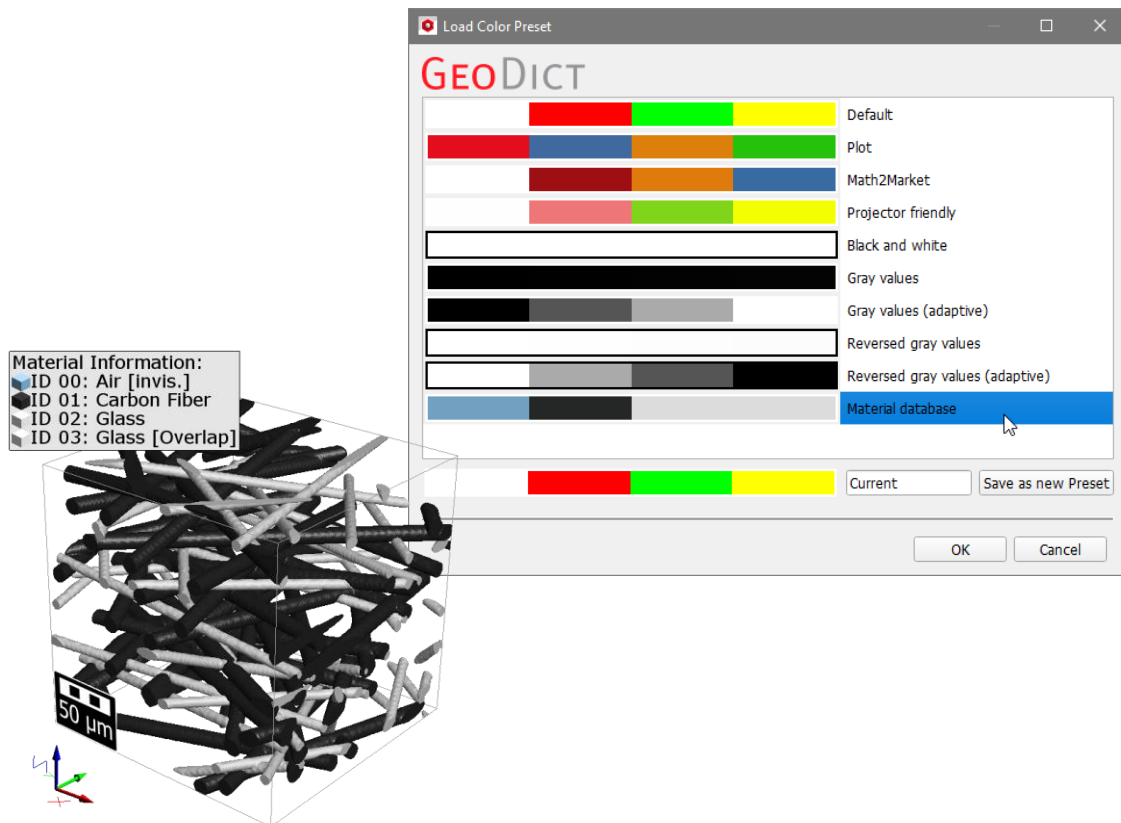


The **Color and Visibility Settings** dialog shows the colors currently assigned to the Material IDs and the Constituent Materials.

To use the colors defined in the GeoDict Material Database, click **Load Preset** and then, choose **Material Database** in the **Load Color Preset** dialog. Confirm the choice with **OK** and close the **Color & Visibility Settings** with the **Close button** 



For example, the preset color for *Glass* in the material database is a light grey, as shown here.



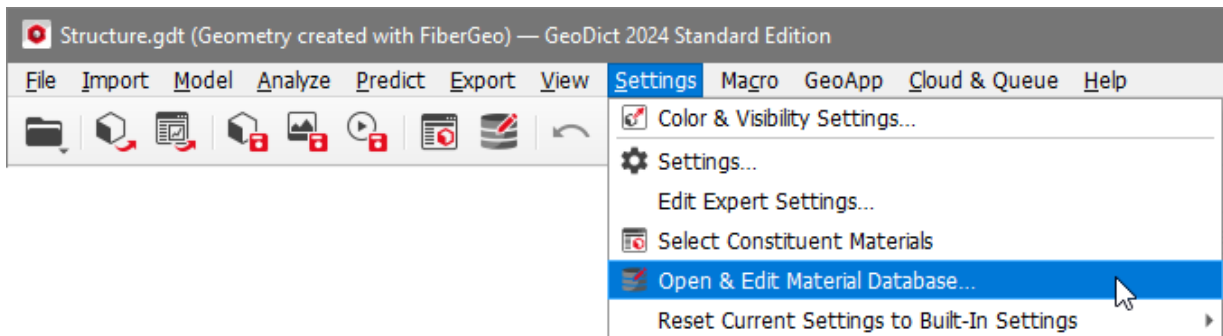
EDIT AND EXPAND THE GEODICT MATERIAL DATABASE

The **GeoDict** Material Database installed with **GeoDict** can be viewed, edited, and expanded. In the following, it is explained how to access the Material Database, which information is stored in the Material Database, how to edit the properties of materials already included in the **GeoDict** Material Database and how to create new constituent materials.

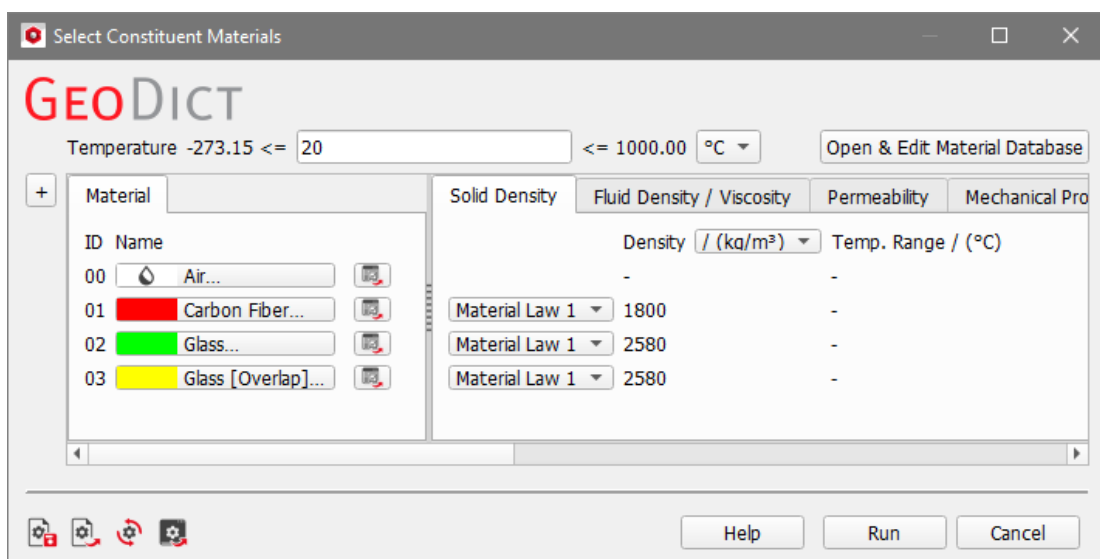
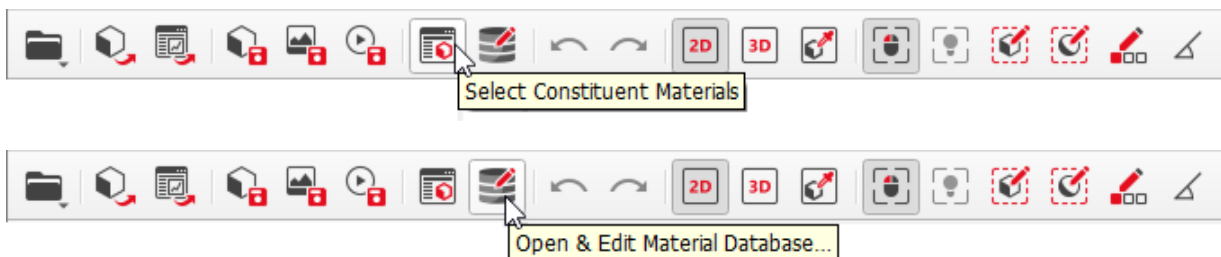
ACCESS THE MATERIAL DATABASE

