Mineral Compositions Visualization Implementing the Spinel Prism

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Abstract. An important problem in Mineralogy, is to accomplish an adequate representation of a great amount of data coming from different geological environments, in order to characterize a particular geologic region in terms of its tectonic setting. With such Databases of mineral compositions it is possible to define the compositional fields that constitute a reference pattern to classify an unclassified data sample. Mineralogic patterns are represented in ad-hoc tree dimensional spaces that could be prismatic or tetragonal. In this context we developed the Spinel Prism Viewer, a Geological Visualization Application consisting on a 3D Viewer which allows the user to watch, explore and interact with the Spinel Prism and different Datasets at the same time. The Viewer provides projection tools in 2D and 3D, helping the users to understand the tectonic identity of a particular mineral composition represented on the view.

Key words: Scientific Visualization, Interactions, Spinels, Geological Sciences.

1 Introduction

Scientific visualization is the use of computer graphics to create visual images which aid in the understanding of complex, often massive numerical representations of scientific concepts or results [1]. Such numerical representations, or datasets, may be output of numerical simulations as in Computational Fluid Dynamics (CFD), Molecular Dynamics (MD) or engineering in general, measured data as in geological, meteorological or astrophysical applications.

Visualization is essential in interpreting data for many scientific problems. It transforms numerical data into a visual representation which is much easier to understand for humans. Other tools such as statistical analysis may present only a global or localized partial view on the data [2].

The exploration of Datasets originated from Natural Sciences, and Geological Sciences in particular, involves the application of interactive visualization tools and techniques. In this paper we study visualization if an special group of minerals called Spinels. Minerals that integrate the group of Spinels represent a great compositional variety linked to their genesis. This implies the fact that some minerals of the group, chromite minerals in particular, have been used as "Petrogenetic indicators"[6, 3, 4], since they provide vital information regarding the tectonic setting of the rocks present in an area, in the context of global tectonics.

To achieve a significant evaluation of data samples in this context, it becomes necessary to have a big number of data coming from different geological environments. With such databases of mineral compositions it is possible to define the compositional fields that constitute a reference pattern to classify an unclassified data sample.

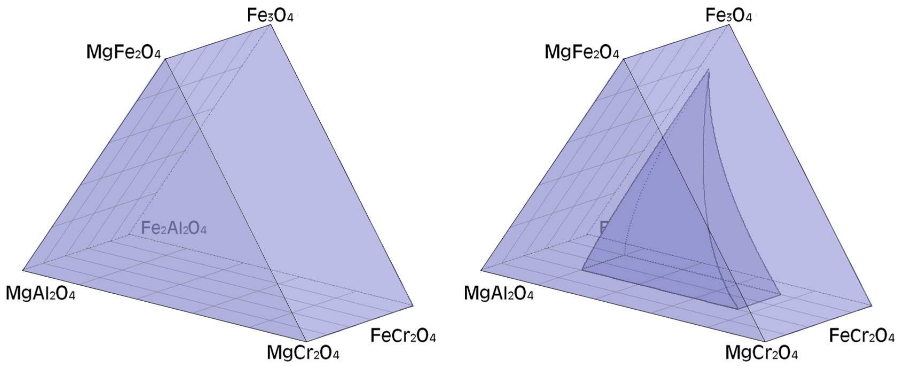
Without a doubt, building a referential field with such a big amount of data, (more than 20.000), and at the same time include in a graph the data of a new population are tasks that require a big amount of time inversion if they are not implemented on an automated way. All this has set the necessity to visualize data on their natural domain, making easier the comparisons and integration of multiple Datasets.

Taking all of this into account we developed a Geological Visualization Application called Spinel Prism Viewer. The application consists on a 3D Viewer which allows the user to watch, explore and interact with the Spinel Prism and different Datasets at the same time. The Spinel Prism Viewer provides the capability of project Datasets over the different faces of the prism in 2D and 3D, helping the user to understand easily the mineralogic composition represented on the view.

