

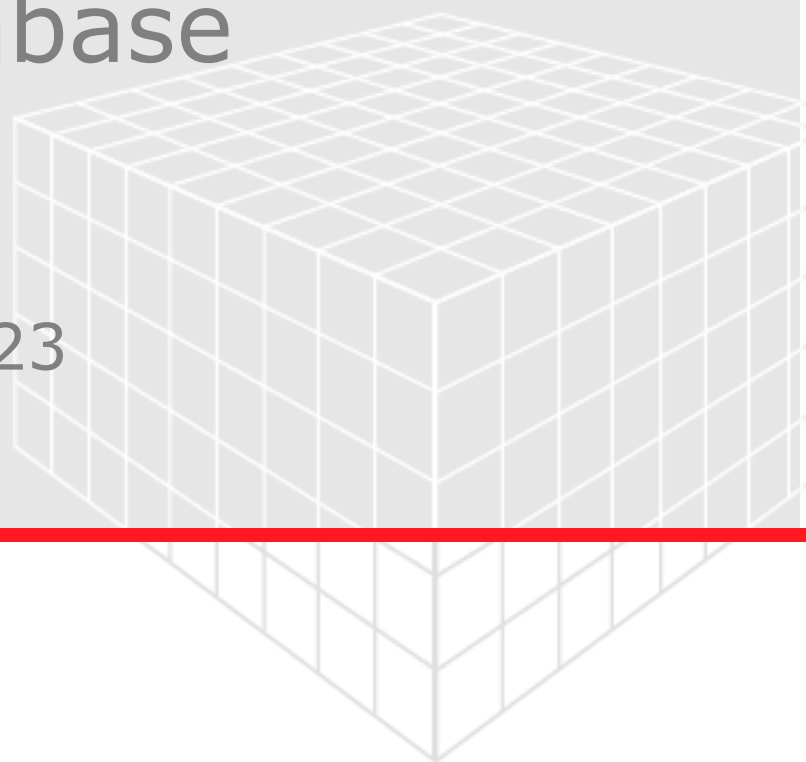
GEO DICT

Material database

User Guide

GeoDict release 2023

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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

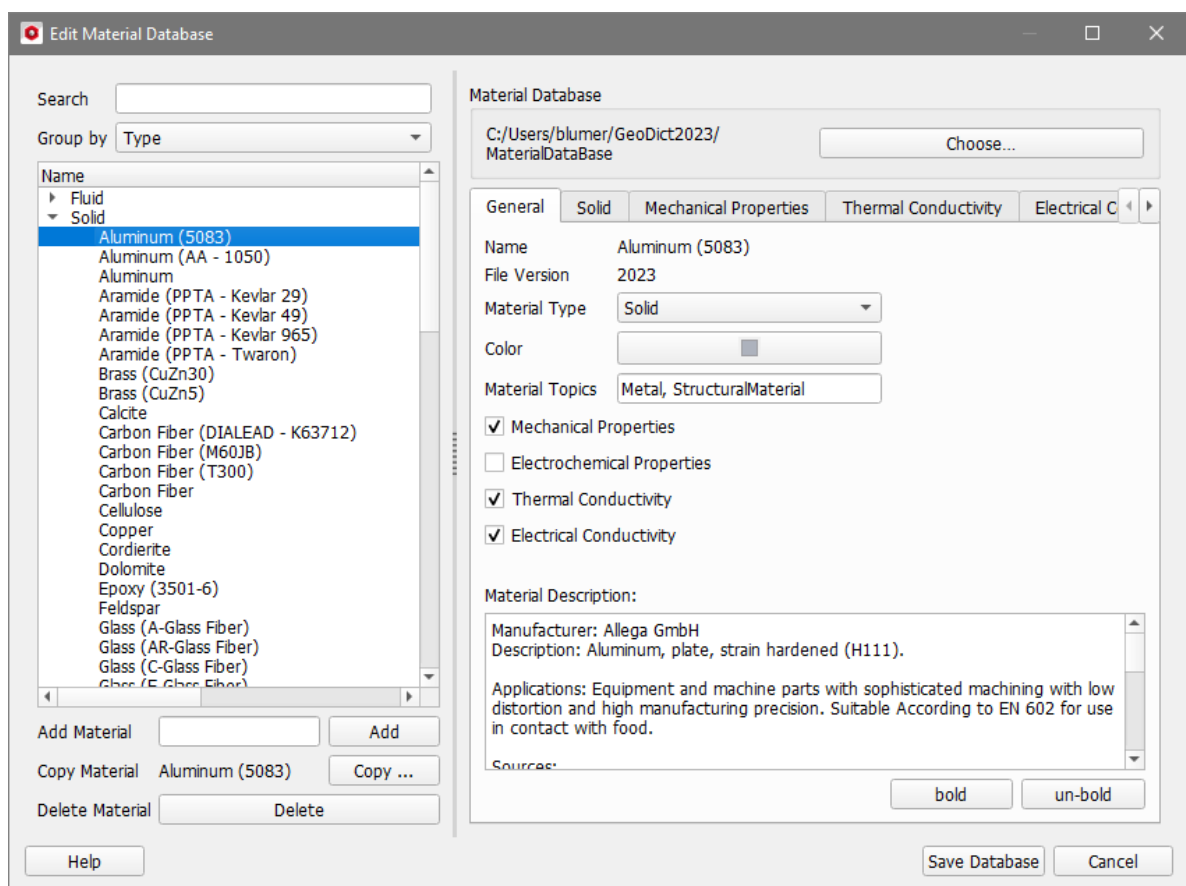
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THE GEO_DICT MATERIAL DATABASE

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 for the simulation run. However, it is always possible to change the materials and their properties prior to simulation.

MATERIALS IN GEODICT

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 must be defined. Additionally, **Mechanical Properties**, **Electrochemical Properties**, **Thermal Conductivity**, and **Electrical Conductivity** can be selected as optional parameters.

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

The screenshot shows the 'Fluid' tab of the material properties dialog. The 'Material Type' is set to 'Fluid'. Under 'Material Topics', the following options are available and unchecked: Mechanical Properties, Electrochemical Properties, Thermal Conductivity, and Electrical Conductivity. The 'Color' is set to 'Dark gray'.

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

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

The screenshot shows the 'Solid' tab of the material properties dialog. The 'Material Type' is set to 'Solid'. Under 'Material Topics', the following options are available and unchecked: Mechanical Properties, Electrochemical Properties, Thermal Conductivity, and Electrical Conductivity. The 'Color' is set to 'Dark gray'.

- **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.

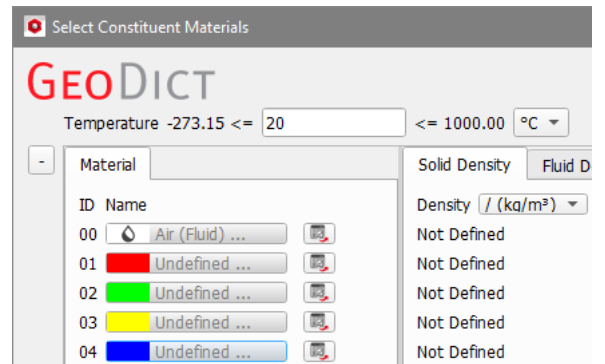
The screenshot shows the 'Porous' tab of the material properties dialog. The 'Material Type' is set to 'Porous'. Under 'Material Topics', the following options are available and unchecked: Permeability, Mechanical Properties, Electrochemical Properties, Thermal Conductivity, Electrical Conductivity, and Porosity and Tortuosity. The 'Color' is set to 'Dark gray'.

Materials can either be selected from the GeoDict material database or **Manual** 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.

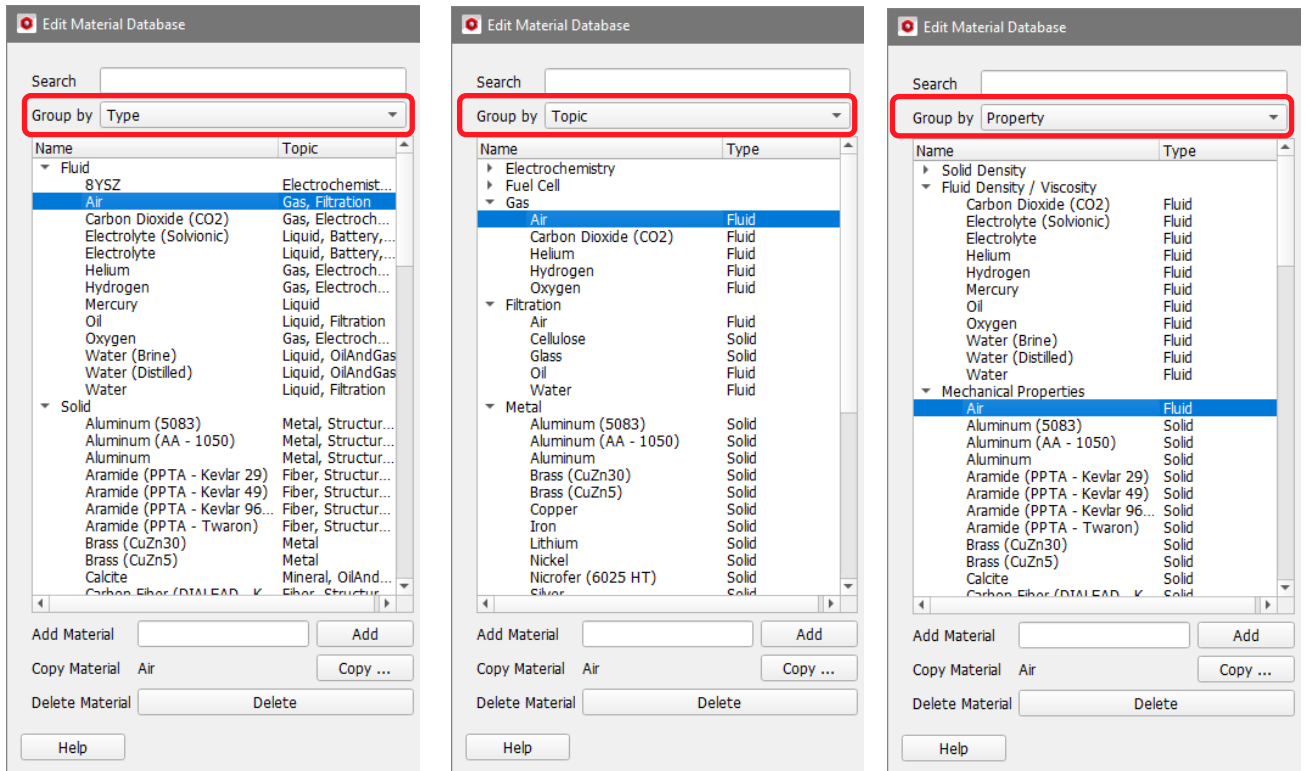
Manual materials allow to quickly set the needed parameters, whereas using materials from the material database allows to reuse them for further simulations. Furthermore, materials defined in the GeoDict material database may have more complex properties than **Manual** materials. For example, when defining a manual material in the **ElastoDict** settings, it is not possible to select nonlinear material laws.

