



## SpinelViz: An interactive 3D application for visualizing spinel group minerals

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### ABSTRACT

SpinelViz is an application for the visualization of the spinel group minerals in three dimensions. SpinelViz uses the spinel prism to display mineral composition datasets from different tectonic settings. The application projects data onto 2D and 3D plots. Such projections are used to classify spinels based on geochemical data. The spinel mineral group exhibits a wide range of solid solutions and has been the subject of many thermodynamic studies. Spinel, particularly chromites from mafic–ultramafic igneous rocks are used to discriminate among various tectonic settings. Their existence in ultramafic rocks and their resistance to alteration make them excellent tectonic tracers and a very important tool in search for economic deposits of the platinum group elements (PGE) and Ni–Cu–PGE. SpinelViz provides a set of functionalities that helps users to manipulate their datasets for both 2D and 3D visualization and 2D projections.

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### 1. Introduction

Visualization is essential for data interpretation in many scientific problems (Koutek, 2003). It displays numerical data into a visual representation that makes them much easier to understand. Scientific Visualization is concerned with techniques that allow scientists and engineers to gain better information from the results of simulations and computations (Bonneau et al., 2005). It uses computer graphics to create images which aid in the understanding of complex and often massive numerical representations of scientific concepts or results (McCormick, 1988). Visualization is becoming an essential tool toward understanding and interpreting datasets from different scientific fields, including geosciences data (Mackinlay, 1986; Card et al., 1999).

In this paper we develop a visualization approach for the spinel mineral group. Spinel minerals exhibit a wide compositional range based on the modified spinel prism (Stevens, 1944; Irvine, 1965, 1967) and are routinely used to compare datasets of spinel chemical analyses. Different regions have been delineated based on the composition of spinels according to their tectonic settings

(Barnes and Roeder, 2001). Some minerals of the group, particularly chromites, have been used as “petrogenetic indicators” (Irvine, 1965, 1967; Evans and Frost, 1975; Sack, 1982; Sack and Ghiorso, 1991; Haggerty, 1991; Castro et al., 1997). This is due to the fact that chromites associated with mafic–ultramafic rocks, although being normally accessory phases (< 2 vol%), are very sensitive to conditions present during the crystallization of these rocks; therefore, they provide vital information regarding the tectonic settings in which their host rocks were formed. The evolution of fluid phases involved in the metamorphism of serpentinites can also be established based on the study of chromian spinels (Hoffman and Walker, 1978). They are also invaluable tools in the exploration for economic deposits of the platinum group elements (PGE) and Ni–Cu–PGE.

Barnes and Roeder (2001) compiled a database comprising of more than 26 000 analyses of spinels from igneous and meta-igneous rocks. The database is used to delineate and construct characteristic compositional fields for spinels of various tectonic settings and magma compositions. Manipulating, analyzing and charting such a large dataset is often a time consuming process. Hence arises the need to visualize the data which makes the comparison and integration of the data much easier.

It is a common practice to plot spinels on the oxidized magnetite prism (Magnetite, Magnesioferrite, Spinel, Hercynite, Chromite, Magnesiochromite), which provides a reasonable and easily interpretable 3D chart (Haggerty, 1991). Such plots are now extremely widespread even though they are difficult to generate by hand and, therefore, they are obvious candidates for computerization.

Geoscientists mostly use binary and ternary plots to evaluate correlation between chemical elements or oxides.

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For example, IGPet,<sup>2</sup> MinPet,<sup>3</sup> MinCalc (Bernhardt, 2007),<sup>4</sup> GCDkit (Janousek et al., 2006),<sup>5</sup> etc. have been developed for better data analysis and representation. In 1990 an integrated package of ten Macintosh programs for producing igneous petrology information was published (Williams et al., 1990). This package contains two programs, called SPINEL and SPINELTAB, to plot spinel analyses in two particular 3D compositional prisms. The functionality of these programs includes the capability to enlarge or shrink the plot, choose the angle of view and distinguish up to five distinct groups of spinel analyses by means of different symbols. It is important to emphasize that the SPINEL and SPINELTAB programs are not spinel visualization applications, but they are oriented to plot and analyze spinel datasets.