2 Application Field

An important problem in Mineralogy is to achieve an adequate representation of mineral compositions, in a way that groups of samples can be intuitively matched against a given pattern. Mineralogic patterns are represented in ad-hoc tree dimensional spaces that could be prismatic or tetragonal. In this paper we are studying the prismatic representation, where each apices of the prism are determined by the composition of the Data Sample Group (Figure 1(a)). These Prism is called Spinel Prism.

In Figure 1(b) we can see a prismatic space of oxide composition. An established "historical" set of samples of a given mineral belonging to rocks from a particular tectonic setting conforms a trend within the composition space. This trend is a volumetric pattern compositions or proportion of oxides that characterizes that particular mineral, and can be represented as a solid within the composition 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) .

Fig. 1. Prismatic Space [6]

Data from a given set of unclassified samples may be represented in this space with an adequate icon, and the classification problem is now to visually determine if these icons lay within the pattern or not. However, the set of samples is normally a huge, of variable size and subject to change. Then, a better representation aid should be to find and adequately represent a set of samples as a whole.

2.1 Sample Representation within the Spinel Prism

In this section we want to introduce the process of positioning a sample within the Prism(Figure 3). In the prismatic representation, each apices of the prism is determined by the composition of the minerals of the Spinel Group. In this case to represent the samples on the prism the Magnesium (Mg), Iron (Fe), Chrome (Cr) and Aluminium (Al) proportions are taken into account. As illustrated in Figure 3, the ternary on the left of the prism has Mg as the common element, and the ternary to the right has Fe^{2+} as the common element [3].

To understand how a data sample is positioned within the Spinel Prism and only as an example, projections of a particular data sample over the faces of the Prism are shown. In this case, we consider a data sample composed by the following values for each component:

- $Magnesium(Mg) = 12\%$
- $Iron(Fe) = 18\%$

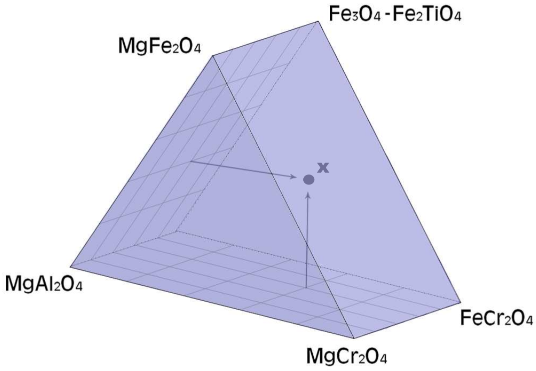


Fig. 2. A data sample within the Spinel Prism.

– $Aluminium(Al) = 21\%$
– $Chrome(Cr) = 32\%$

An useful projection of this particular data is shown in Figure 3(a). The projection on this face is given by the following expression:

$$\frac{2Fe^{3+}}{2Fe^{3+} + Al + Cr} \tag{1}$$

Equation (1) defines where the sample is going to be positioned according to the edge determined by the $FeAl_2O_4$ and Fe_3O_4 apices of the Spinel Prism.

$$\frac{Fe^{2+}}{Fe^{2+} + Mg} \tag{2}$$

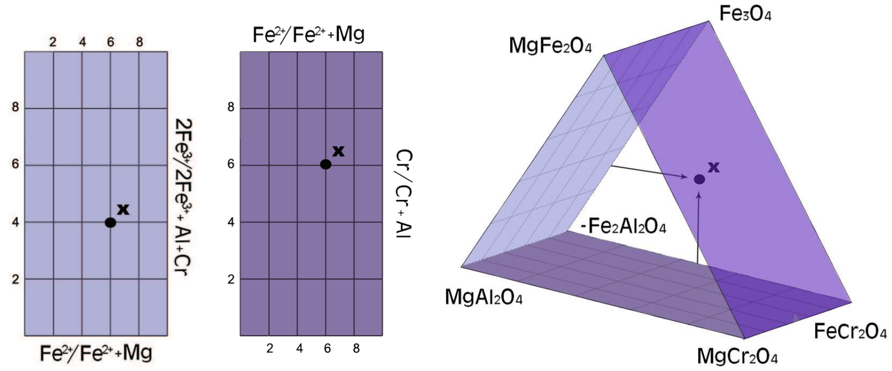
Equation (2) defines where the sample is going to be positioned according to the edge determined by the $MgAl_2O_4$ and $FeAl_2O_4$ apices of the Spinel Prism. Figure 3(b) shows another useful projection, the projection on the spinel prism base. In this case the expression (2) detailed above is applied for the edge determined by the $MgAl_2O_4$ and $FeAl_2O_4$, shared by both faces of the Prism, and expression (3) is used to positioning the sample according to the edge determined by the $MgAl_2O_4$ and $MgCr_2O_4$ apices.