In some cases, the material for a given material ID might be unclear. Then, the material is **Undefined**.

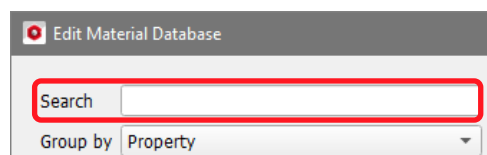
Choose a material for these IDs before running simulations on the structure.



The materials in the material database 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 16). When choosing **Property**, all materials are grouped for which a corresponding property is defined.



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

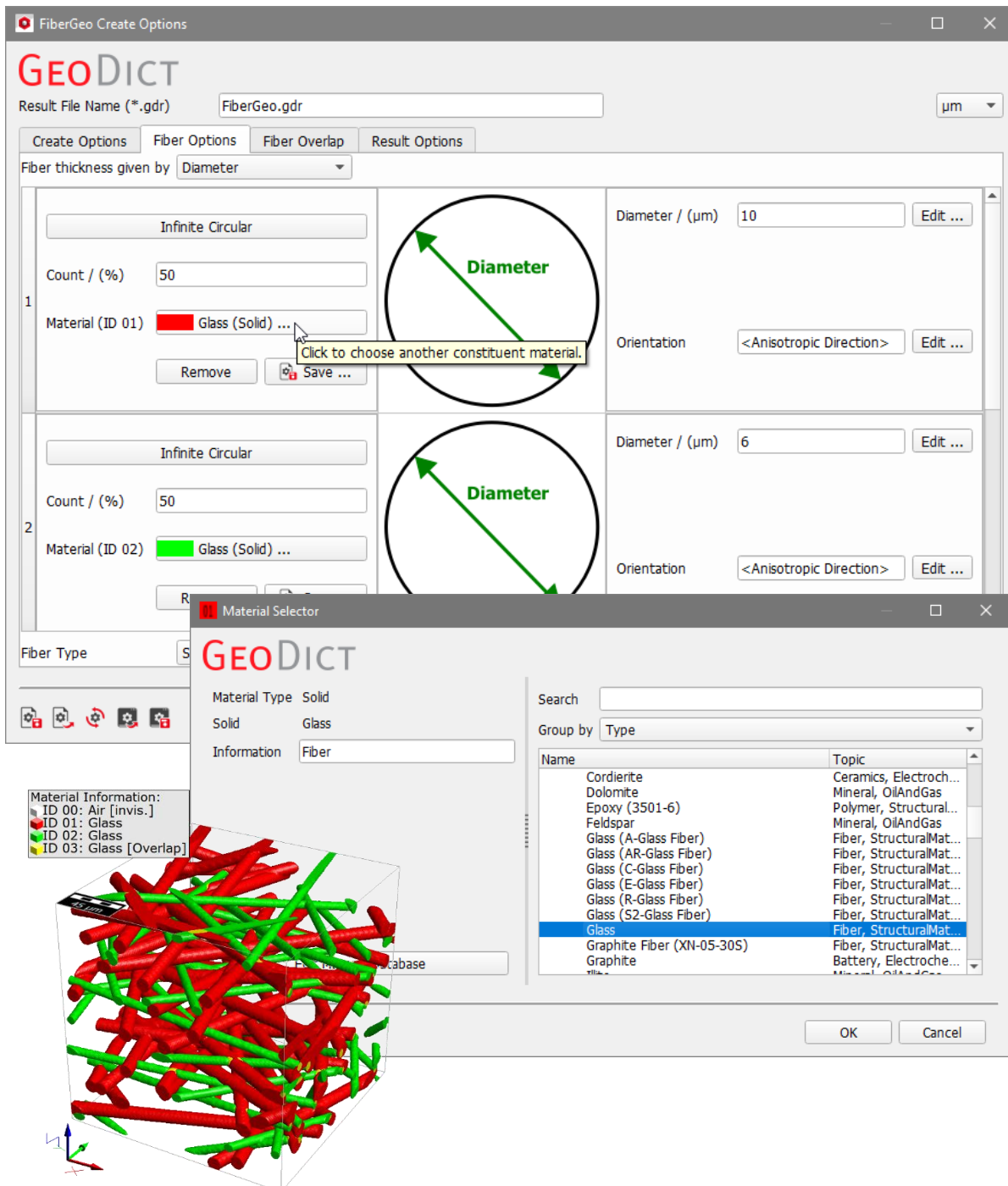


SETTING THE CONSTITUENT MATERIALS IN GEO-DICT

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

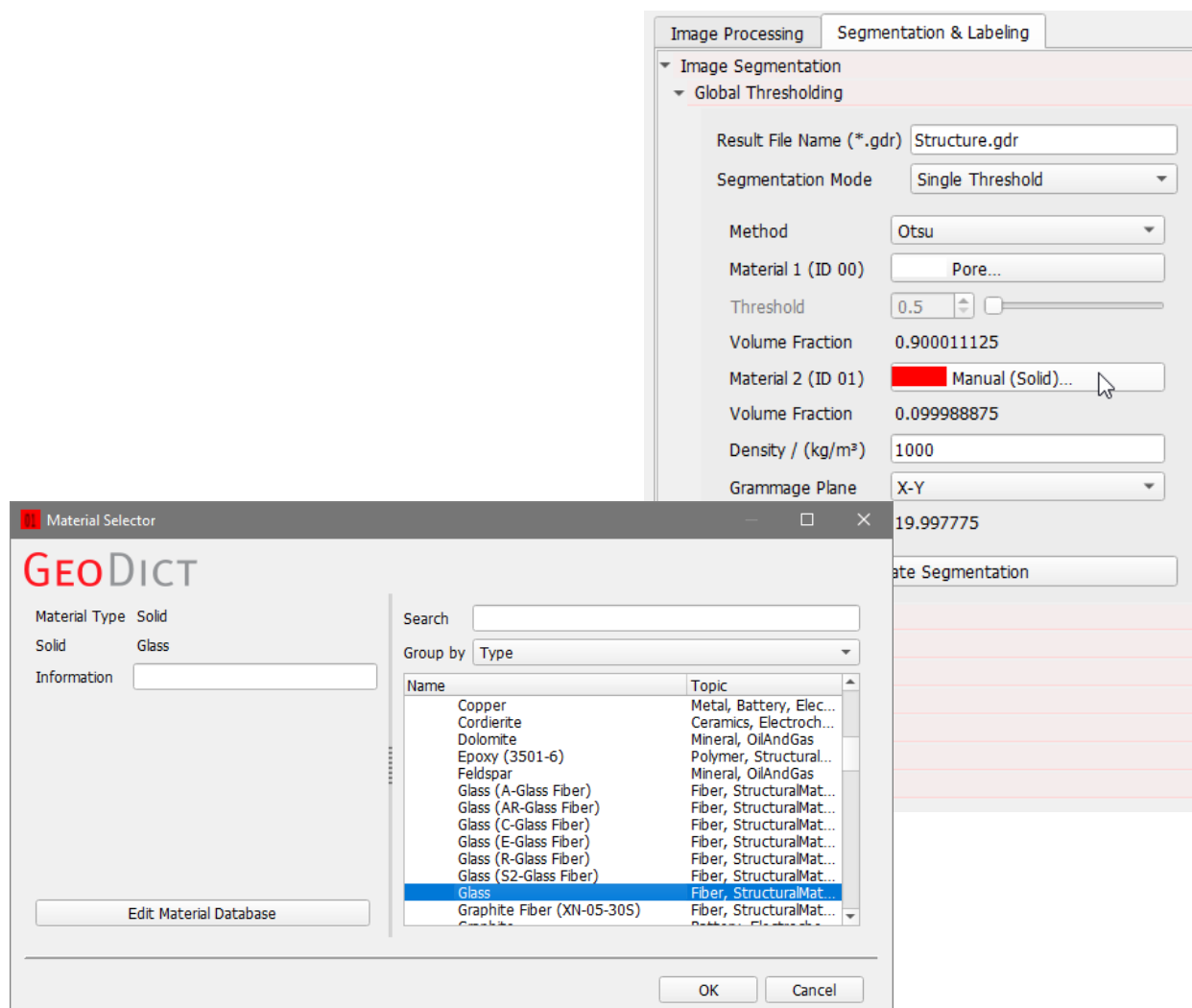
An example for the selection of the constituent materials in FiberGeo is shown below. For each fiber type, the material can be selected by clicking the corresponding button. The **Material Selector** dialog opens, and all materials stored in the current material database are available.



SETTING MATERIALS DURING IMPORT

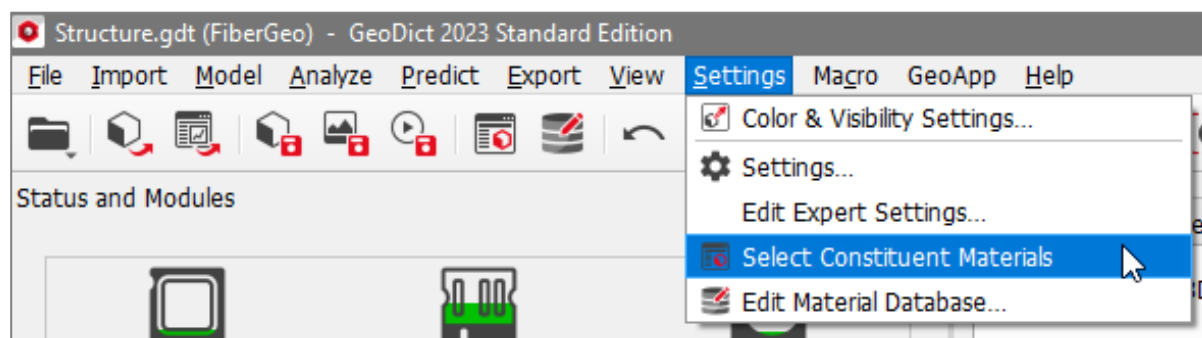
When a structure is imported in GeoDict (e.g., from a μ CT-scan), its constituent materials can be set during the import.

