Colouring Schemes

Colouring schemes: Multiple colouring schemes can be applied to simulation results to investigate different areas of interest. These are also full customisable in the visualiser.

In order to highlight and investigate features exhibited by simulated crystals, a number of colouring schemes have been added into the visualiser. In addition to XYZ coordinates, all XYZ files output by *CrystalGrower* also include a species type and species number identifier for each set of coordinates. Species type is generally an identifier for objects that are of completely different shapes, whereas species number is an identifier for species of the same type in slightly different positions or orientations (an example for LTL is shown in Figure 6). These identifiers ensure the placement of correct species at the listed XYZ coordinates and refer back to the coordinates of individual objects in the .vis file.

By placing objects according to their species type, they can also be assigned different colours to allow easy identification. This is known as “type” colouring in the visualiser e.g. colouring by tile type or molecule type colouring depending on the selected operating mode (Figure 6, Centre). Alternatively, all objects can be assigned a single colour, known as “block” colouring in the visualiser.

During simulation, species can be identified according to crystal facet planes and separated into layers dependent on each facet’s d-spacing by invoking the “facet find” routine in *CrystalGrower*. XYZ files produced in this mode will include an additional column of data referred to as a species’ layer number. Files of this type allow colouring of crystal species

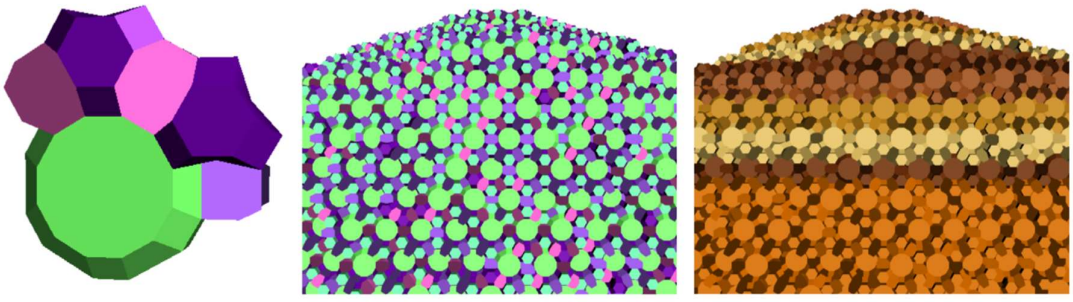

***Figure 6, Left**: The natural tile components of an LTL unit cell. Tiles coloured the same are the same species type (i.e. the same shape) but at different symmetry positions – a different species number. **Centre**: An LTL crystal surface coloured by tile type. **Right**: An LTL crystal surface coloured by layers, with layer separation decided by a facet’s d-spacing, produced using the “facet find” routine in the CrystalGrower simulation package.*

(molecules or tiles) by identified facets, known as “layer” colouring in the visualiser (Figure 6, Right). A set of 4 colours are cycled between in layer colouring, cycling to the next colour in the sequence upon crossing a distance equal to the d-spacing of the plane assigned as a crystal face. If the number of distinct crystal layers on a facet exceeds 4 and a facet was assigned to show > 4 layers while using facet find, the sequence of colours is repeated as necessary. Species may occasionally fall between two planes or exist on roughened areas of crystal where a smooth facet cannot be identified. These species are assigned a value indicating their layer type is “unassigned” and are coloured by a colour outside of the layers colour sequence allowing for easy identification (default = pink).

An additional “layer” is present if users apply a second sweep to their simulation for internal defects. This layer is coloured red by default and represents the species that are adjacent to a missing unit in the crystal structure. For tile structures these species can be fully condensated at the vertices by other neighbouring tiles, but have a neighbouring tile missing via a tile face. These species are separated to allow them to easily be filtered out or studied in greater detail. Numerically, layers 1-4 are surface species belonging to identified facets, layer 5 contains species that do not fit into an identified layer (be that due to their presence on a facet that was not identified, or being located within the crystal as an internal defect) and layer 6 contains species that are “indirect” defects.

This colour scheme is particularly useful for comparing simulated crystals against experimental AFM data, allowing crystal terraces to be located quickly and for information like terrace step heights and crystal surface terminations to be investigated. Each of the discussed colour schemes can be used with all operation and drawing modes of the visualiser.

An additional colour scheme is available for molecular (atoms and bonds) where species are coloured by atom type (examples are shown for urea and calcite in Figures 1 and 3, respectively). Atom types are defined for each molecule type during the structure read in phase. Each atom type is counted as a separate display list during the visualisation process described above, meaning each atom type can be assigned a different colour. Default colours for elements are saved in a database within the visualiser (this colour scheme is shown in Figure 7) and used when atom types are called within the program, all bond types are coloured black by default.