$$\frac{Cr}{Cr + Al} \tag{3}$$

Finally, equations 1, 2 and 3 gives the coordinates of the data sample within the Spinel Prism.

3 Related Work

In the Visualization field, no research devoted to this particular group of minerals is known. Geological Scientists use to work with the prismatic space doing



(a) (b) (c)

Fig. 3. Plotting procedure for compositions in the multicomponent Spinel Prism. Coordinates of a the data sample detailed above. The position of the sample is determined by equation (1) $2Fe^{3+}/2Fe^{3+} + Al + Cr = 0.4$, equation (2) $Fe^{2+}/Fe^{2+} + Mg = 0.6$ and equation (3) $Cr/Cr + Al = 0.6$ [3].

different projections over the faces of the Prism as it was explained on section 2.1. To achieve these projections several applications has been developed, most of them implement triangular diagramming in two dimensions. Clearly a tree dimensional interactive visualization might be very useful to Geological Scientists who need to study Spinels Datasets, because although 2d projection tools exist, they don't provide any interaction over the view or the capabilities of integrate projections with the spinel prism in order to get a better idea of the visual context. Until the moment no tree dimensional application has been developed yet.

4 Spinel Prism Visualization Application

The Spinel Prism Viewer presented provides an interactive visual representation of these group of minerals that constitute Tectonic Tracers using the Spinel Prism. The application was customized to handle specific types of data, allowing the analysis of special relationship between data. It presents Mineralogic Datasets within the Spinel Prism following equations 1, 2 and 3 (section 2.1), providing interactions to the user to allow navigation over the prismatic space and exploration of data.

In Figure 4 a screen capture of the Spinel Prism is shown, in this case a data set is plotted inside the prism.

The Application was implemented in C#, using the Microsoft .NET Framework [9] and the OpenGl API [8]. To use OpenGl with any .NET programming language, a wrapper is needed. We adopt the CsGL wrapper [7], which provides support for OpenGL 1.1 and numerous extensions.

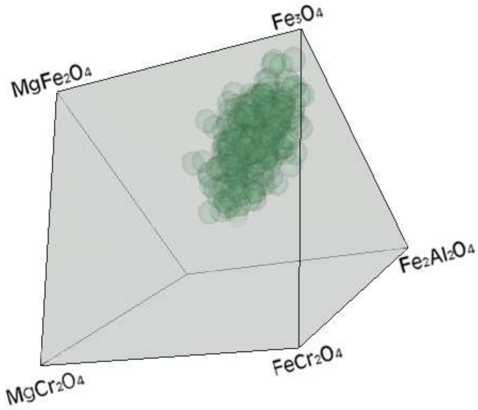


Fig. 4. Spinel Prism Viewer.

The Spinel Prism Viewer composed by tree main components: the Mathematics Framework, The Visual Representation and the Interactions sets.

5 Mathematical Framework

The mathematical framework is a major component of the Spinel Prism Application. The goal of the Math Framework is to provide a specific solver for the mathematical problems in the application domain. These problems include the calculation of coordinates and projection of each data sample within the Spinel Prism; which constitute very important for the correct result of the visualization.

The fact that projections are shown on 3D and 2D adds an additional difficulty to calculations, so it seems attractive to separate the Mathematics Framework as a independent module.