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



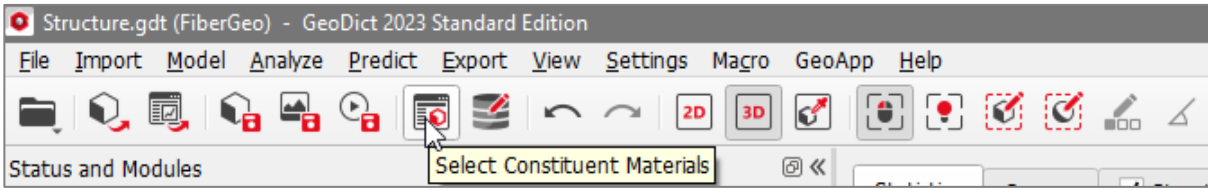
SETTING MATERIALS FOR THE CURRENT STRUCTURE

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

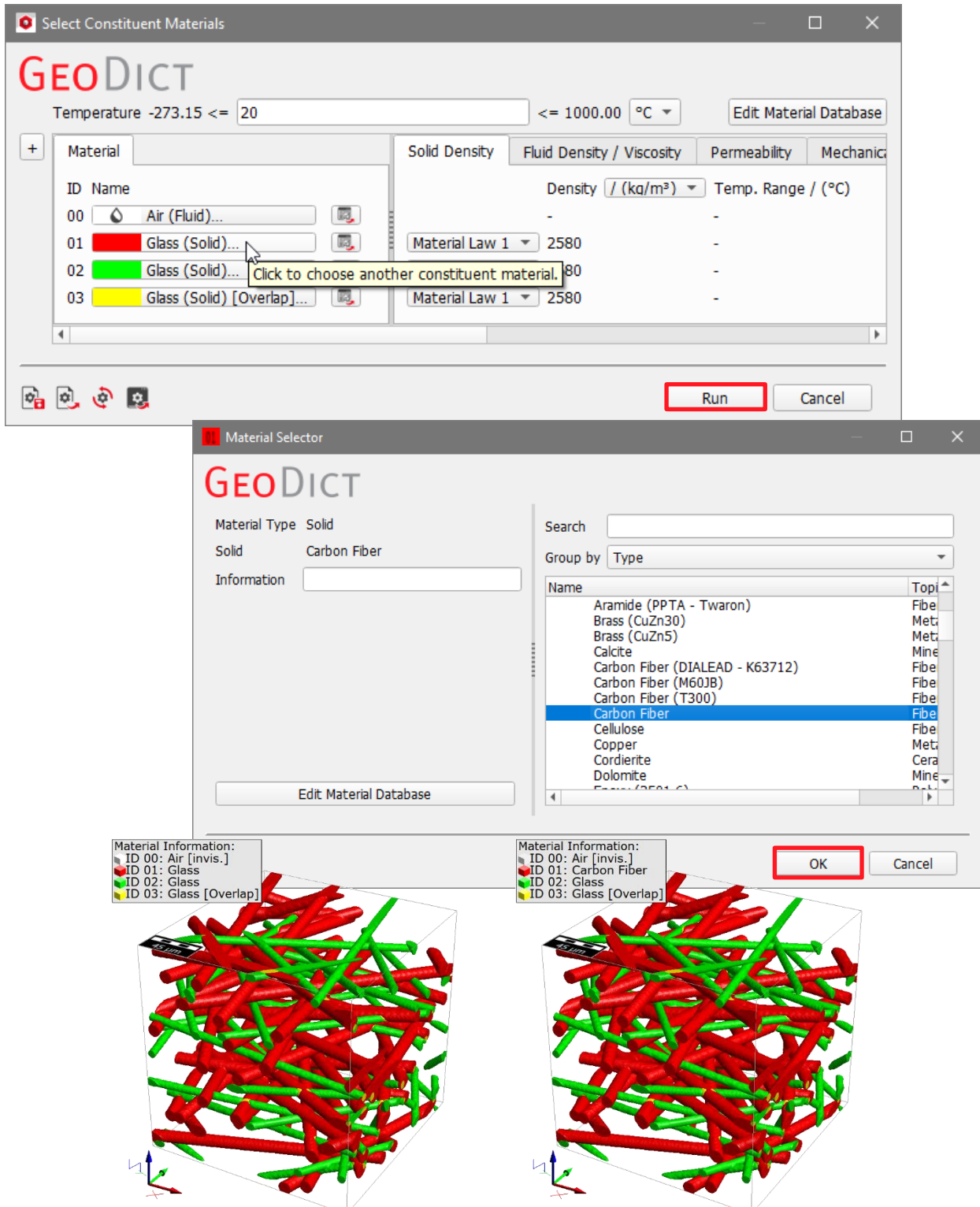


The GeoDict Material Database

Alternatively, click the corresponding icon in the toolbar.



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

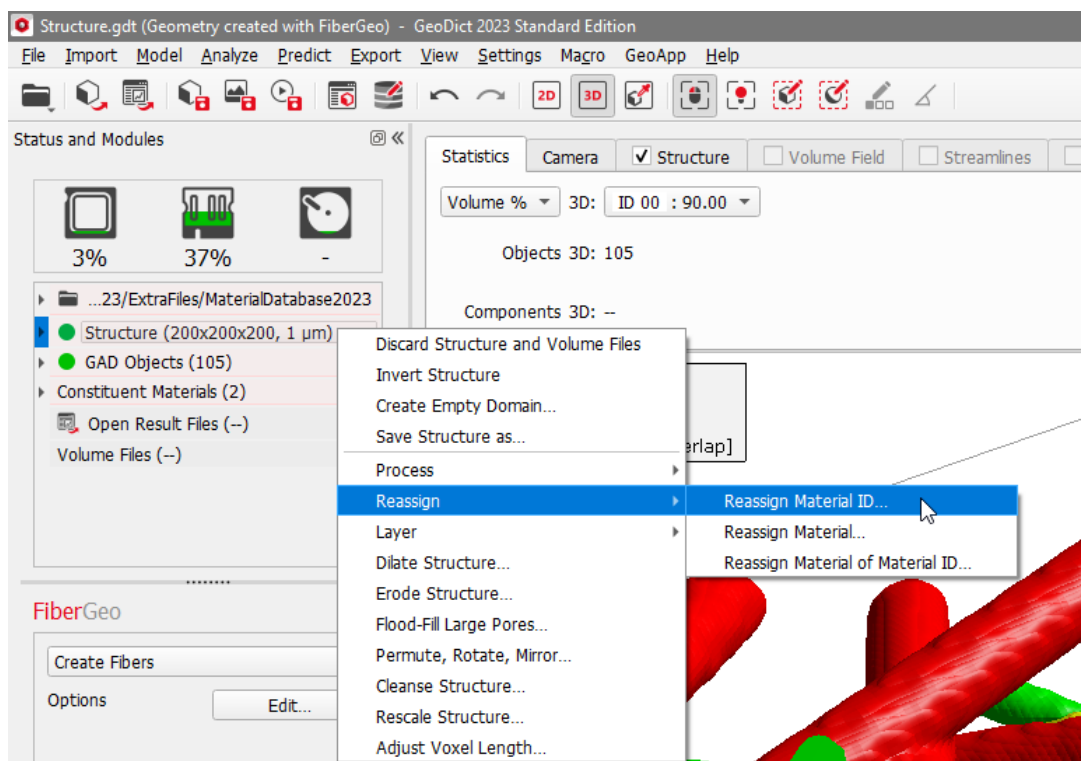


REASSIGNING MATERIALS AND MATERIALS IDS

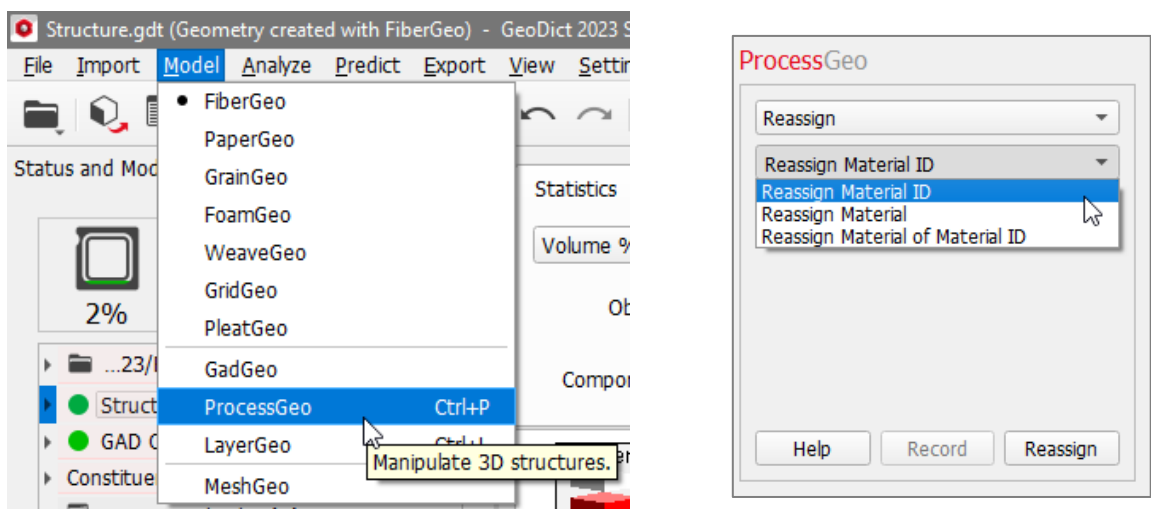
One option to change materials in the structure is the **Select Constituent Materials** dialog, as described [above](#). Depending on the use case, there are other options available through the **ProcessGeo** module.

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 handbook](#) of this 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.

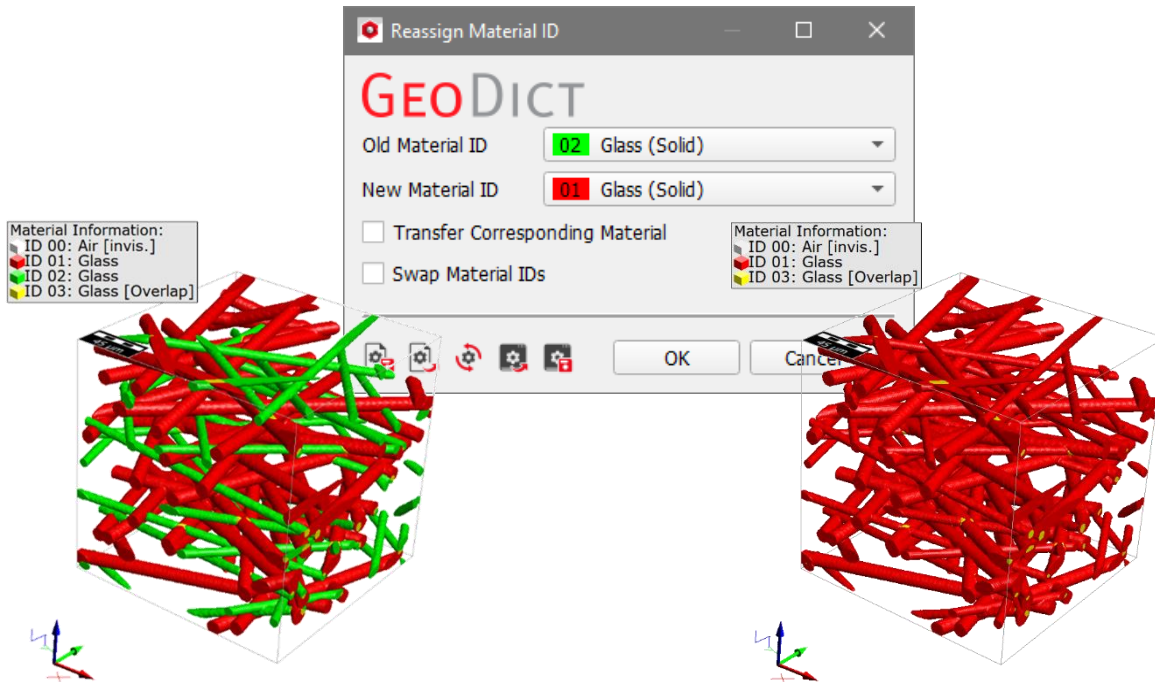


Alternatively, these options are also available from the menu bar by selecting **Model** → **ProcessGeo** → **Reassign**.