There are several options to access the Material Database in **GeoDict**:

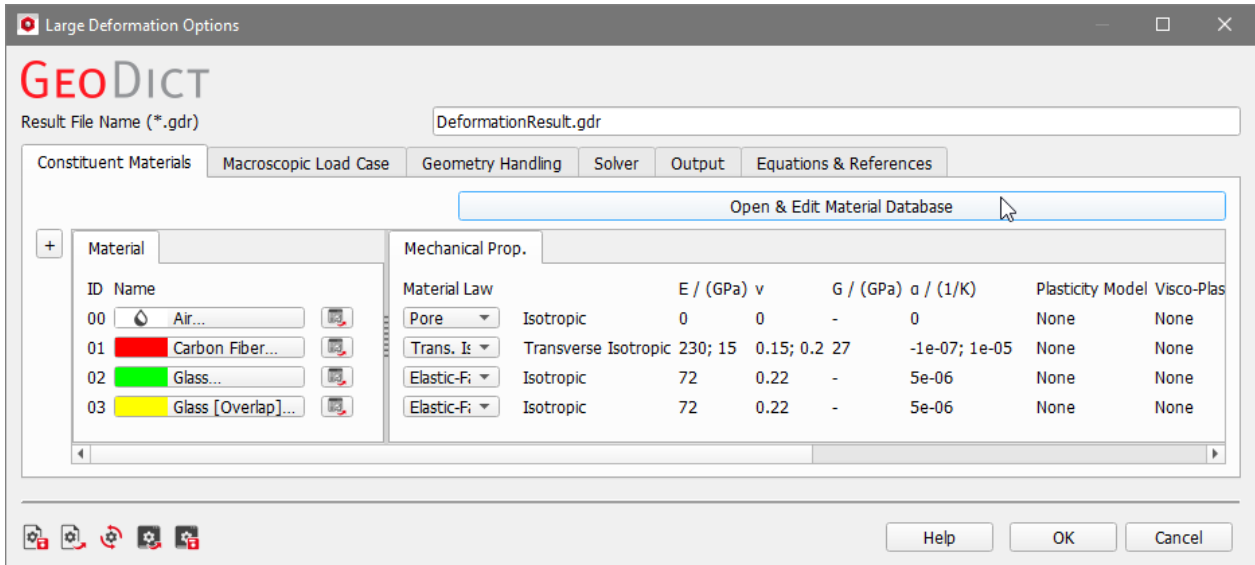
1. Select **Settings** → **Open & Edit Material Database...** in the menu bar.



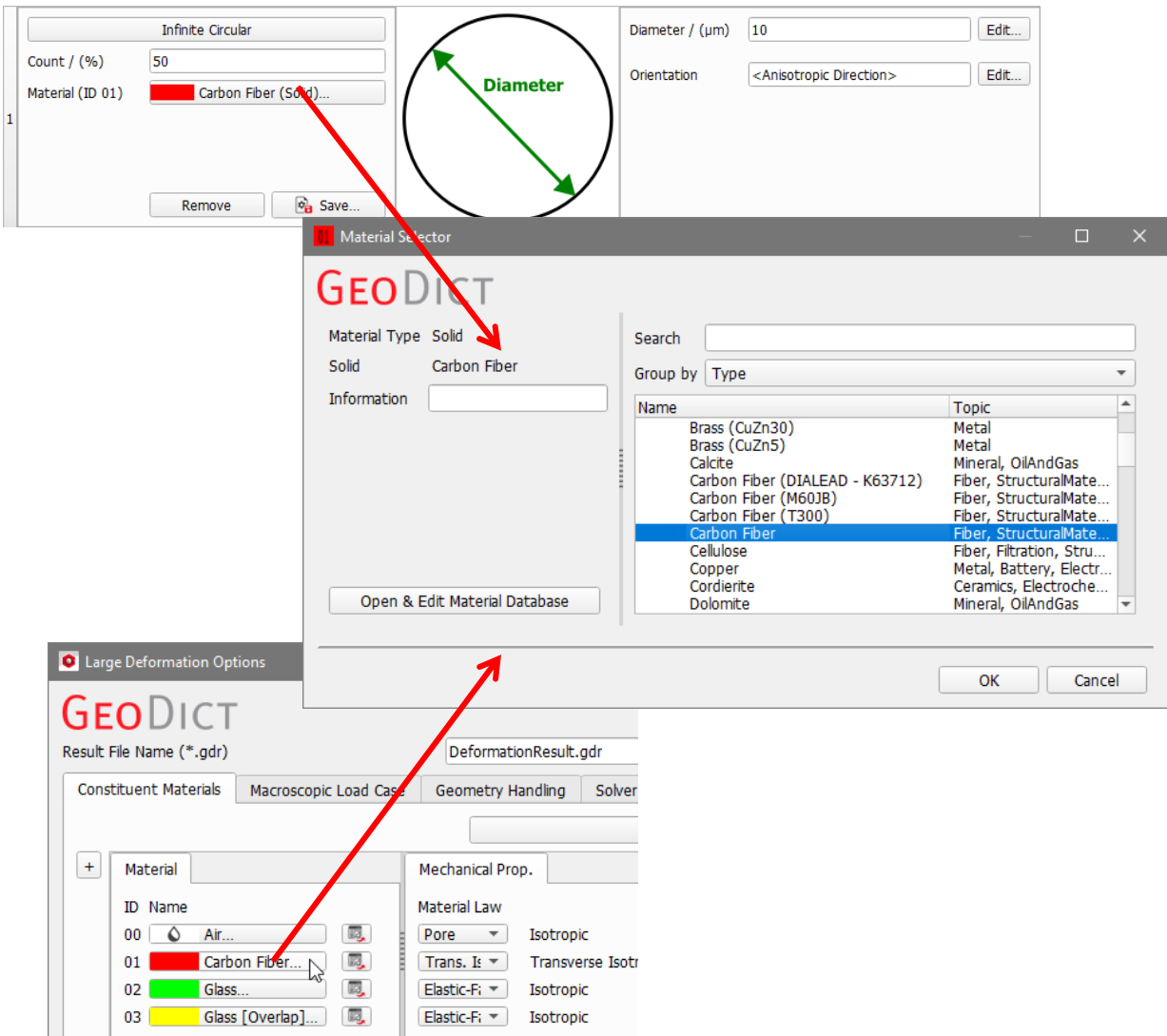
2. Click the **Open & Edit Material Database** icon in the toolbar.
3. Click the **Select Constituent Materials** icon in the toolbar and click **Open & Edit Material Database** in the Select Constituent Materials dialog.



- Click the **Open & Edit Material Database** button located in the **Constituent Materials** tab of the **Solver Options** for the predictor modules (**ElastoDict**, **ConductoDict**, **FlowDict**, **DiffuDict**, **FilterDict**, etc.):