All colouring modes are fully customisable. A user can select to change the colours of individual species types, atom types, bond types or layer types (as well as the background colour) using a colour picker (Figure 8, Left) or change all colours simultaneously by loading

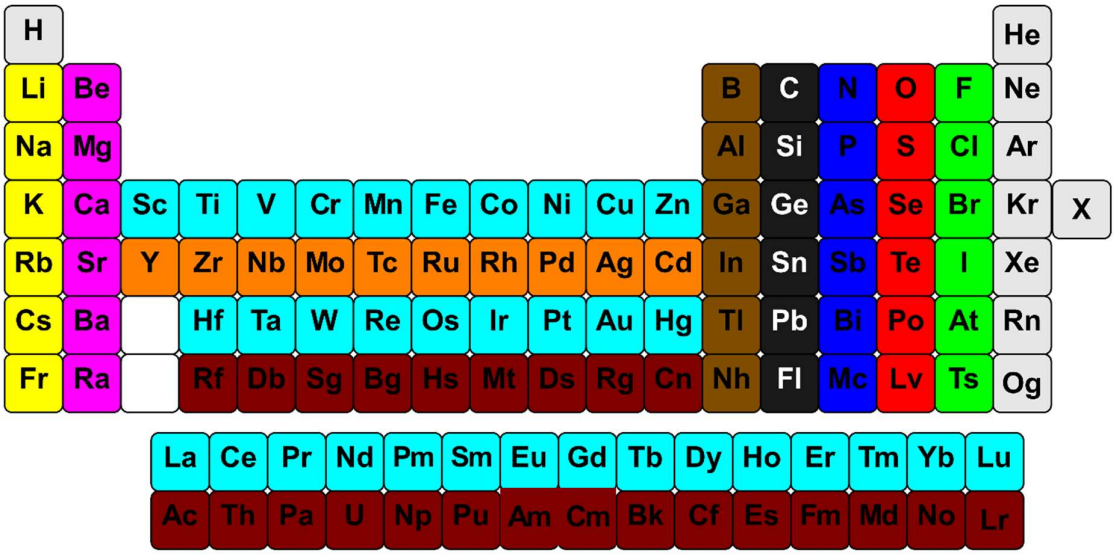

***Figure 7**: The periodic table coloured according to the default element colours within the visualiser. All element colours are fully customisable by the user. Element "X" denotes a generic growth modifier species with the same sphere size and colour as Kr.*

a text file of RGBA (red, green, blue, alpha) values (Figure 8, Right). All RGBA values in this file are decimal equivalents of the usual format where 255 is the maximum possible value for a colour component e.g. 51 in the standard format would equate to 0.2 in the decimal format. In place of the ".txt" file extension, the file extension used for colour files is ".col" to assist in locating colour files when filtering by file type. The visualiser is also capable of saving a set of custom colours in the ".col" file format for easy setup on subsequent visualisations of the same structure. Custom colour options are all located under the "Colouring" drop-down menu.

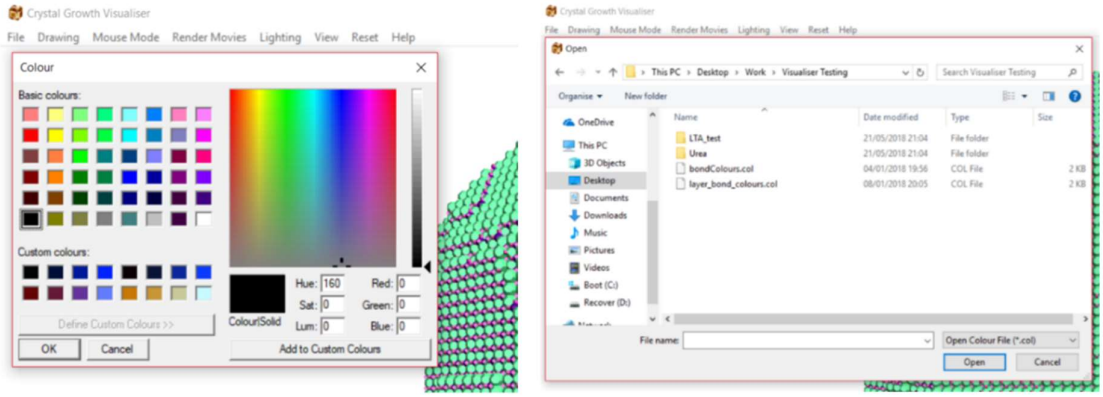

***Figure 8, Left**: The colour picker window for changing a single selected species' colour. **Right**: The file explorer window for loading a colour (.col) file containing RGBA values for changing a set of colours.*

All options related to colouring modes are found in the “Drawing” drop-down menu on the visualiser toolbar. The options for each operating mode are separated into further drop-down menus: “Tile Crystals” and “Net Crystals” for the tiles and net operating modes, respectively. Options related to selecting custom colours are also located in the “Drawing” drop-down menu, under the option “Custom Colours”. The option to save a custom colour file is instead located under the “File” menu with the option “Save Colour File”.