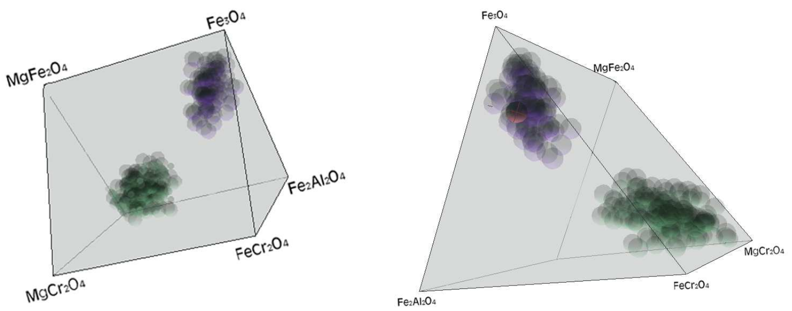
6 The Visual Representation

The visual representation involves the definition of the spatial substrate, the asociation of visual elements to represent data elements and the graphical attributes of those elements.

An important task of our application is to achieve an adequate representation of mineral compositions, in a way that groups of samples can be intuitively matched against a given pattern. Spinel Prism Viewer represents the mineralogic composition of each data sample with an Sphere within the Prism. The position of the Sphere is given by equations 1, 2 and 3 (section 2.1).

In order to achieve a significant evaluation of unclassified samples, it is necessary to be provided with a big number of spinel compositions coming from different geological environments , in order to define compositional fields that constitute a reference pattern to classify an unclassified sample. To represent these patterns the Spinel Prism Viewer use transparency over the Spheres; allowing a set of data samples situated on neighborhood positions to constitute a volume within the Prism. Data samples from different patterns are represented with different colors, allowing the visualization of two or more referential patterns within the same prismatic space (See Figure 5(a)).

To see if a data sample belongs to a certain pattern, the Application represents the data set with a different color from the color used for the patterns (See Figure 5(b)), and with the help of transparency the user can navigate over the 3D space to realize if the data sample lay inside a pattern or outside. As an example of these feature Figures 6(a) and 6(b) illustrate the application of the zoom interaction over the scene, allowing the user to get closer to the data sample to verify if it belongs to a pattern or not. In this case, by getting closer to the sample, we realize that in fact it belongs to one of the two given patterns.



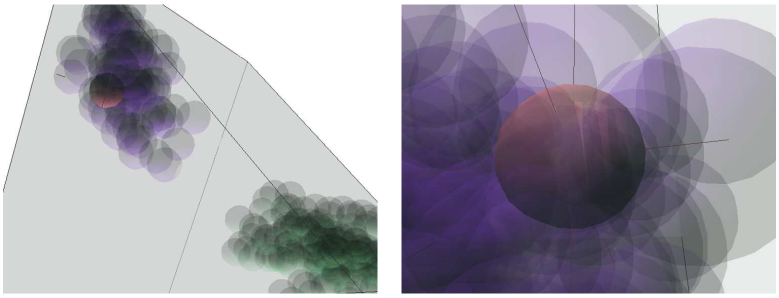
(a) (b)

Fig. 5. Spinel Prism Viewer allows the user to load more than one pattern. Figure (a) illustrates this capability, showing two different patterns inside the prism . Notice that the patterns can be differentiated by the color of the Spheres. One pattern has been drawn in green and the other in purple. In Figure (b) a new data sample has been added in red color.

7 Interactions

The most important application goal is to provide a 3D visualization of the prismatic space, allowing the user to interact with the visualization for a better understanding to obtain different perspectives of the position and projection of data set. The Spinel Prism Viewer provides a set of basic interactions, like rotation, geometric zooming, and translation of the scene, which allows the user to navigate across the scene and explore the data from different points of view.

The Viewer also supplies some particular interactions specific to the application field:



(a) (b)

Fig. 6. Zooming over the prismatic space. Figure (a): Zoom interaction applied to the scene, attempting to get closer to the data sample. On Figure (b), with more zoom, is clear that the data sample lays inside the purple pattern.

Show/Hide Projections 2D The projection of each data sample within the Spinel Prism is a very important task. Our approach provides the user with two ways to see, explore and analyze these projection. The fist approach consists of 2D projection of the five faces of the Prism with the corresponding data sample projected over them. These 2D projections are shown on a different window, and can be closed and opened at any time within the application execution (See figure 7(b)).