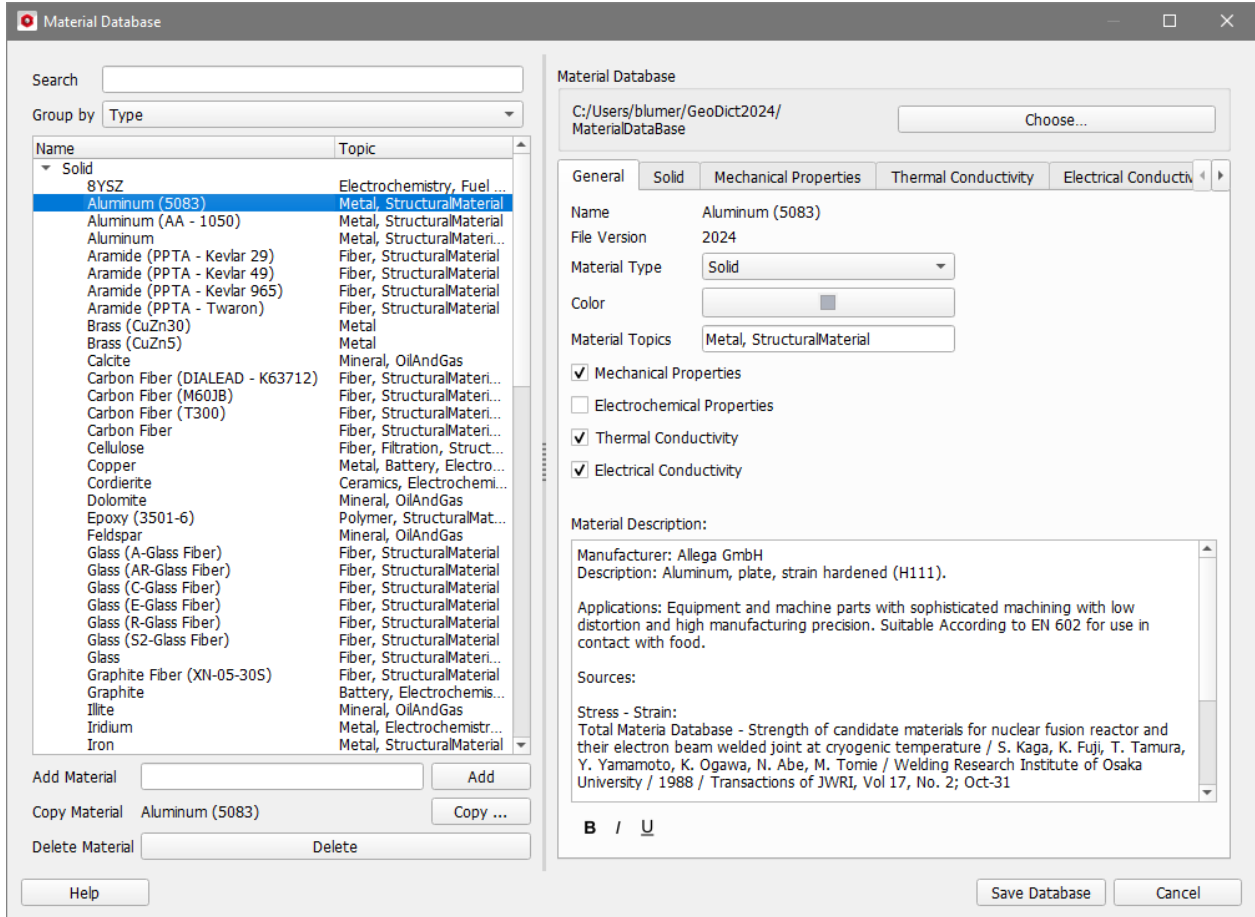


- Click any material button in generator or predictor modules, and then click **Open & Edit Material Database** in the **Material Selector** dialog box.



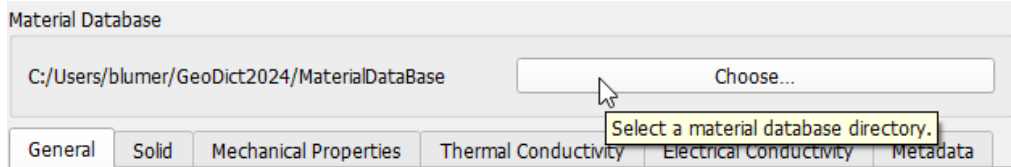
For the predictor modules (**ElastoDict**, **ConductoDict**, **FlowDict**, **DiffuDict**, **FilterDict**, etc.), the material buttons are located in the **Constituent Materials** tab of the **Solver Options**.

After clicking **Open & Edit Material Database**, the **Material Database** dialog opens:



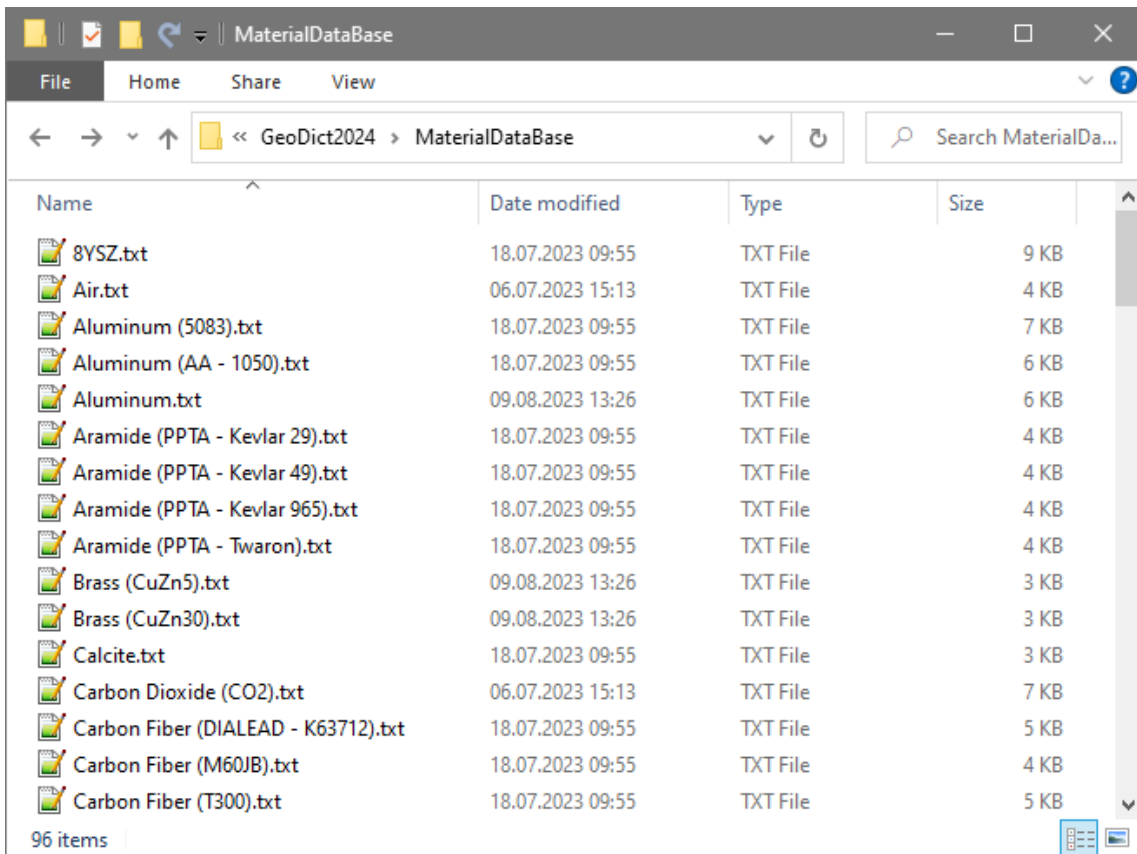
CHOOSE A MATERIAL DATABASE

On the upper right corner of the **Material Database** dialog, click **Choose...** to select a material database. A material database is a folder containing various *.txt files, one for each material (see also page [26](#)). Selecting a material database thus means to set the path to a material database directory.



The default path for the supplied GeoDict Material Database is

- C:\Users\username\GeoDict20XX\MaterialDataBase for Windows
- /home/username/.geodict20XX/MaterialDataBase for Linux



If the default material database needs to be recovered, it can be copied from the GeoDict installation directory, e.g., from:



An arbitrary folder can be chosen as Material Database. For example, a shared network folder could be chosen as material database folder. This way, the same database can be accessed by multiple GeoDict users.

If the current material database folder is deleted, it is automatically recovered from the installation folder at the next start of GeoDict.