Here, we present a Geological Visualization Application called SpinelViz. The application consists of an interactive 3D viewer which allows the user to view and explore the spinel prism with different datasets at the same time. SpinelViz provides the capability to manipulate, view, plot, and project data on 2D and 3D which helps the user to gain a better insight of the data distribution.

This paper is an extension of a previous work (Ganuza et al., 2009) that focused on a set of basic functionalities and different data representations for datasets of spinel mineral group compositions. Based on the obtained results, we choose the most suitable for the design of a 3D Spinel Prism Viewer tool. Whereas such a work was strongly focused on the data representation, our current work describes the SpinelViz. This application provides a rich set of functionalities required by the geologists who helped in its design and development.

## 2. Program scope

In Mineralogy, an important problem is to achieve an adequate representation of mineral compositions in a way that groups of samples can be intuitively matched against a given pattern.

Considering that the spinel mineral group has a formula  $XYO_4$ , with SpinelViz it is possible to plot any solid solution with changes in  $X$  and  $Y$  in one single diagram. This is a great advantage due to the complex chemical variability displayed by this group of minerals, variability that reflects different genetic conditions which has also a direct relationship to the tectonic environment where they were crystallized. Therefore, the chart allows potential users to visualize populations with different genesis and tectonic settings in one single plot.

As has been mentioned, it is a common practice to plot spinels in the oxidized magnetite prism (Fig. 1(a)). Fig. 1(b) shows a prismatic space of oxide composition. An established “historical” set of samples of a given mineral belonging to rocks from a particular tectonic setting forms a trend within the compositional space. This trend is a volumetric pattern composition or proportion of oxides that characterizes that particular mineral, and can be represented as a solid within the compositional space. Data from a given set of unclassified samples may be represented in this space with an adequate icon, and the classification problem consists in visually determine whether these icons lay within the pattern or not. In this context SpinelViz uses a graphic object to represent the mineral composition of each data sample within the prism. To represent patterns, SpinelViz uses transparency on the graphic objects, allowing a set of data samples

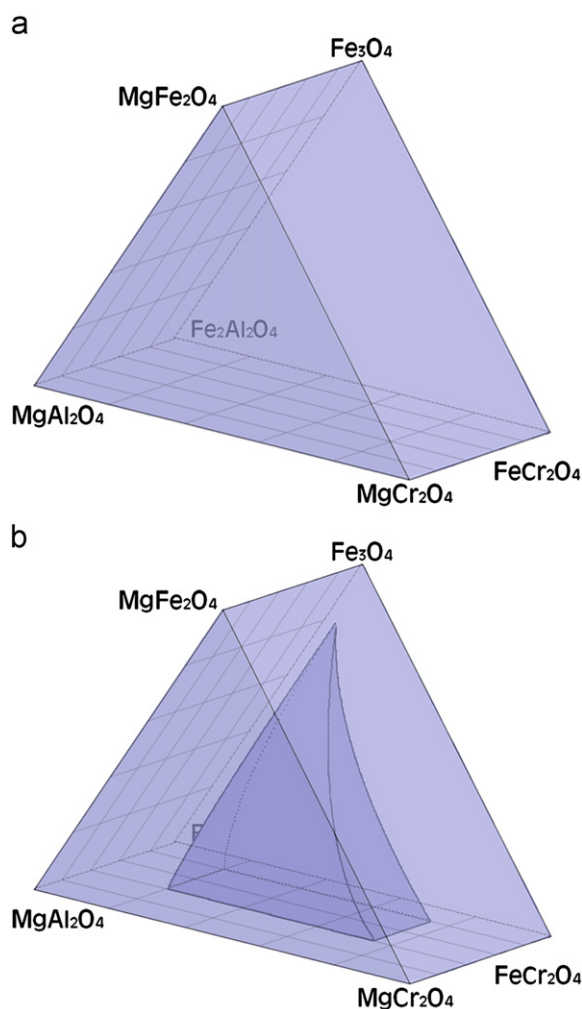


Fig. 1. Prismatic space. (a) Prismatic composition space of standard mineral. (b) A prismatic composition space of standard mineral oxides, and the volumetric pattern that identify minerals from a particular rock (basalts in this case).

situated on neighboring positions to constitute a volume within the prism (Fig. 2(a)).