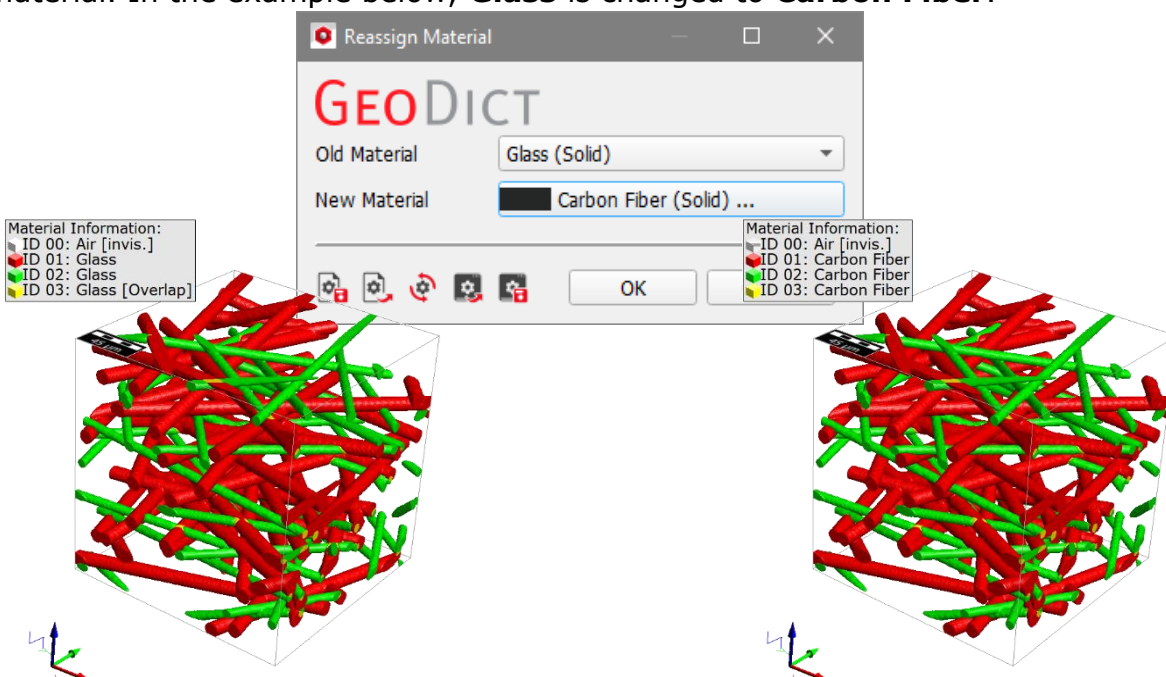
REASSIGN MATERIAL ID

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.



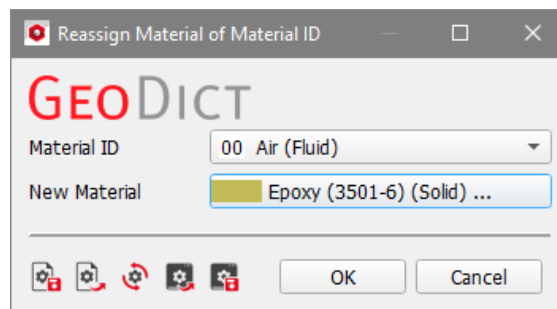
REASSIGN MATERIAL

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**.

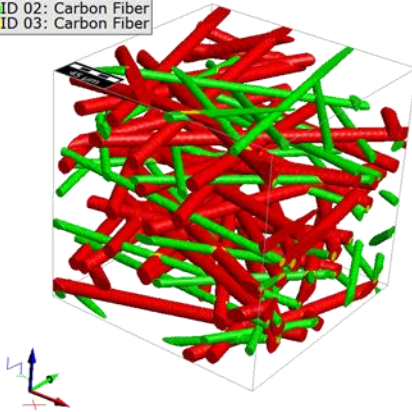


REASSIGN MATERIAL OF MATERIAL ID

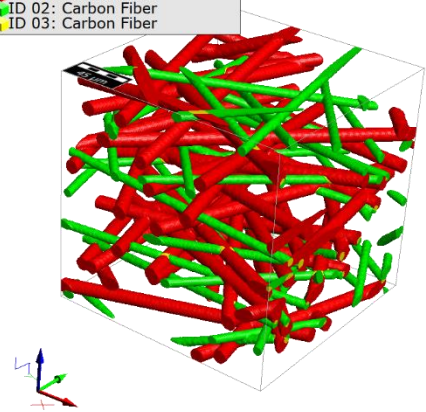
Reassign Material of Material ID corresponds to the option available in the **Select Constituent Materials** dialog. As shown in this example, the material is changed for one selected material ID (here: *Air* to *Epoxy* for Material ID 00).



Material Information:
ID 00: Air [invis.]
ID 01: Carbon Fiber
ID 02: Carbon Fiber
ID 03: Carbon Fiber




Material Information:
ID 00: Epoxy (3501-6) [invis.]
ID 01: Carbon Fiber
ID 02: Carbon Fiber
ID 03: Carbon Fiber

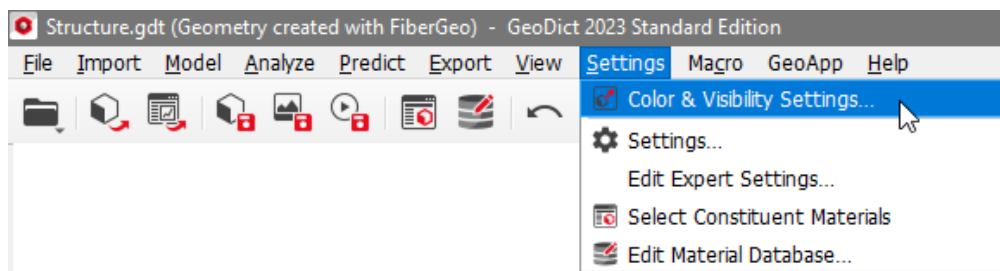


MATERIAL COLORS IN GEODICT


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 16). In the following, it is described how to use these stored material colors for display.

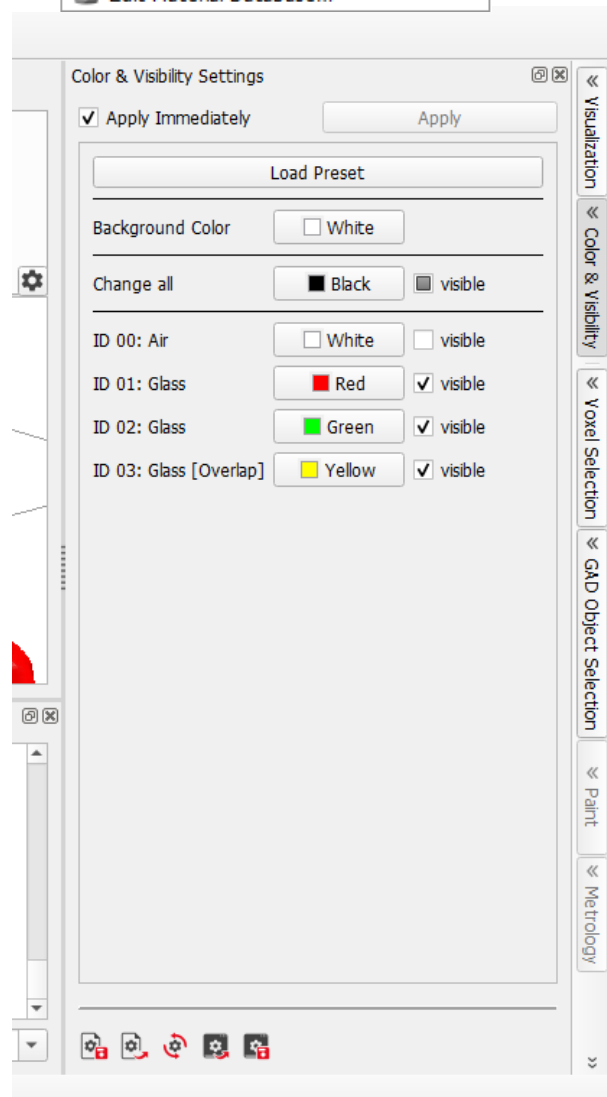
COLOR SELECTION

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.