Materials can be added to the Material Database in two ways:

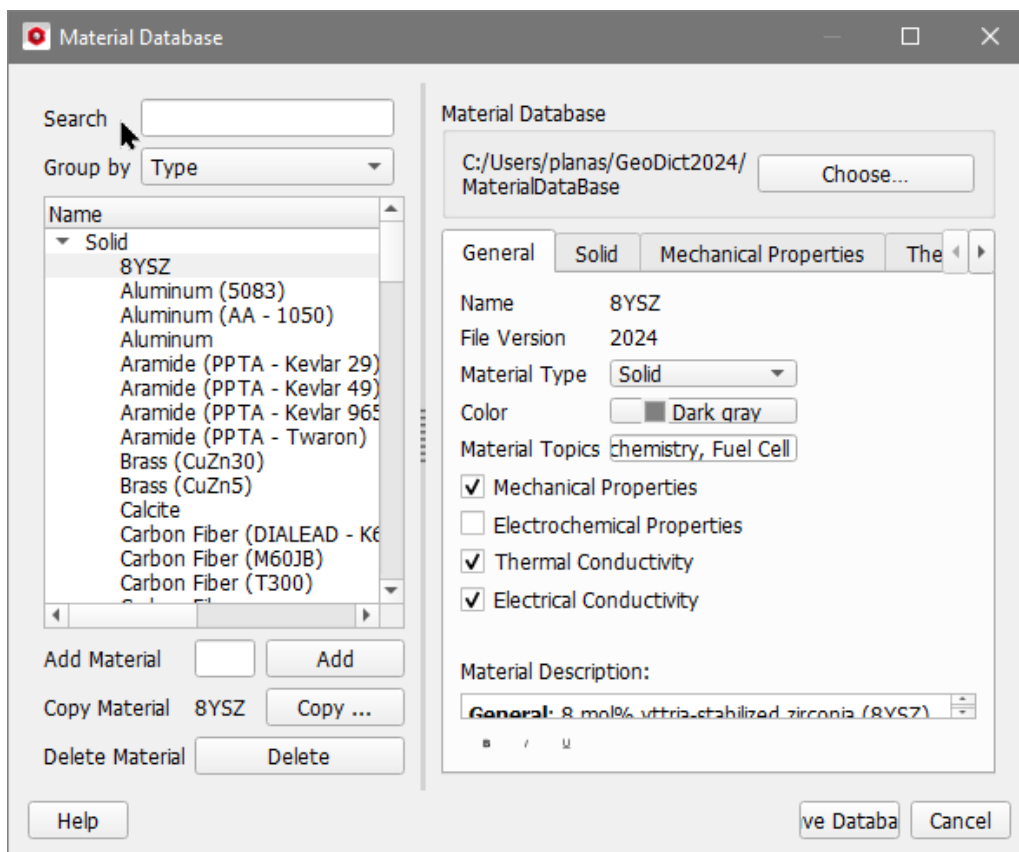
1. Add or copy materials in the material database dialog (see page [24](#))
2. Copy the corresponding *.txt files from another material database into the MaterialDataBase folder.

In this way, it is also possible to create a new material database with materials that are not shipped with **GeoDict**.

HOW TO USE THE MATERIAL DATABASE

The **GeoDict** Material Database dialog consists of two main panels. In the panel on the left side materials can be searched, grouped, added (see page [24](#)), copied (see page [24](#)) or deleted. On the right side, the currently chosen material can be edited (see page [19](#)).

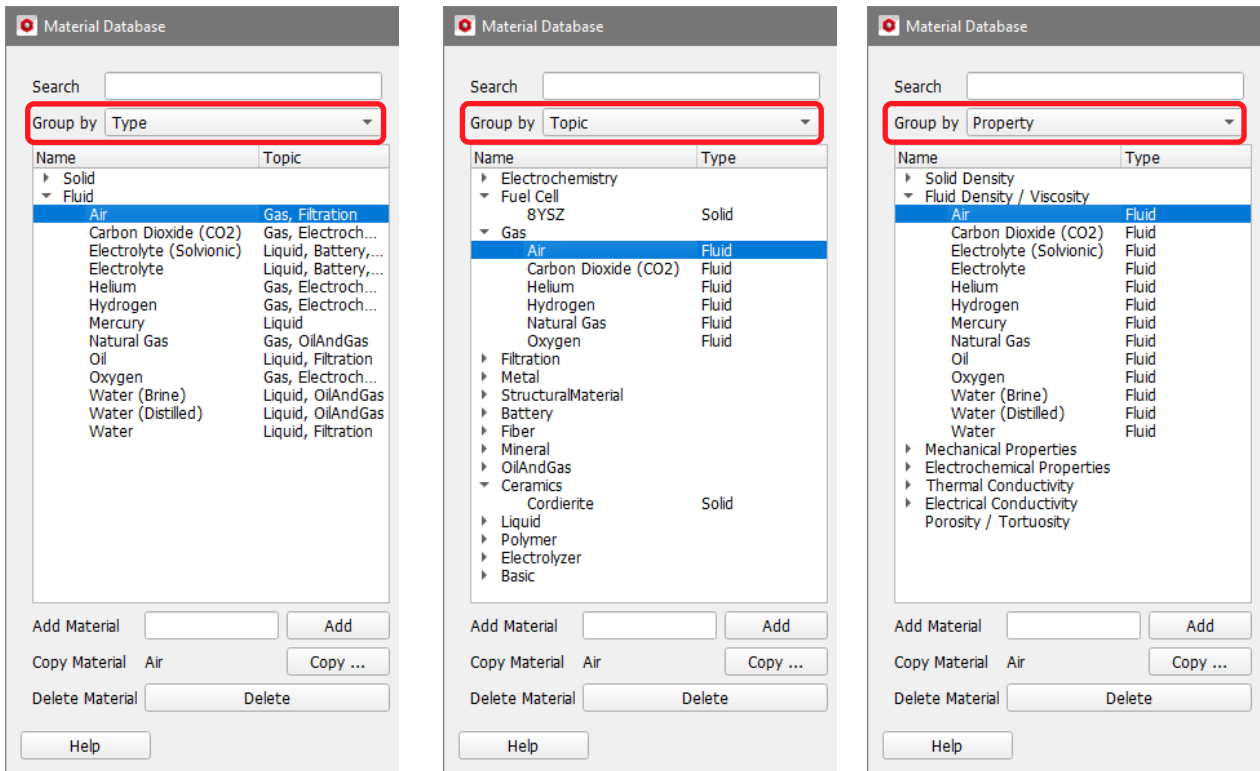
The material database can be searched with the search box at the top of the material database dialog.



Alternatively, the materials can be grouped by **Type**, by **Topic** or by **Property**.

The **Types** are **GeoDict**'s material categories (**Fluid**, **Solid** and **Porous**), while the **Topics** can be user-defined (See page [19](#)).

When choosing **Property**, all materials are grouped for which a corresponding property is defined.



Clicking on a material selects this material and its list entry is highlighted in blue.

With the **Delete** button the selected material is removed from the chosen material database. This means the *.txt file is deleted from the material database folder.

The **Help** button gives directly access to this User Guide.