Show/Hide Projection 3D The 3D projection is basically a 2D projection integrated in the 3D scene with the Spinel Prism. 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 and situated behind it. This integration brings the user a better idea of the context of each projection, and allows interactions with the Spinel Prism and projections at the same time (See figure 7(c)).

Show/Hide Grid The Viewer allows the user to activate and hide referential Grids on the faces of the prism. These referential grids are used to give the user a notion of the mineralogic composition of a sample according to the projection of it over the faces of the prism. Referential grids are shown on Figures 3(b) and 3(a).

Change/Select Color of Spheres This interaction provides the user the capability of changing the color of a whole pattern, a set of data samples, or a unique sample.

Load a unique data sample This interaction adds an unclassified data sample (which components are giver by the user) to the Spinel Prism. This new sample is represented, as any sample, with a Sphere, and paint on a different color to be easily differentiated to all the other samples already drown on the scene. This is one of the most important interaction of the application because allows the user to integrate a data sample with different patterns, and find out if a data sample belongs to a given pattern or not. Thanks to the different color, and the use of transparency, zooming, and rotation of the scene, the user can get closer to the new data sample and discover if its placed inside pattern or not, as has been seen on figure 6.

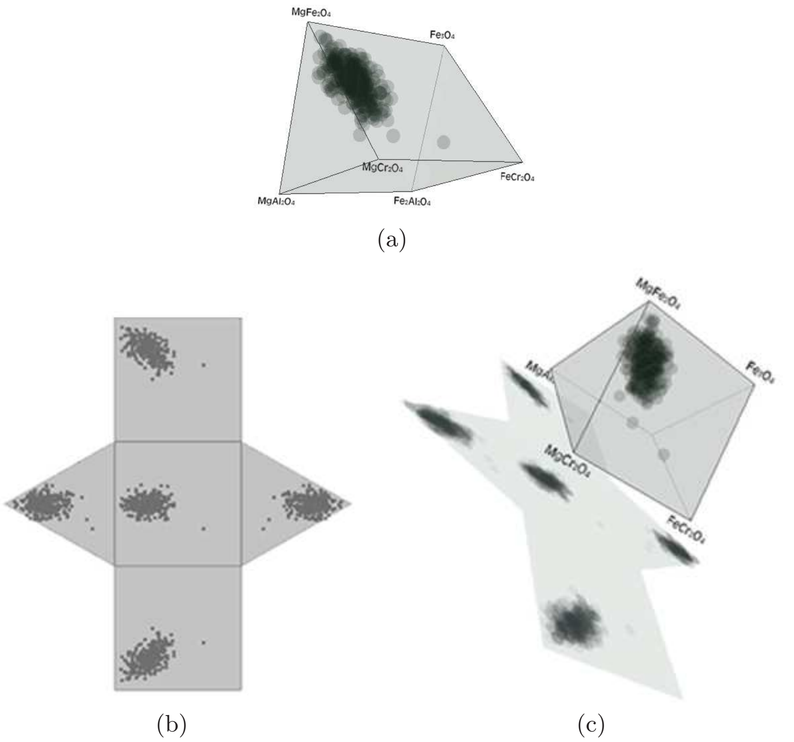


Fig. 7. Spinel Prism Projection Example. Figure (a) shows the data set to be projected, figure (b), shows a screen capture of the 2D projection of the data set; and figure (c) shows the 3D projection of the data set integrated with the Spinel Prism.

8 Conclusions and Future Work

The Spinel Prism Viewer: is a visualization tool intended to help users to explore geological Datasets within a prismatic space. As been said before, no geological visualization tools using the spinel prism have been developed, and geological scientists use 2D triangular plots to obtain the projections. Spinel Prism Viewer not only represents the prismatic space on tree dimensions, but also provides a rich interaction set, allowing the user to interact with the view gaining insight about the representation of mineral compositions. Besides interactions, we pretend to include volume rendering, and explore other ways to represent data patterns, as closed surface or volume rendering. As future work, we intend to extend the interactions set, including tools which allow to get more information of each data set on demand of the user. For example, we aim to include an interaction that shows the mineralogical composition of a sample when the user select it. Finally, some user evaluation is expected to be done, in order to obtain a quantitative measure of the effectiveness of our Application.

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