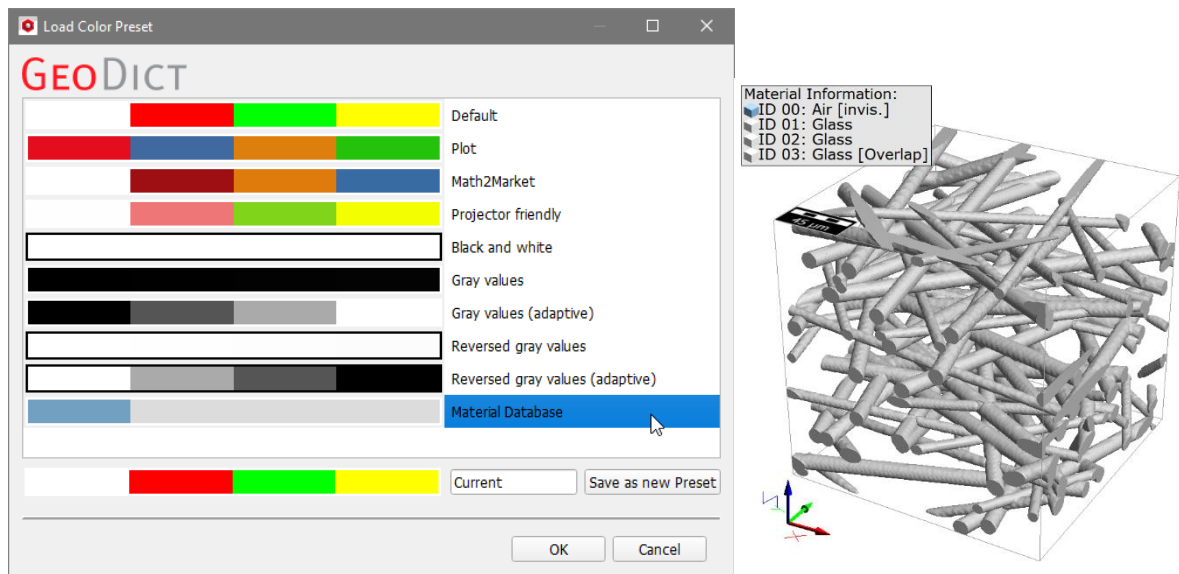


The **Color and Visibility Settings** dialog shows the colors currently assigned to the Material IDs and the Constituent Materials.

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**  in the top right.



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



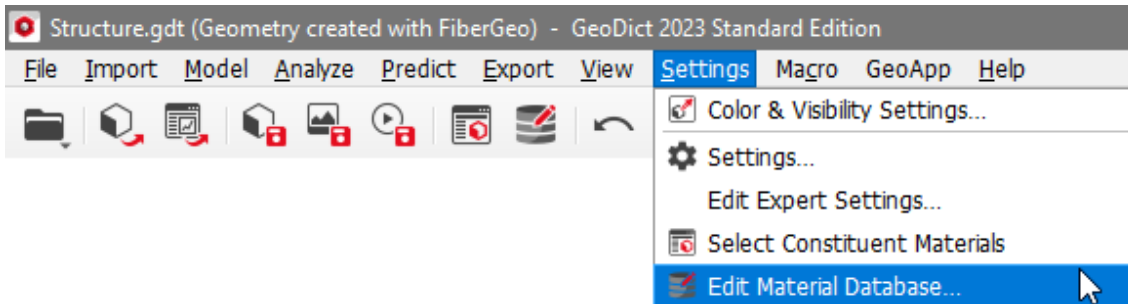
EDIT AND EXPAND THE GEODICT MATERIAL DATABASE

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

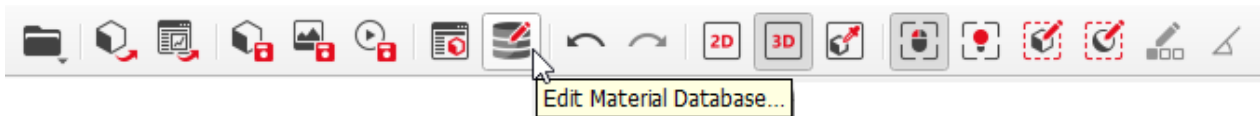
ACCESS THE MATERIAL DATABASE

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

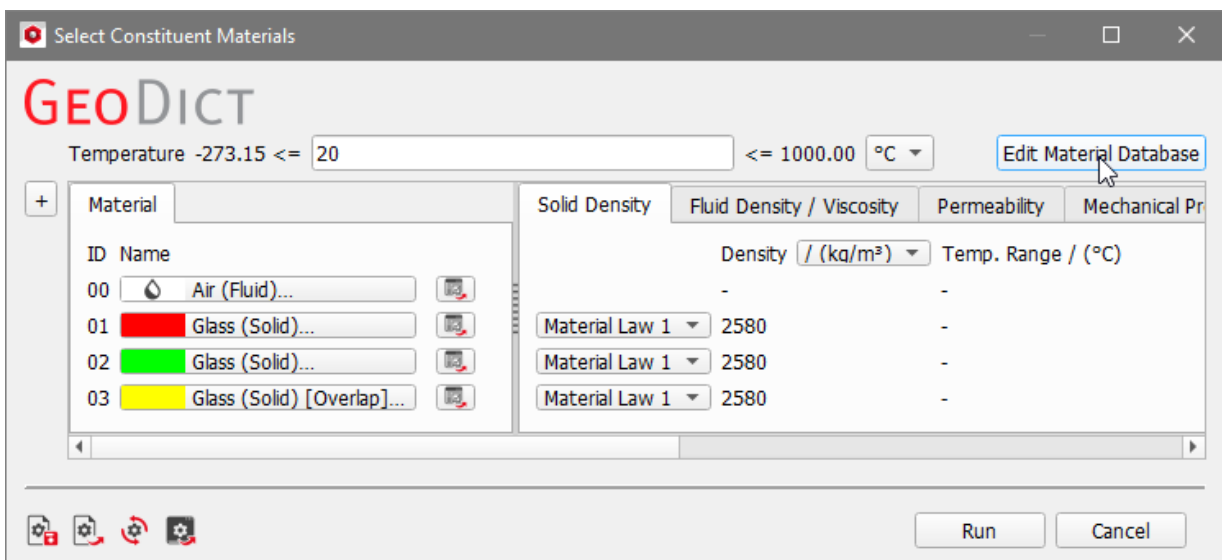
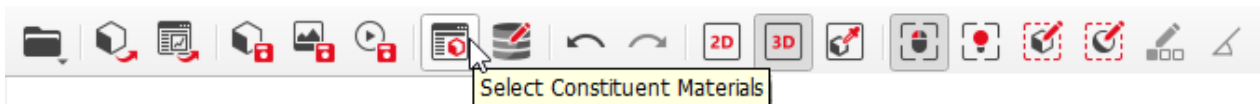
1. Select **Settings** → **Edit Material Database...** in the menu bar



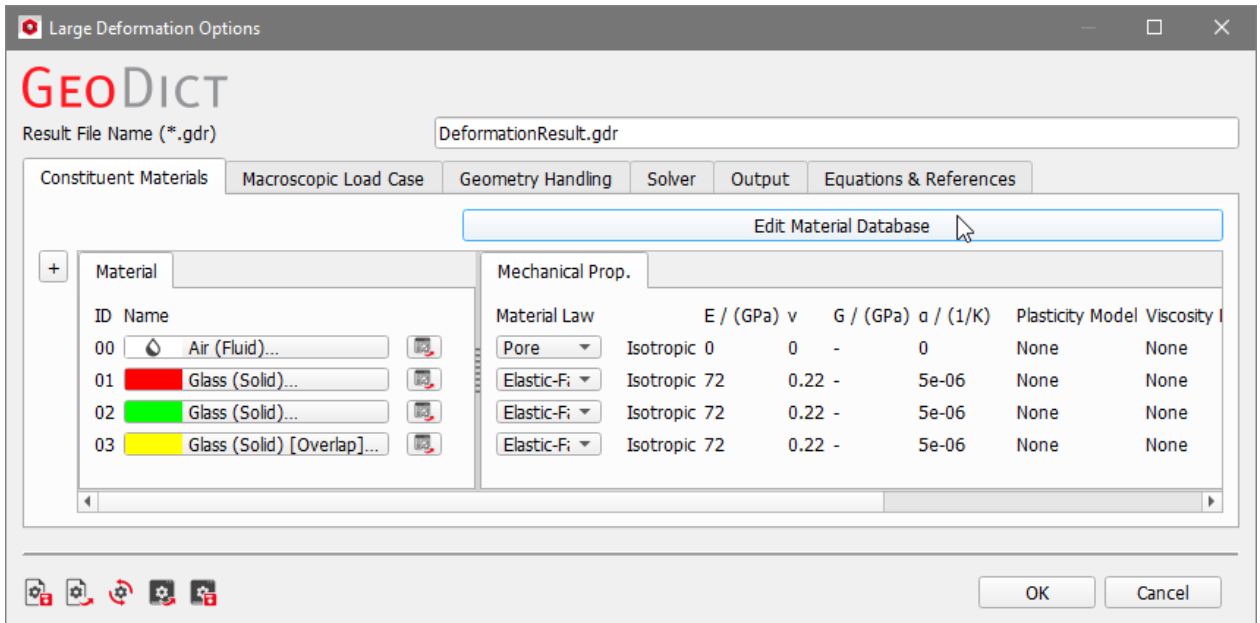
2. Click the **Edit Material Database** icon in the toolbar



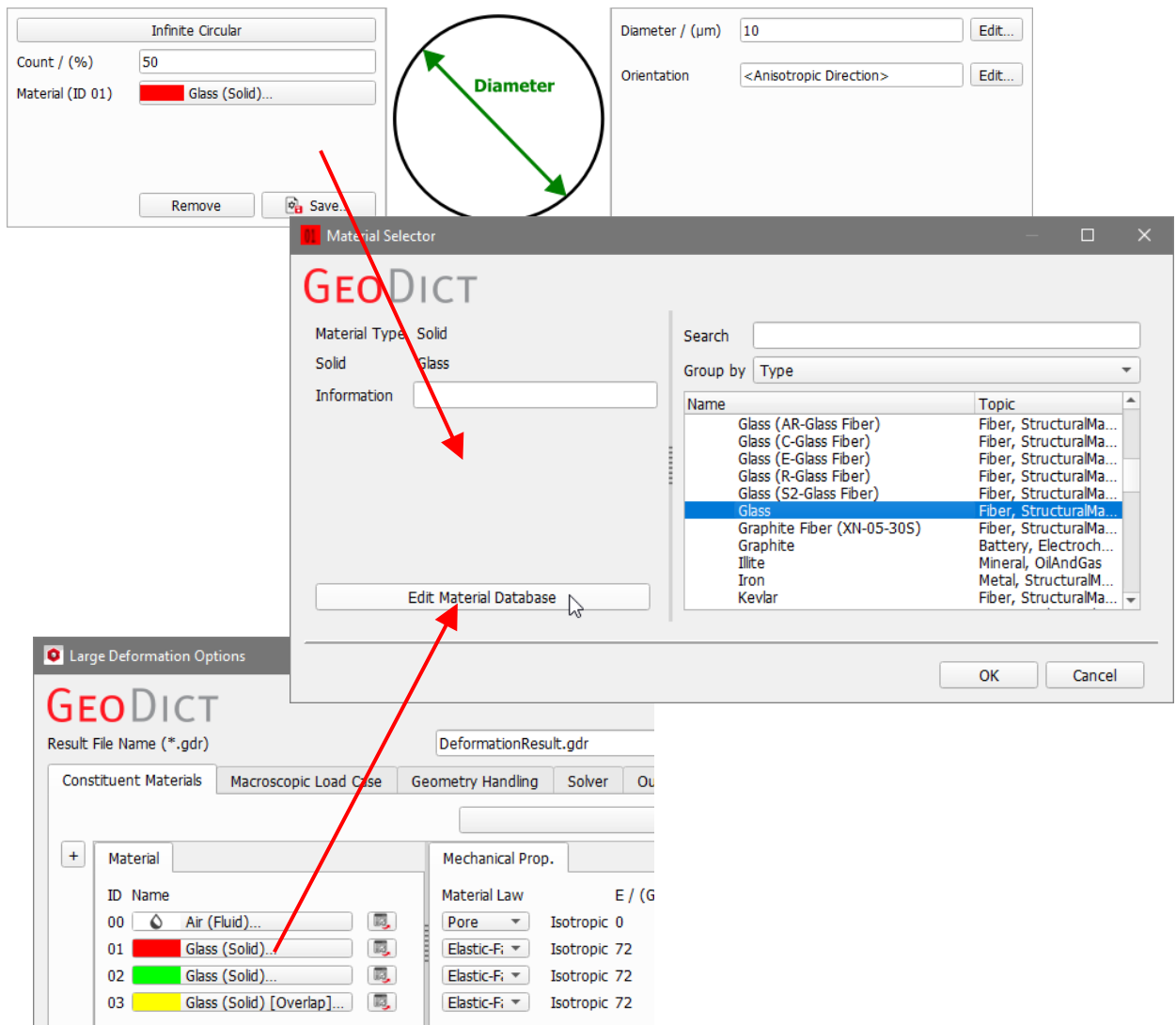
3. Click the **Select Constituent Materials** icon in the toolbar and click **Edit Material Database** in the Select Constituent Materials dialog