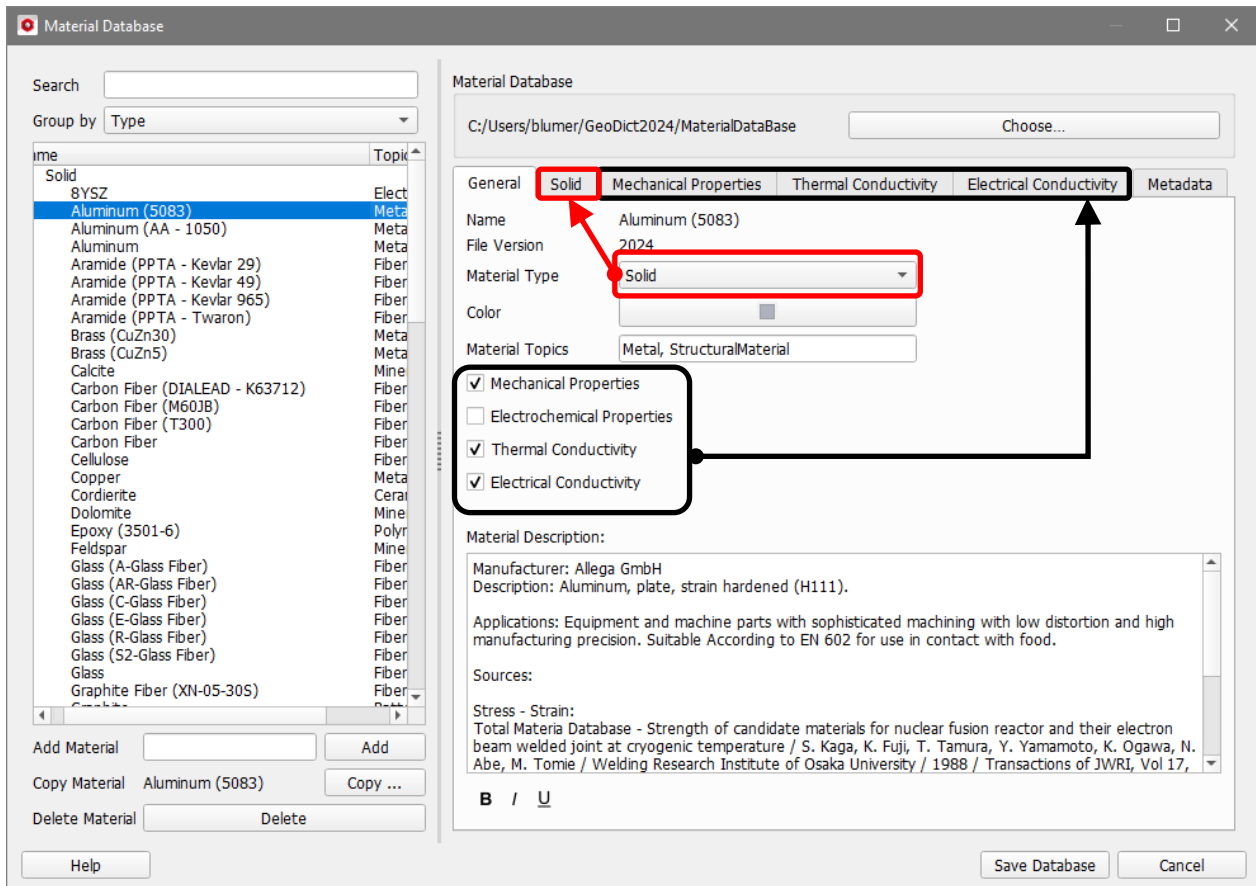
After editing is done, click **Save Database** to save the changes to the database (see also page 26) and close the Material Database dialog window. With **Cancel** the dialog window is closed without saving the changes.

EDIT EXISTING MATERIAL DATABASE ENTRIES

The material database can be edited by modifying or adding properties of constituent materials through the **Material Database** dialog.

In the left panel, click to highlight and choose one of the materials in the current **GeoDict** material database.

In the right panel, under the **General** tab, the **Material Type** (Solid, Fluid, Porous), its assigned **Color**, the **Material Topics** (e.g., Battery, Electrochemistry), the material **Properties**, and the **Material Description** can be edited.

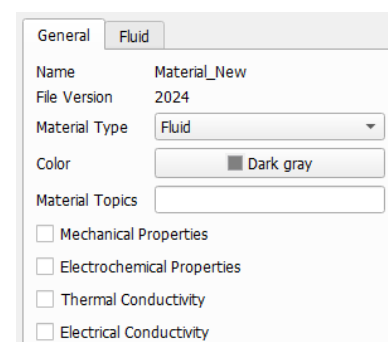


GENERAL

Three material types are available in **GeoDict**: **Fluid**, **Solid** and **Porous**. Depending on the material type, different material properties can be assigned.

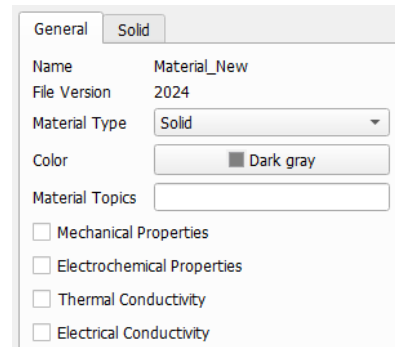
- For a **Fluid**, the density and the dynamic and kinematic viscosity are defined in the **Fluid** tab. Additionally, **Mechanical Properties**, **Electrochemical Properties**, **Thermal Conductivity**, and **Electrical Conductivity** can be selected as optional parameters.

Density, **Dynamic Viscosity**, **Kinematic Viscosity**, **Thermal Conductivity** and **Electrical Conductivity** can be temperature dependent, and the mechanical properties contain the option to add a thermal expansion coefficient.



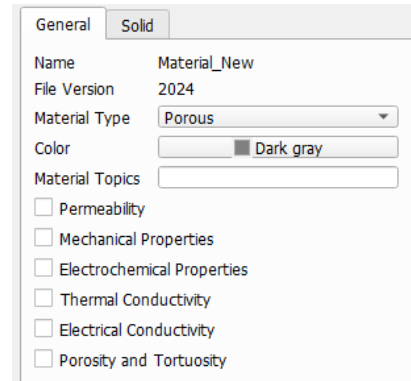
- For **Solid** materials, only the density must be defined in the **Solid** tab. Additionally, **Mechanical Properties**, **Electrochemical Properties**, **Thermal Conductivity**, and **Electrical Conductivity** can be selected as optional parameters.

Density, **Thermal Conductivity** and **Electrical Conductivity** can be temperature dependent, and the mechanical properties contain the option to add a thermal expansion coefficient.

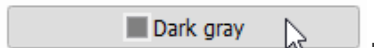


- Porous** materials have the same options as **Solid** materials, but they additionally allow to define the **Permeability** and **Porosity and Tortuosity**.

The **Porosity** and **Tortuosity** cannot be set to be temperature dependent.



The material color can be changed by clicking on the corresponding button, e.g.,



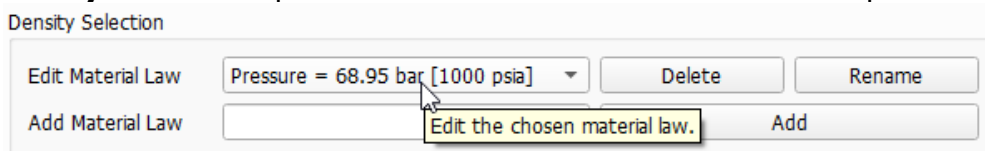
The other tabs depend on the material properties that are selected under the **General** tab. Available are **Mechanical Properties**, **Electrochemical Properties**, **Thermal Conductivity** and **Electrical Conductivity**. Additionally, for Porous material types, the **Permeability** and the **Porosity and Tortuosity** can be chosen.

In the **Material Description** panel the references for the predefined material properties can be found. This text box can be edited by the user to add more comments on the material.

SOLID AND FLUID PROPERTIES

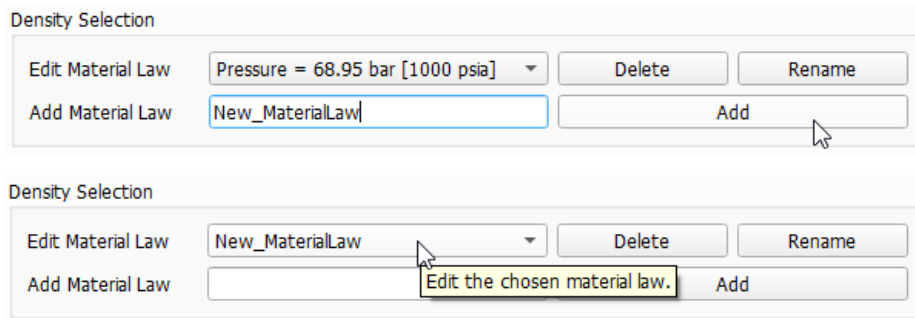
Depending on the chosen Material Type, the second tab is called Solid (for Solid and Pore) or Fluid (for Fluid). Here, the density and, for fluids, the dynamic and kinematic viscosity are defined. Multiple **Material Laws** can be created for different application cases or physical conditions. For example, the physical properties may change for varying pressure values. Thus, for different pressure values an individual material law can be defined.

In the **Density Selection** panel select a material law from the drop-down menu.



Below, the current values are shown and can be edited. The selected material law can be deleted with **Delete** and a new name can be given with **Rename**.

To create a new material law, type its name in the **Add Material Law** box and click **Add**. Then, the values can be entered below and a material law with the entered name is listed under **Edit Material Law**.