The application allows distinguishing up to ten groups of spinels for analysis. Data samples from different patterns are represented with different colors and shapes, allowing the visualization of more than one reference pattern within the same prismatic space (Fig. 2(b)). The application assigns a set of default colors to the represented datasets, but the user is able to change them when he/she considers that others will communicate the meaning of the data most effectively.

To determine whether a data sample belongs to a certain pattern, the user can choose a different color from the colors used for the patterns, and, with the help of the transparency, navigate over the 3D space to realize if the data sample lays inside or outside a determined pattern (Fig. 3).

## 3. Starting the program

SpinelViz should be copied on a PC folder, no installation process is necessary. A version of the Microsoft .NET Framework 2.0<sup>6</sup> or younger is required to use SpinelViz. To start the application, execute the Prisma.exe file. Once the interface of SpinelViz is loaded (Fig. 4),

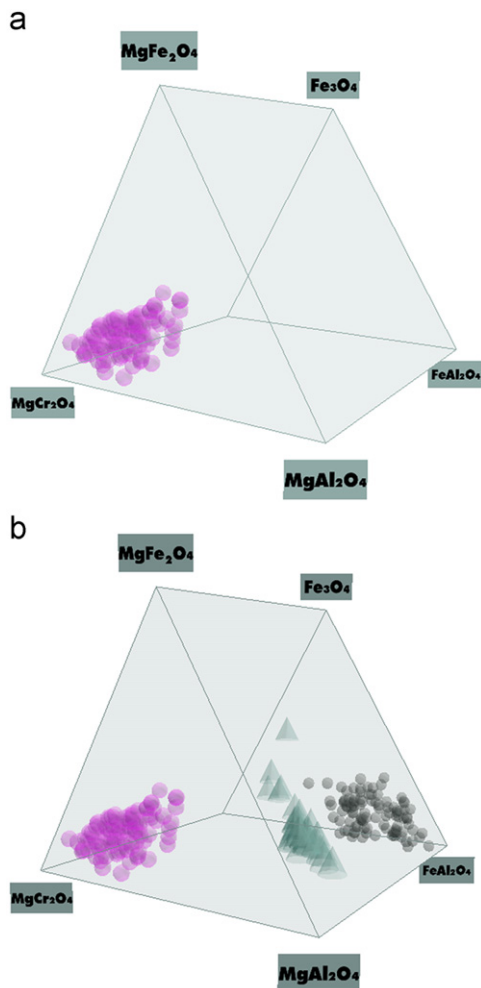
<sup>2</sup> IGPet, Igneous Petrology Software. Rockware (<http://www.rockware.com>).

<sup>3</sup> MinPet, Minealogical and petrological data processing system. MinPet Geological Software Inc (<http://www.minpet.com>).

<sup>4</sup> MinCalc, a software tool for mineral analyses data processing. (<http://www.earth.ox.ac.uk/davewa/pt/mincalc.html>).

<sup>5</sup> GCDkit, GeoChemical Data toolkit. Vojtěch Janoušek, Colin M Farrow and Vojtěch Erban (<http://www.gcdkit.org/>).