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



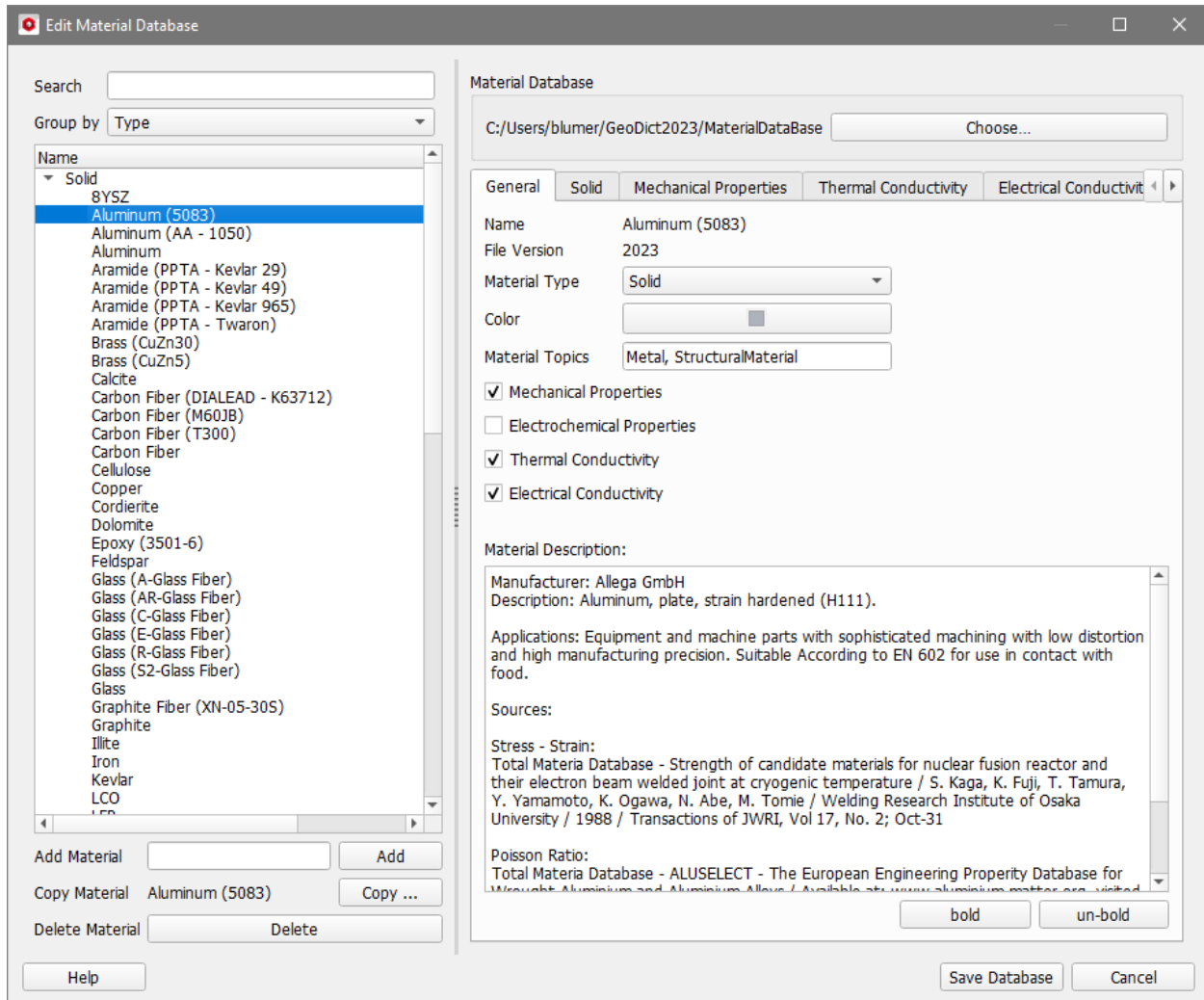
- Click any material button in generator or predictor modules, and then click **Edit Material Database** in the **Material Selector** dialog box.



The GeoDict Material Database

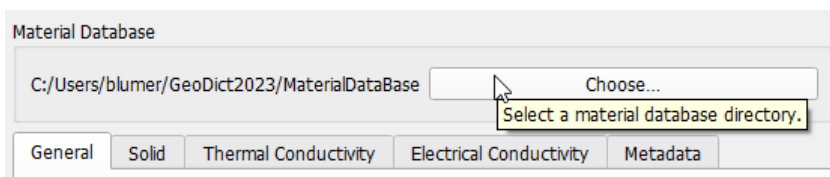
For the predictor modules (**ElastoDict**, **ConductoDict**, **FlowDict**, **DiffuDict**, **FilterDict**, etc.), the material buttons are located in the **Constituent Materials** tab of the **Solver Options**.

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



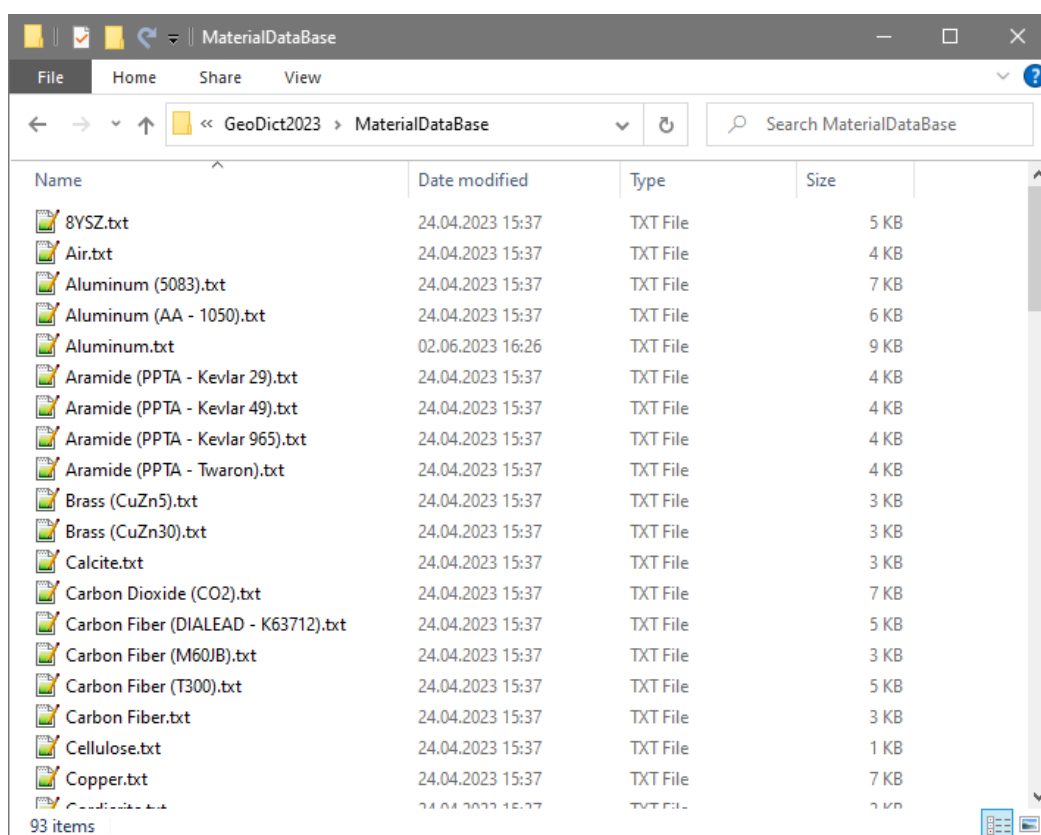
CHOOSE A MATERIAL DATABASE

On the upper right corner of the **Edit Material Database** dialog, click **Choose...** to set the path to a material database directory.

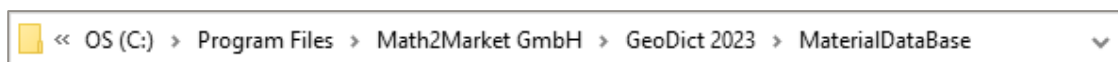


The default path for the **GeoDict** Material Database is

- `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**.