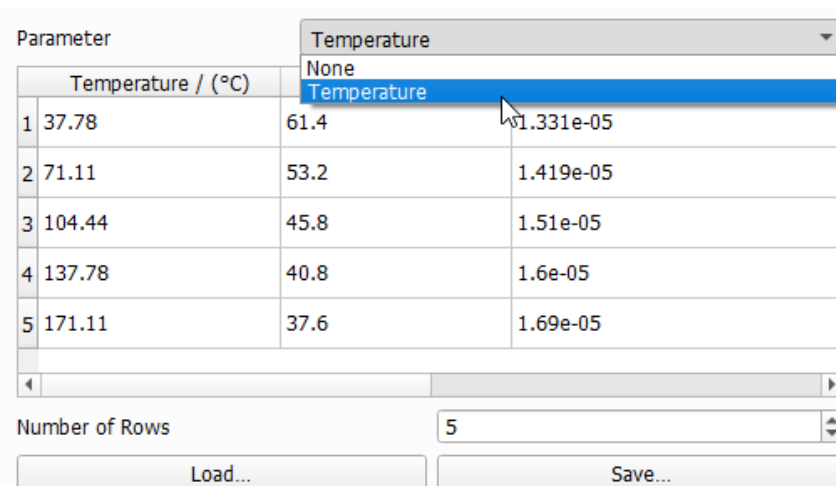


From the **Parameter** drop-down menu choose if the density (and viscosity for fluids) should be temperature dependent or not. In the latter case, simply enter in the corresponding values.

For the parameter **Temperature**, a table allows to enter the corresponding density and viscosity values for different temperature values. This table can be saved as ASCII *.txt file and such a file with values can also be loaded into the material database.

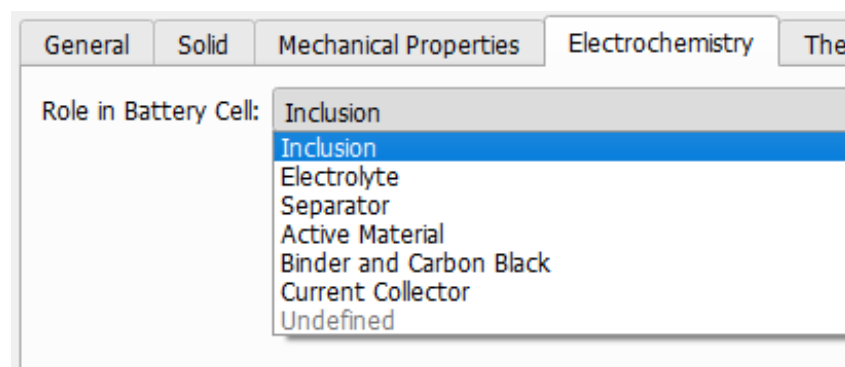
MECHANICAL PROPERTIES

Under **Mechanical Properties**, multiple material laws can be defined. Later, one of them can be selected to run a simulation. For further information about how to define the Mechanical Properties of materials, refer to the [ElastoDict](#) handbook of the User Guide.



ELECTROCHEMICAL PROPERTIES

In the **Electrochemical Properties** section, the parameters are set depending on the role of the material in a lithium-ion battery cell. First, select the role from the drop-down menu.



Enter the parameters if necessary. For some roles (e.g., Separator), no parameters need to be entered. More details about the parameters can be found in the [BatteryDict](#) handbook of the User Guide.

THERMAL CONDUCTIVITY

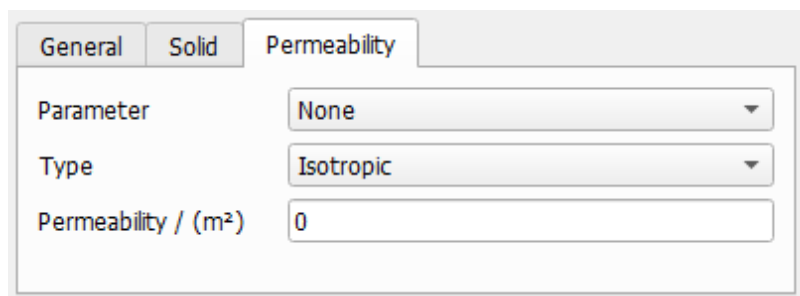
Thermal conductivity is used, e.g., in [ConductoDict](#) and can be temperature dependent or not. It can be isotropic, transverse isotropic or orthotropic and the material laws can be edited as described above on page [20](#). More information on Thermal conductivity can be found in the [ConductoDict](#) handbook of the User Guide.

ELECTRICAL CONDUCTIVITY

Electrical conductivity works analogously to thermal conductivity and details can also be found in the [ConductoDict](#) handbook of the User Guide.

PERMEABILITY

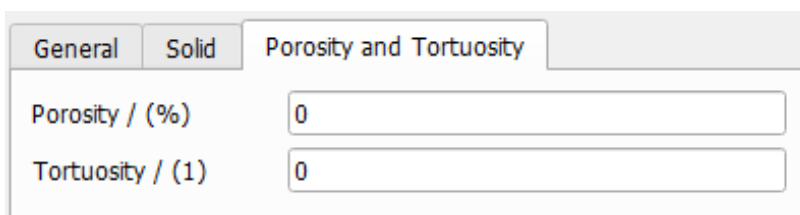
The Permeability can have the parameter Temperature or none. It can be the same in all directions (**Isotropic**) or can be different in X, Y, and Z direction (**Anisotropic**). The tab works analogously as described above on page [20](#).



The screenshot shows a software interface with three tabs: 'General', 'Solid', and 'Permeability'. The 'Permeability' tab is active. It contains three input fields: 'Parameter' with a dropdown menu set to 'None', 'Type' with a dropdown menu set to 'Isotropic', and 'Permeability / (m²)' with a text input field containing the value '0'.

POROSITY AND TORTUOSITY

Porosity and Tortuosity can only be entered as scalar values with no parameters.

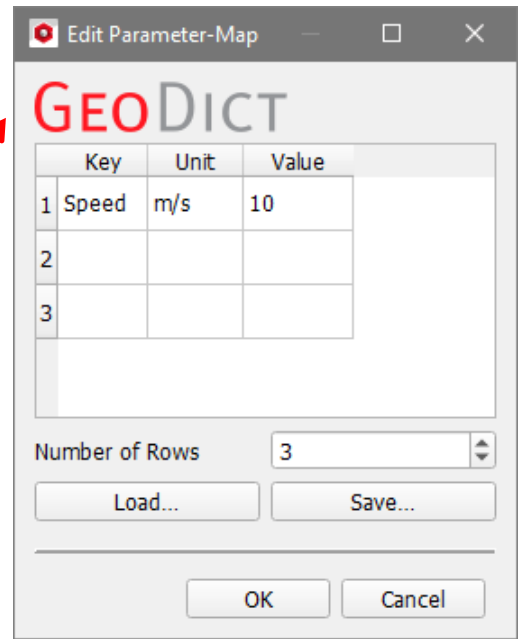
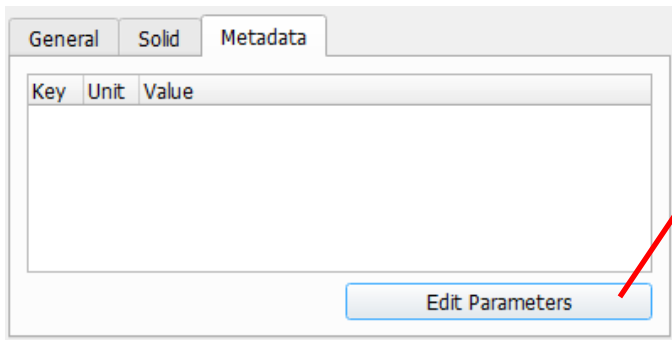


The screenshot shows a software interface with three tabs: 'General', 'Solid', and 'Porosity and Tortuosity'. The 'Porosity and Tortuosity' tab is active. It contains two input fields: 'Porosity / (%)' and 'Tortuosity / (1)', both with text input fields containing the value '0'.

METADATA

In the metadata tab, custom properties can be defined, e.g., it is possible to add new physical properties. They can be accessed, e.g. through a Python interface.