<sup>6</sup> Available on-line at <http://www.microsoft.com/net>



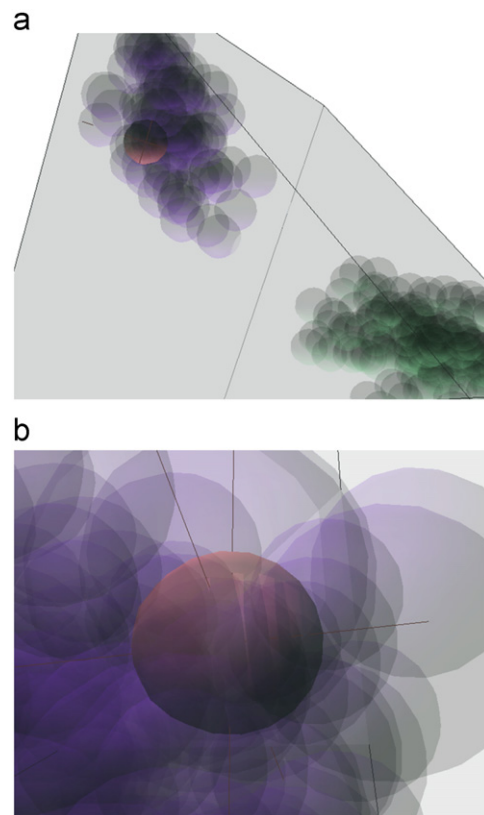
**Fig. 2.** SpinelViz. Representation of patterns. (a) A dataset within the spinel prism. The dataset conforms a volumetric pattern. (b) SpinelViz. Three patterns with different visual representations within the spinel prism.

the application is ready to be used. In order to integrate the 3D view of the prism and other important information, the user interface was designed as a combination of three main sections: the visualization area, the pattern information area and the utilities area.

To use SpinelViz, data should be compiled in a Microsoft Excel™ spreadsheet (\*.xls) that should have the format depicted in Fig. 5. The columns correspond, in general, to the final element values that compose each sample. The first column contains the sample name and the next columns have the oxides. The first row of the spreadsheet is reserved for labels. In the first cell of the first row (cell A1) the word “sample” should be written and the following ones must contain a label for each oxide. It is not required that the oxides follow a fixed order, but, at least, the six oxides of the Magnetite or Ulvospinel representation must be present. Each data sample corresponds to a row in the .xls file. That is, for a dataset of ten samples the file must contain at least 11 rows. The labels corresponding to the oxides in the first row of the file are detailed in Table 1. The first cell of unused rows or columns should be empty, but zero could be written.

#### 4. Functionalities

At first, when the interface of SpinelViz is loaded (Fig. 4), the empty spinel prism is shown, and the application is ready to be used as described in the following subsections.



**Fig. 3.** Zooming into the prismatic space allows the user to get closer to the data sample to verify if it belongs to a pattern. (a) Zoom applied to the scene, attempting to get closer to the data sample. (b) By zooming, we realize that the data sample lays inside the purple pattern. So, the data sample belongs to it. (For interpretation of the references to color in this figure caption, the reader is referred to the web version of this article.)

##### 4.1. Loading patterns and samples

A dataset can be loaded using the menu bar and selecting the option “Patterns”–“Load” (Fig. 6). This opens a new window that allows the data file (e.g., data.xls) to be chosen. This loaded file can represent an established reference pattern, a common dataset or a single data sample. This action adds a new item to the pattern list on the pattern information area (Fig. 7) detailing the name of the pattern and information about its visual representation.

A loaded dataset can be deleted from the pattern list and from the prismatic space. This action can be performed by selecting the corresponding pattern from the pattern list and clicking over the “delete” button (Fig. 7). This operation cannot be undone; if the user needs to use a deleted pattern it must be loaded again.

The user can hide a dataset if necessary without deleting it permanently; then he/she is able to show it again on the prismatic space without reloading it. This action can be performed by pressing the “show/hide” button in the pattern information area (Fig. 7).

##### 4.2. Modifying the visual representation of patterns and samples

When loading a pattern, the application draws all the samples of the dataset with a predetermined color, shape and size. In order to achieve an effective comparison between different patterns, it is necessary to provide the functionality to change these attributes promoting the task of highlighting and distinguishing a pattern. In the pattern information area of SpinelViz’s interface, the user can change the size, color and shape used to represent the data samples of a selected pattern. To change the size of data