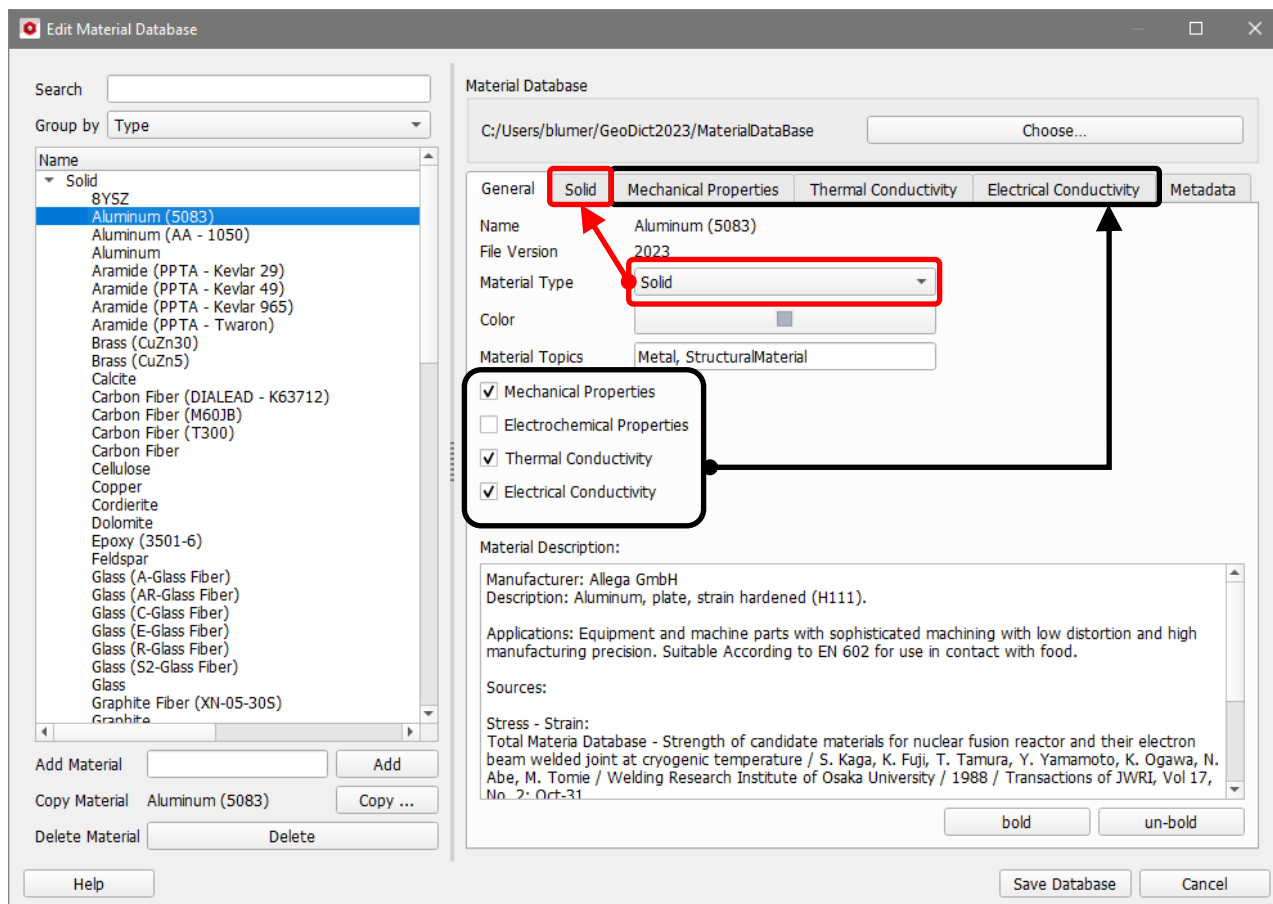
Materials can be added to the Material Database in two ways:

1. Add or copy materials in the material database dialog (see page [18](#))
2. Copy the corresponding *.txt files from another material database into the MaterialDataBase folder.

EDIT EXISTING MATERIAL DATABASE ENTRIES

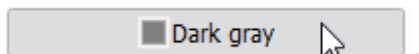
The material database can be edited by modifying or adding properties of constituent materials through the **Edit Material Database** dialog as follows:

1. In the left panel, click to highlight and choose one of the materials in the current GeoDict material database.
2. 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.



Depending on the selection of material type, the next tab after the **General** tab is titled **Solid** or **Fluid**, and the parameters that apply in each case can be edited. For Solid Materials, a fixed density or a temperature dependent density can be entered. For Fluid Materials, a density and the dynamic and kinematic viscosity can be set, which might also be temperature dependent. Porous materials work analogously to solid materials.

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 defined.

MECHANICAL PROPERTIES: MULTIPLE MATERIAL LAWS

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 this User Guide.

In the material database, it is possible to:

- Edit an existing material law by choosing it under **Edit Material Law** and editing the corresponding parameters below:

Mechanical Properties Selection

Edit Material Law: Elastic (dropdown menu)

Add Material Law: (empty text box)

Buttons: Delete, Rename, Add

Tooltip: Edit the chosen material law.

- Add a new material law by entering its name in the box **Add Material Law** and clicking **Add**. Afterwards, a material law with the entered name is listed under **Edit Material Law** and can be edited as described above.

Mechanical Properties Selection

Edit Material Law: Elastic (dropdown menu)

Add Material Law: Plastic (text box)

Buttons: Delete, Rename, Add

Mechanical Properties Selection

Edit Material Law: Plastic (dropdown menu)

Add Material Law: (empty text box)

Buttons: Delete, Rename, Add

Tooltip: Edit the chosen material law.

ELECTROCHEMICAL PROPERTIES

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

General | Solid | Mechanical Properties | **Electrochemistry** | T

Role in Battery Cell: Inclusion (dropdown menu)

Options in dropdown: Inclusion, Electrolyte, Separator, Anode Active Material, Cathode Active Material, Binder and Carbon Black, Current Collector, Undefined

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](#).

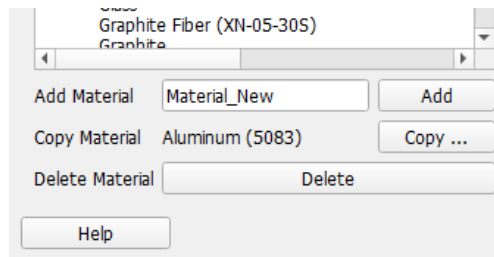
ADDING NEW MATERIALS TO THE DATABASE

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

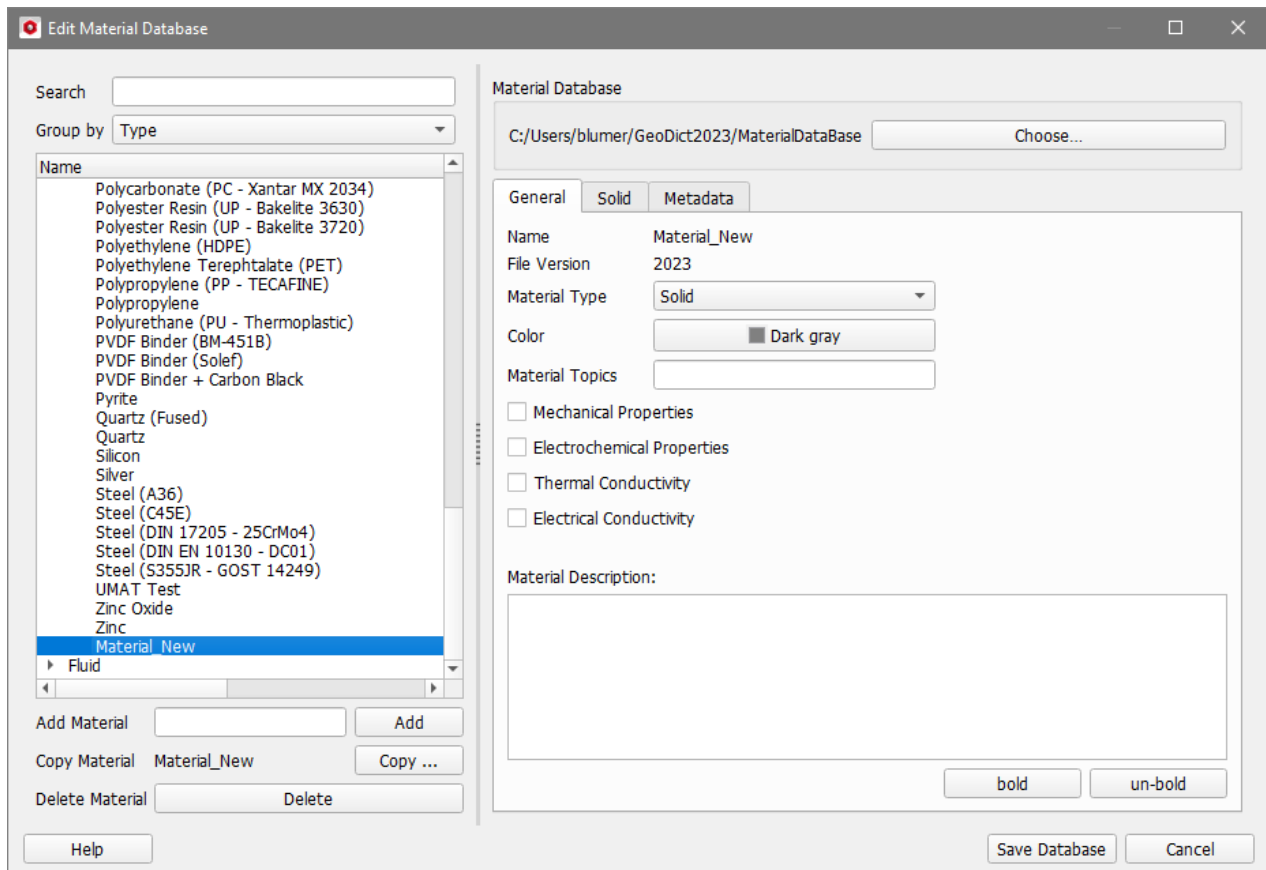
CREATING NEW MATERIALS

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.



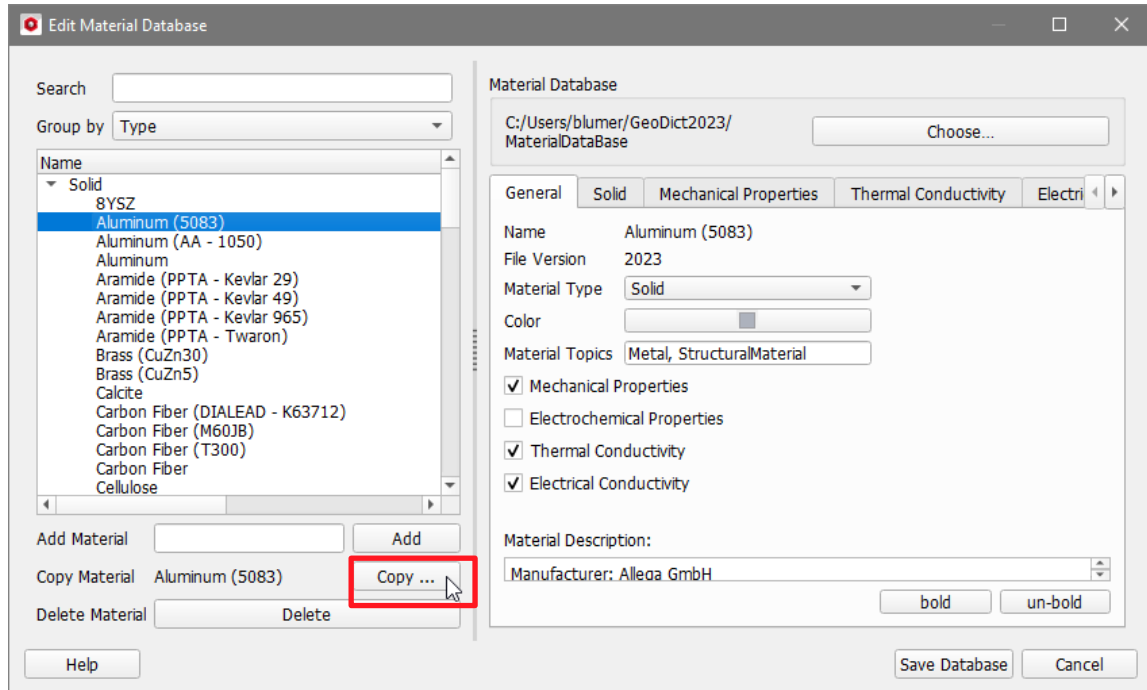
When a material is newly created, its **Material Type** is set to **Solid** per default and therefore it appears under the **Solid** tree listed at the very end.