Click on **Edit Parameters** to open the **Edit Parameter-Map** dialog. Enter a **Key**, a **Unit**, and a **Value** for this key in the chosen unit. The metadata will also be saved in the text file for the material as **Parameter Map**.

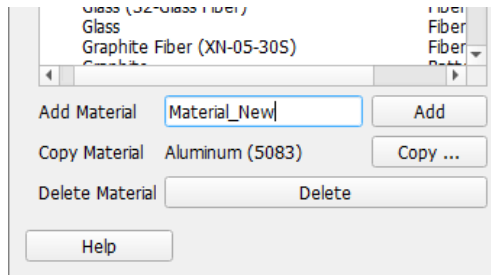


ADDING NEW MATERIALS TO THE DATABASE

The material database can be expanded by adding new constituent materials or by copying (and editing) existing materials in the **Material Database** dialog.

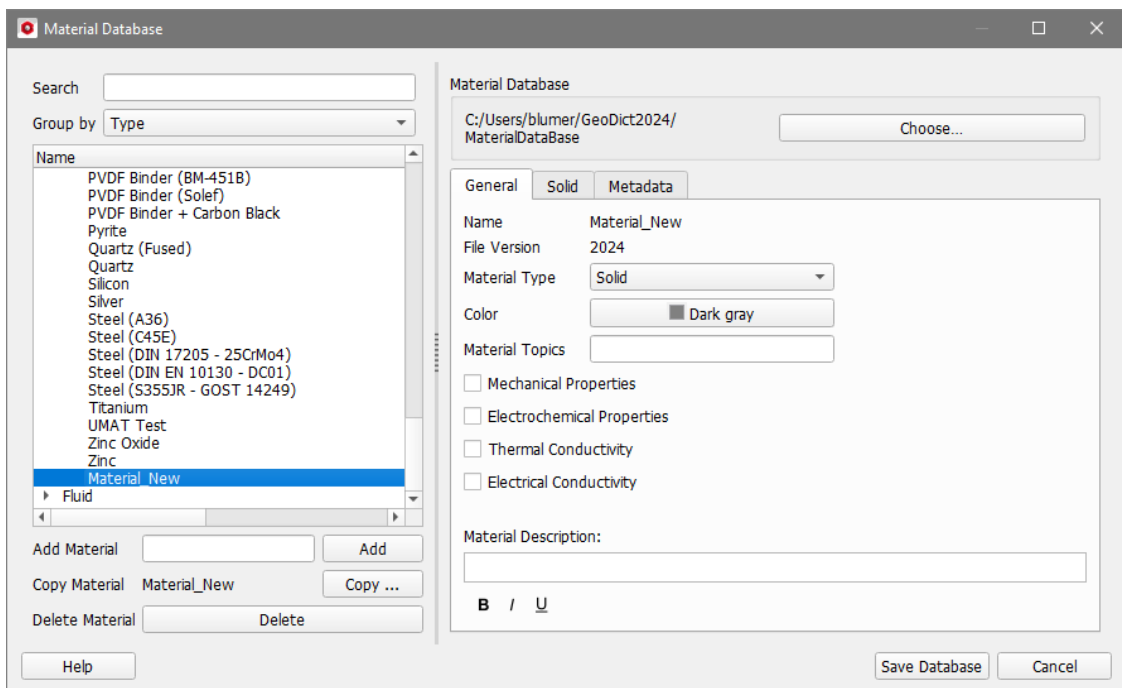
CREATING NEW MATERIALS

To add a new material to the database, enter a name for the new material in the corresponding box in the lower left corner of the dialog (e.g., **Material_New** in the example below). Click **Add**.



Material_New appears listed in the left panel and default values appear in the right panel under the General and the Solid tabs.

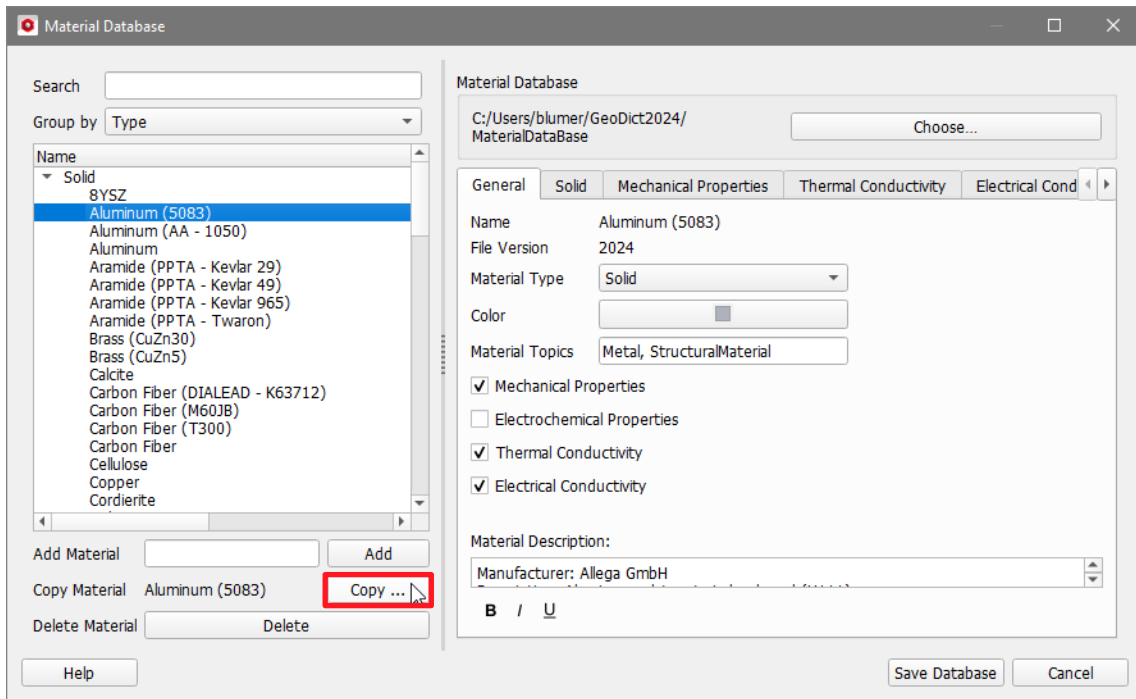
When a material is newly created, its **Material Type** is set to **Solid** per default and therefore it appears under the **Solid** tree listed at the very end.



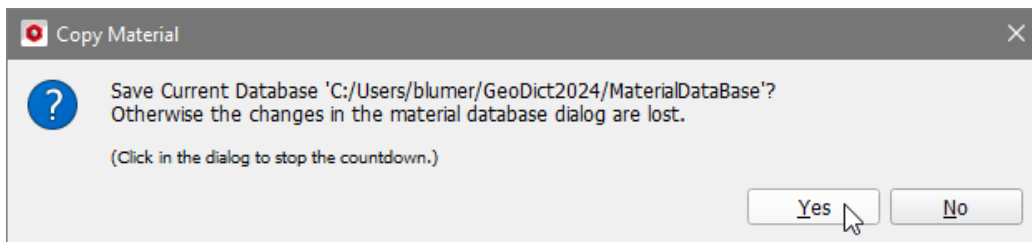
In the next step, the **Material Type** and its properties can be set under the corresponding tabs (see the corresponding paragraph on page 19).