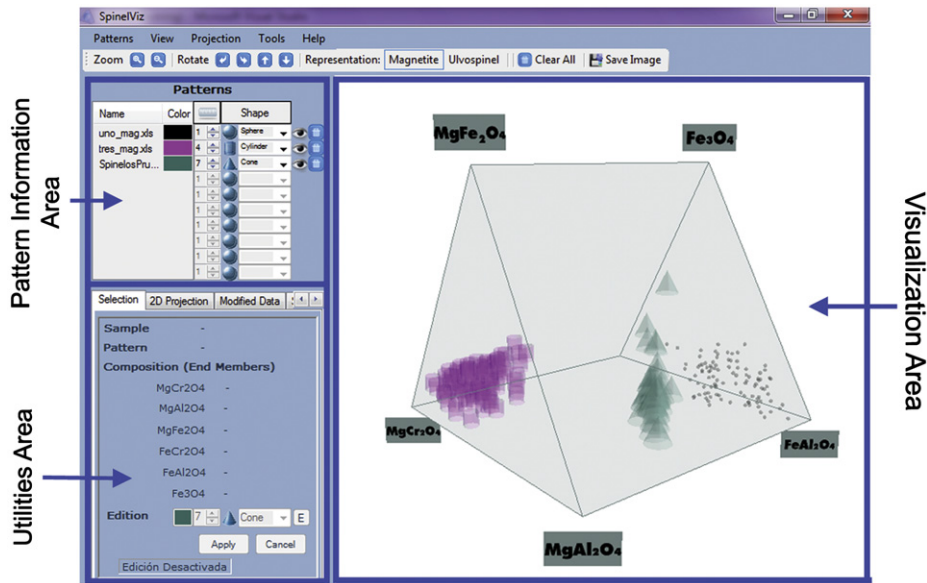


Fig. 4. The application user interface was designed as a combination of three main sections: the visualization area, the pattern information area and the utilities area.

	A	B	C	D	E	F	G	H	I	J	K	L	M
1	sample	MgAl <sub>2</sub> O <sub>4</sub>	FeAl <sub>2</sub> O <sub>4</sub>	MnAl <sub>2</sub> O <sub>4</sub>	MgFe <sub>2</sub> O <sub>4</sub>	Fe <sub>3</sub> O <sub>4</sub>	MnFe <sub>2</sub> O <sub>4</sub>	MgCr <sub>2</sub> O <sub>4</sub>	FeCr <sub>2</sub> O <sub>4</sub>	MnCr <sub>2</sub> O <sub>4</sub>	Fe <sub>2</sub> TiO <sub>4</sub>	Zn-Spinel	MgTiO <sub>4</sub>
2	4.34,3sp5	0,100	0,300	0,004	0,100	0,200	0,000	0,100	0,200	0,002	0,002	0,036	0,298
3	4.34,3sp	0,100	0,100	0,007	0,100	0,100	0,001	0,500	0,100	0,005	0,008	0,031	0,192
4	4.34,3sp6	0,050	0,200	0,006	0,050	0,200	0,001	0,300	0,200	0,005	0,006	0,030	0,244

Fig. 5. Example of a data.xls file.

Table 1  
Oxides' Labels for .xls input files.

Oxide	Label
Spinel	MgAl <sub>2</sub> O <sub>4</sub>
Hercynite	FeAl <sub>2</sub> O <sub>4</sub>
Magnesianferrite	MgFe <sub>2</sub> O <sub>4</sub>
Magnetite	Fe <sub>3</sub> O <sub>4</sub>
Magnesianchromite	MgCr <sub>2</sub> O <sub>4</sub>
Chromite	FeCr <sub>2</sub> O <sub>4</sub>
Ulvospinel	Fe <sub>2</sub> TiO <sub>4</sub>
Inverse spinel	MgTiO <sub>4</sub>

By using the selection tab, the user can change the visual attributes (such as color, size and shape) of the selected sample (Fig. 10). The modifications applied on the visual representation of a particular data sample can be undone; when this occurs, that sample acquires the same visual representation that the rest of the dataset to which it belongs.

#### 4.3. Obtaining details of a data sample by demand

By selecting a sample within the prism, additional information relating to it is provided on the selection tab of the utilities area. This tab provides information about the selected data sample, information related to the dataset to which it belongs, the values of its final members and the graphic attributes associated with it. Thereby, the user can get detailed information of each sample located within the prismatic space at any time (Fig. 10).