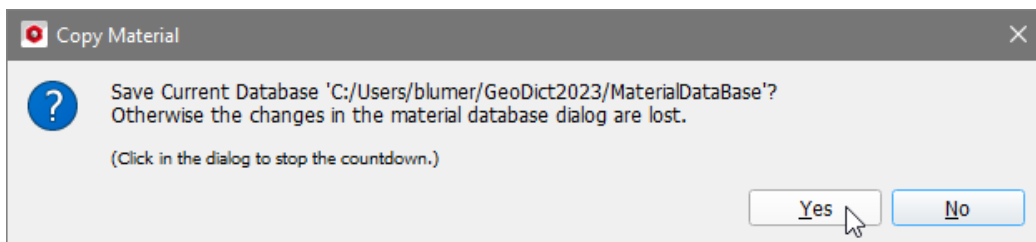
In the next step, the **Material Type** and its properties are set under the corresponding tabs (see the corresponding paragraph on page [16](#)).

COPYING EXISTING MATERIALS

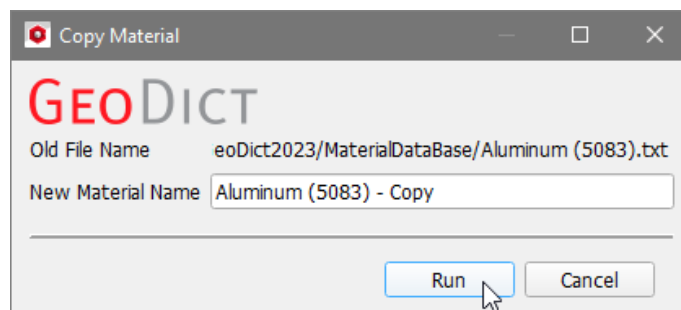
Alternatively, an existing material can be copied by selecting the material and clicking **Copy**



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.

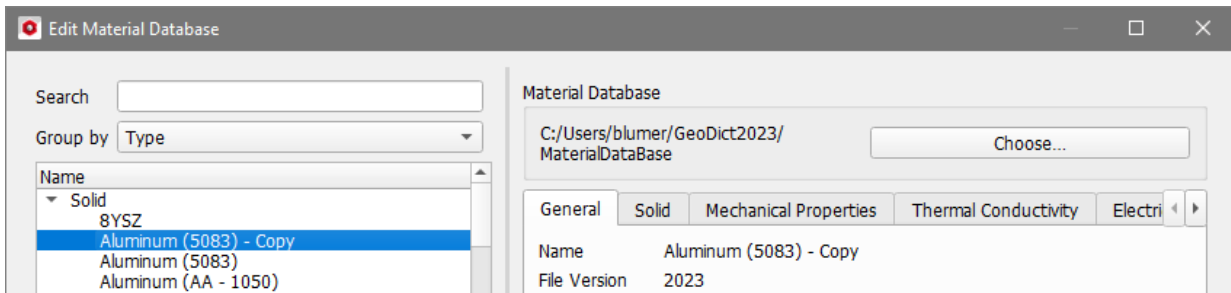


In the next step, the name for the new copy of the material can be selected. In this example, the default name is kept. Click **Run** to create the material.



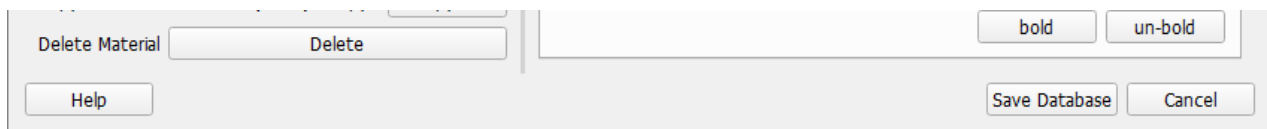
The GeoDict Material Database

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



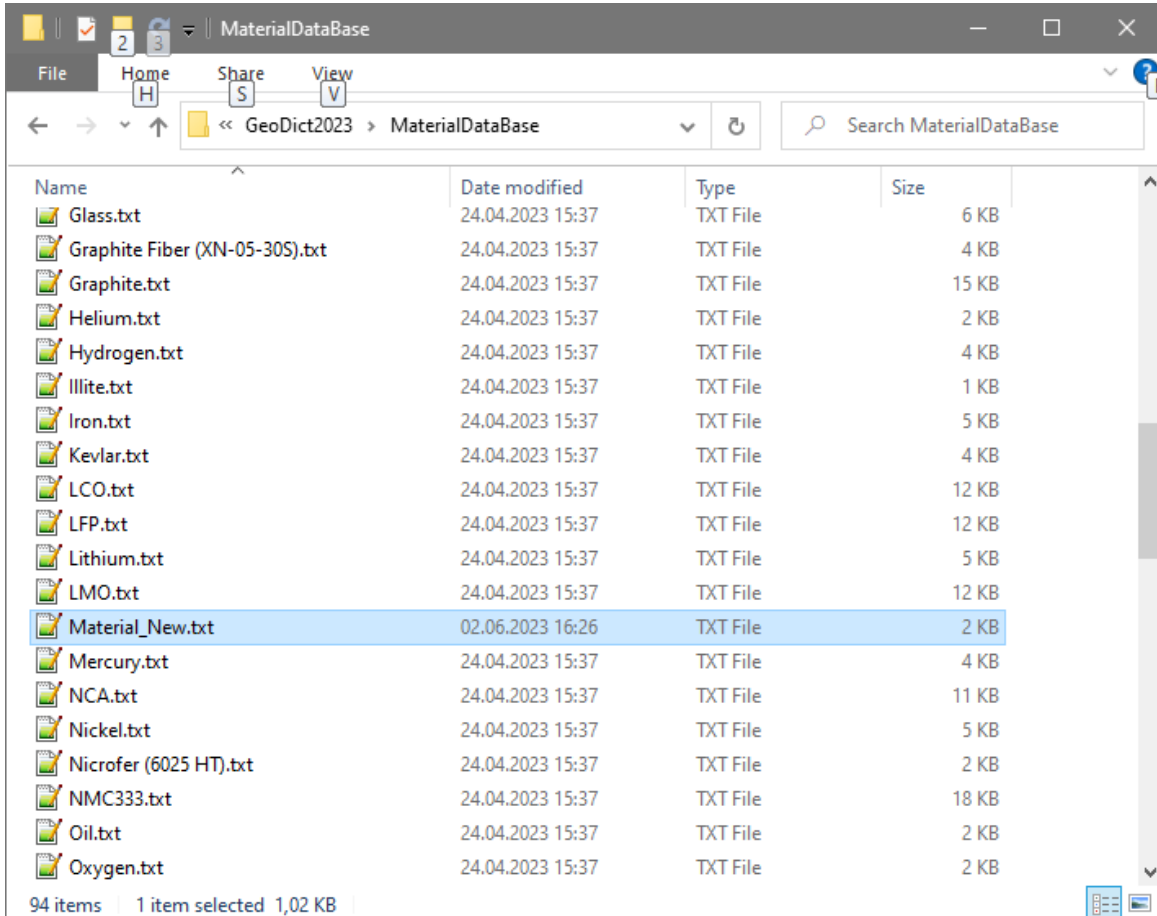
SAVING THE MATERIAL DATABASE

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



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.

```

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                           0,3.9,11.52,13.46,15.27,17.94,19.4,21.5,23.32,24.79,25.89,27.25,28.93,30.04,
64         Stress                           0,0.171,0.232,0.245,0.267,0.278,0.285,0.279,0.288,0.287,0.29,0.286,0.304,0.3
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, AffineLinear, Exponential
73       ViscosityType                      None // Possible values: None, PerzynaLinear, PerzynaNonlinear, MichelSuquet
74       DamageType                         None // Possible values: None, Exponential, Mazar
75       LargeDefoModel                     StVenantKirchhoff // Possible values: StVenantKirchhoff, NeoHook, MooneyRivl
76       InitialYieldStress                 0.115241 [GPa]
77       HardeningType                      Isotropic
78       FirstIsotropicHardening            0.19948 [GPa]
79       SecondIsotropicHardening           8.68635 [1]
80       FailureType                        None // Possible values: None, FailStress
81       HasMeasurement                     true
82     </MaterialLaw1>
83     <MaterialLaw2>
84       Type                              Isotropic
85       Name                              Elasto-Plastic (-196 °C)
86       YoungsModulus                     78 [GPa]
87       PoissonsRatio                      0.33 [1]
88       AllowThermalExpansion              false
89       PlasticityType                     Exponential // Possible values: None, Constant, AffineLinear, Exponential
90       ViscosityType                      None // Possible values: None, PerzynaLinear, PerzynaNonlinear, MichelSuquet
91       DamageType                         None // Possible values: None, Exponential, Mazar
92       LargeDefoModel                     StVenantKirchhoff // Possible values: StVenantKirchhoff, NeoHook, MooneyRivl
93       InitialYieldStress                 0.134927 [GPa]
94       HardeningType                      Isotropic
95       FirstIsotropicHardening            0.340126 [GPa]
96       SecondIsotropicHardening           6.81943 [1]
97       FailureType                        None // Possible values: None, FailStress
98       HasMeasurement                     true
99     <Measurement>
100       Strain                            0,0.42,0.86,1.56,2.75,4.31,5.75,7.43,9.35,11.15,13.08,14.89,17.07,19.25,21.6
101       Stress                             0,0.122,0.156,0.174,0.198,0.221,0.238,0.26,0.288,0.311,0.329,0.347,0.363,0.3
102     </Measurement>
103   </MaterialLaw2>
104 </Elasticity>
105 </Material>
106

```

Python file length: 6,824 lines: 106 Ln: 1 Col: 1 Sel: 0 | 0 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