COPYING EXISTING MATERIALS

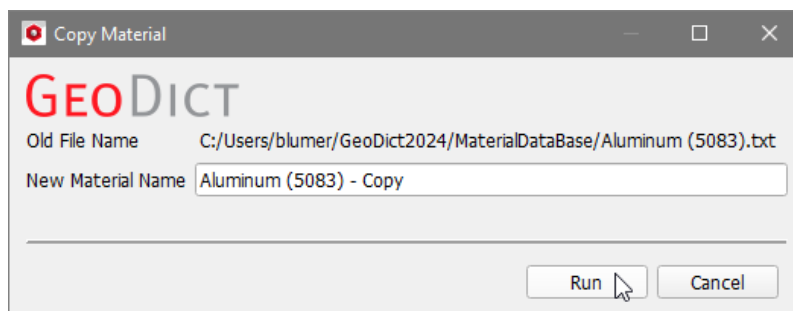
Alternatively, an existing material can be copied by selecting the material and clicking **Copy ...**



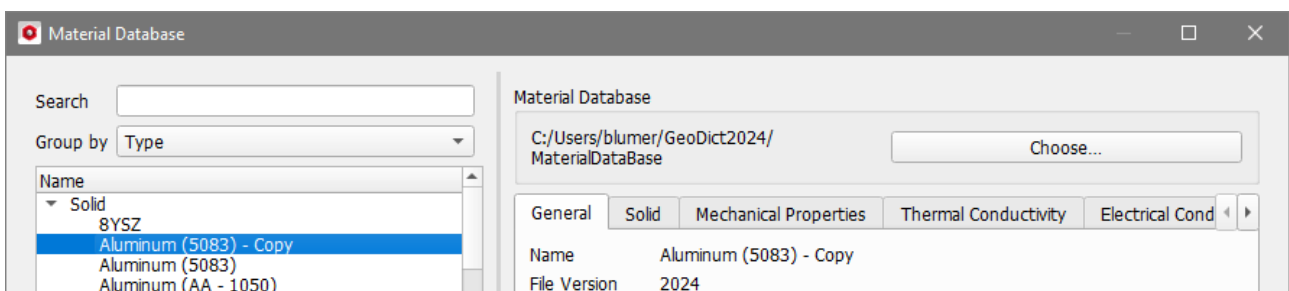
A dialog is shown, which asks if the material database should be saved before adding the copied material. It is recommended to choose **Yes** to proceed.



In the next step, the name for the new copy of the material can be selected. In this example, the default name is kept. Click **Run** to create the material.



Then, the new material is shown in the material database and can be edited as explained before.



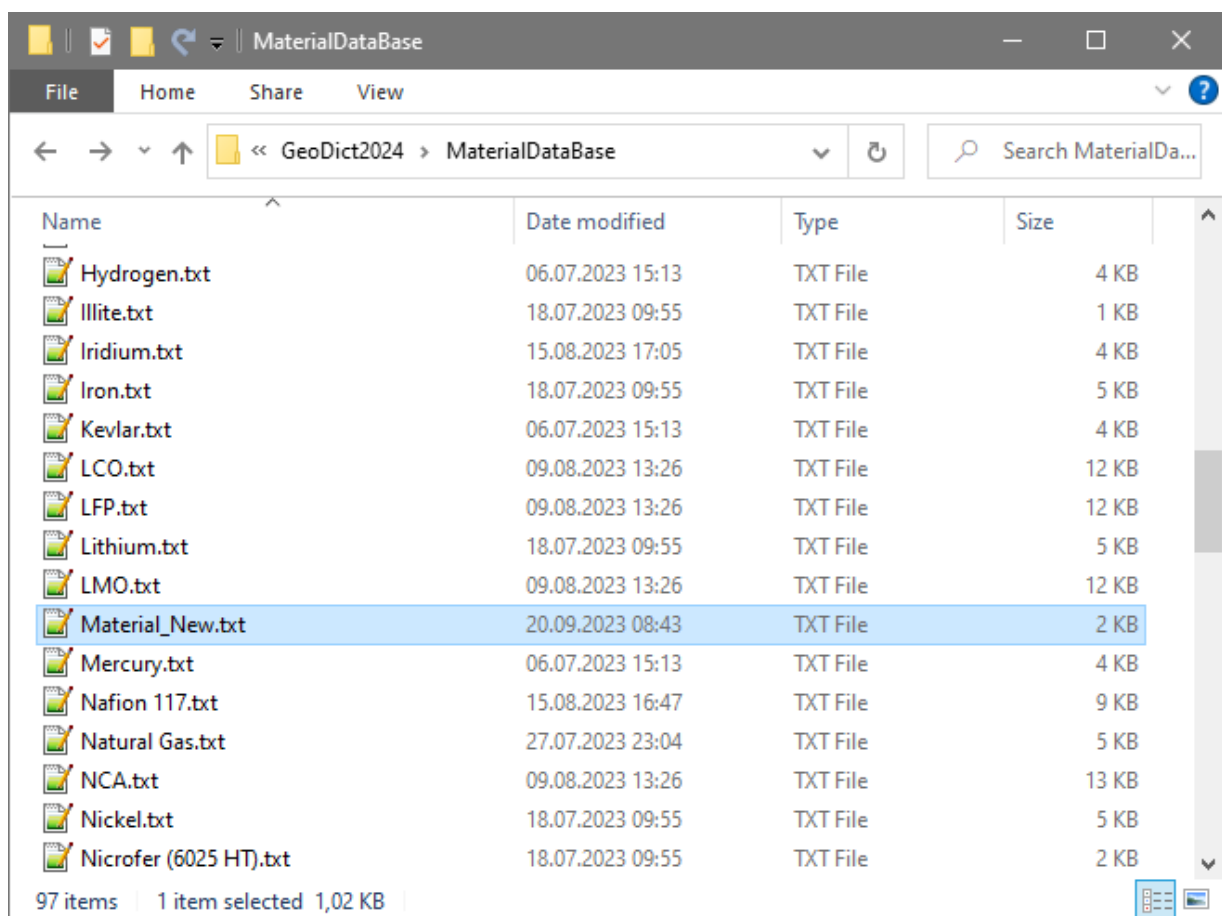
SAVING THE MATERIAL DATABASE

When all parameters are set as desired, either continue with the next material or click **Save Database** at the bottom of the **Material Database** dialog to save all changes to the database and close the window.



The material database entries are stored as *.txt files in the current material database folder (either the default GeoDict material database or a user-selected database).

The filename of the *.txt file is the name of the material in the database (here: Material_New.txt). This text file contains all information about the material database entry. It can be shared to other users and copied to other GeoDict material databases.



These text files can be opened and edited with any text editor, such as Notepad++. All parameters can also be changed directly in the *.txt file. As an example, the file for **Aluminum (5083)** is shown.

```

C:\Users\blumer\GeoDict2024\MaterialDataBase\Aluminum (5083).txt - Notepad++
File Edit Search View Encoding Language Settings Tools Macro Run Plugins Window ?
Aluminum (5083).txt
33 <Material>
34   Type                               Solid
35   <Color>
36     RGB                               173,178,189
37   </Color>
38   Topics                              Metal,StructuralMaterial
39   <Solid>
40     Parameter                          None
41     Density                            2660 [kg/m^3]
42   </Solid>
43   <Thermal>
44     <MaterialLaw1>
45       Name                             Iso. Law
46       Parameter                         Temperature
47       Type                              Isotropic
48       Temperature                       20 [Celsius]
49       Conductivity                       112.5 [W/(mK)]
50     </MaterialLaw1>
51   </Thermal>
52   <Electrical>
53     <MaterialLaw1>
54       Name                             Iso. Law
55       Parameter                         None
56       Type                              Isotropic
57       Conductivity                       16998640 [S/m]
58     </MaterialLaw1>
59   </Electrical>
60   <Elasticity>
61     <MaterialLaw1>
62       <Measurement>
63         Strain                          0,3.9,11.52,13.46,15.27,17.94,19.4,21.5,23.32,24.
64         Stress                          0,0.171,0.232,0.245,0.267,0.278,0.285,0.279,0.288
65       </Measurement>
66       Type                              Isotropic
67       Name                              Elasto-Plastic (20 °C)
68       YoungsModulus                      71 [GPa]
69       PoissonsRatio                       0.33 [1]
70       AllowThermalExpansion               true
71       ThermalExpansion                    2.38e-05 [1/K]
72       PlasticityType                      Exponential // Possible values: None, Constant, A
73       ViscoplasticityType                  None // Possible values: None, PerzynaLinear, Perzyna
Python file      length : 6.976  lines : 108      Ln : 31  Col : 15  Pos : 3.359      Windows (CR LF)  UTF-8-BOM      INS

```

Technical
documentation:

Anne Blumer
Sebastian Rief
Barbara Planas

MATH
2 MARKET

Math2Market GmbH

Richard-Wagner-Str. 1, 67655 Kaiserslautern, Germany
www.geodict.com