#### 4.4. Loading projections

One of the most important features of the application is to provide 2D projected plots of the data, and the integration of these projections in the 3D space. Such projections are used to classify spinels based on geochemical data, minerals that exhibit a wide range of solid solution which has been the subject of many thermodynamic studies.

To see 2D projections, the “projection” tab in the utilities area must be selected (Fig. 11). The 2D projections are calculated automatically when loading a dataset and are available throughout all the application execution, allowing the exploration of the 3D prismatic space and the visualization of 2D projections at the same time. The 2D space where the projections are represented can be translated, rotated and scaled, allowing navigation over the 2D space in order to achieve a more meaningful analysis of the projected data.

samples, a numeric text-box associated to each pattern is provided. To change or select the color of data samples, a color map dialog box can be used by the user to select the most suitable color (Fig. 8). Finally, the data samples can be represented with three different shapes: spheres, cones and cylinders. The user can select and change the shape used to represent the samples of a given pattern in the pattern information area at any time during the execution of the application (Fig. 9).

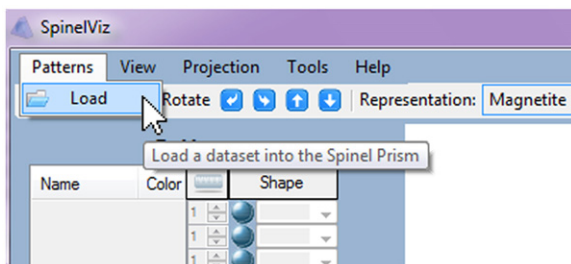


Fig. 6. Loading a dataset into the spinel prism.

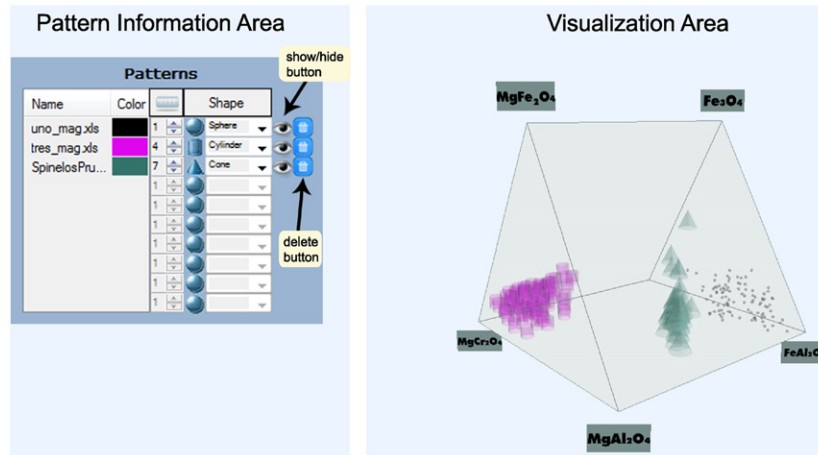


Fig. 7. SpinelViz enables the loading of multiple patterns simultaneously. In this figure three patterns were loaded, each one of them represented with a different shape, size and color. The user is able to change the visual representation of each pattern in the pattern information area.

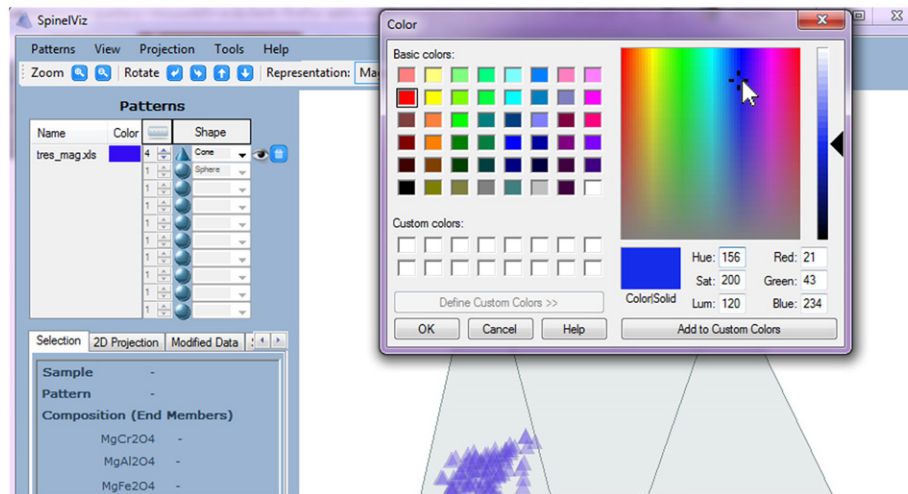


Fig. 8. A color map dialog can be used to choose the color of all the data samples of a pattern.

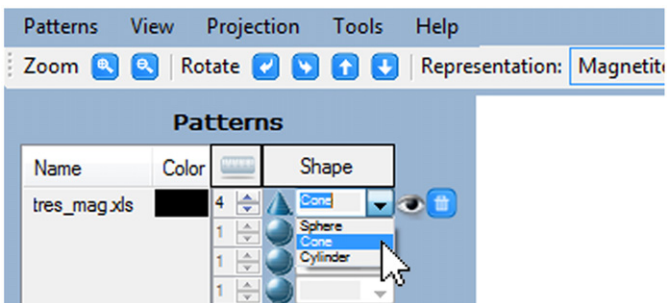
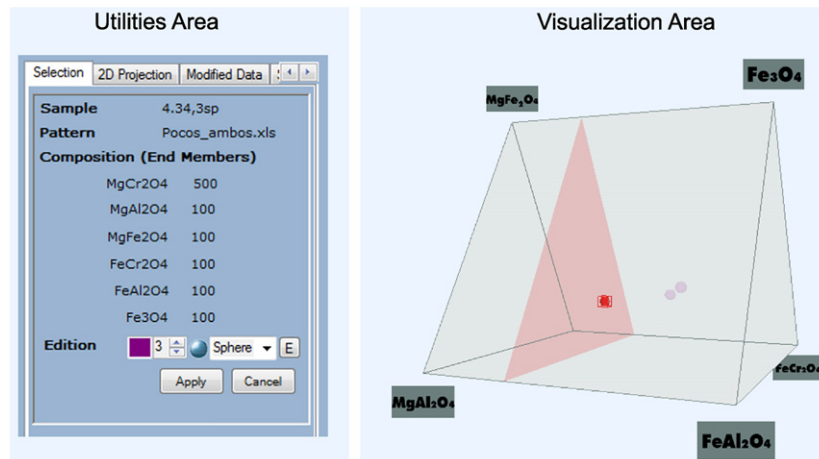


Fig. 9. Changing the shape of all the data samples of a pattern.

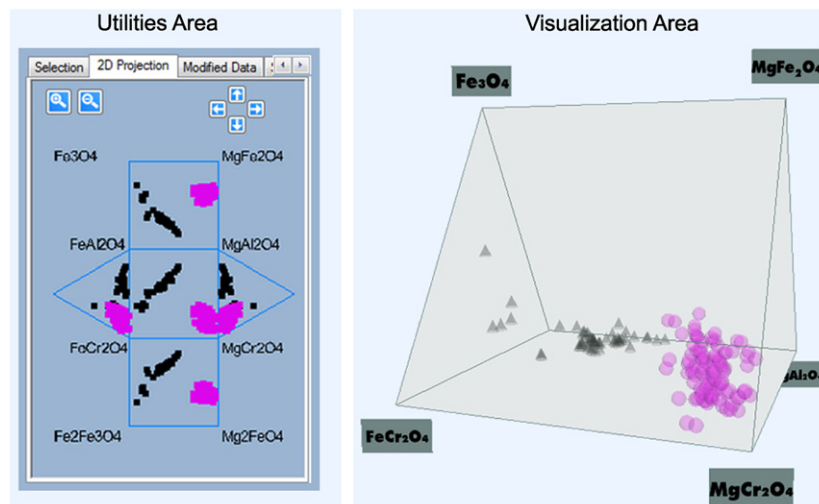
In addition, the application provides the capability to show and hide the 2D projections embedded in the 3D space. A 3D projection is basically a 2D projection integrated in the 3D scene with the spinel prism (Fig. 12). The 3D projection is shown in the same window as the spinel prism, drawing all the projected faces over a plane parallel to the prism base and situated below it. This integration gives the user context of each projection, and enables manipulation of the spinel prism and the projections at the same time.

## 5. Conclusions

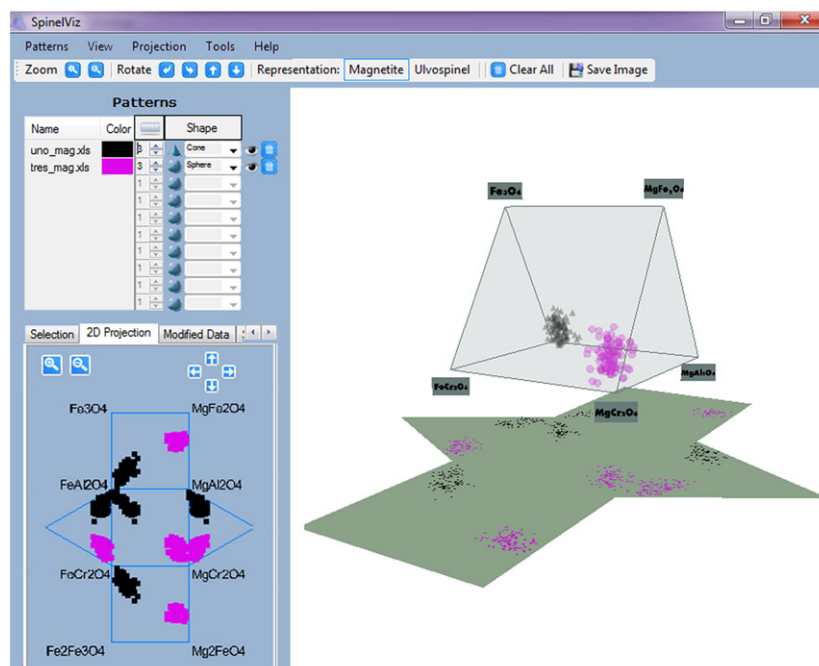
SpinelViz is an application for the visualization of the spinel group minerals in three dimensions. SpinelViz uses the spinel prism to display mineral composition datasets from different tectonic settings, provides the possibility to project and to visualize data within the spinel prism in three dimensions, and make two dimensions projections very easily. Such projections are used to classify spinels based on geochemical data. Spinels, particularly chromites from mafic–ultramafic igneous rocks are used to discriminate among various tectonic settings. Their existence in ultramafic rocks and their resistance to alteration make them excellent tectonic tracers and a very important tool in search for economic deposits of the platinum group elements (PGE) and Ni–Cu–PGE. SpinelViz provides a set of functionalities that help users to manipulate their datasets for both 2D and 3D visualization and 2D projections. Geochemists commonly compile their data with Microsoft Excel™ so SpinelViz uses an Excel source file to upload datasets. With SpinelViz it is possible to plot any solid solution with changes in X and Y in one single diagram, allowing potential users to visualize populations with different genesis and tectonic settings in one single plot. This has impact not only in the academic world but also in the mining sector, due to the fact



**Fig. 10.** By selecting a sample within the prism, additional information relating to it is provided in the selection tab of the utilities area. This tab provides information about the selected data sample, like the dataset to which it belongs, the values of its final members and the graphic attributes associated to it.



**Fig. 11.** 2D projections of the datasets loaded into the prismatic space are drawn in a 2D space (the faces of the prism) and located in one of the tabs in the utilities area.



**Fig. 12.** Several datasets simultaneously loaded into the prismatic space along with the corresponding 3D projection. In the 2D projection tab of the utilities area the 2D projections are shown, allowing the user the exploration of projections in two and three dimensions at the same time.

that these minerals are excellent tracers for a wide variety of economic mineral deposits.

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