The Spinel Explorer - Interactive Visual Analysis of Spinel Group Minerals

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Abstract— Geologists usually deal with rocks that are up to several thousand million years old. They try to reconstruct the tectonic settings where these rocks were formed and the history of events that affected them through the geological time. The spinel group minerals provide useful information regarding the geological environment in which the host rocks were formed. They constitute excellent indicators of geological environments (tectonic settings) and are of invaluable help in the search for mineral deposits of economic interest. The current workflow requires the scientists to work with different applications to analyze spinel data. They do use specific diagrams, but these are usually not interactive. The current workflow hinders domain experts to fully exploit the potentials of tediously and expensively collected data. In this paper, we introduce the Spinel Explorer - an interactive visual analysis application for spinel group minerals. The design of the Spinel Explorer and of the newly introduced interactions is a result of a careful study of geologists' tasks. The Spinel Explorer includes most of the diagrams commonly used for analyzing spinel group minerals, including 2D binary plots, ternary plots, and 3D Spinel prism plots. Besides specific plots, conventional information visualization views are also integrated in the Spinel Explorer. All views are interactive and linked. The Spinel Explorer supports conventional statistics commonly used in spinel minerals exploration. The statistics views and different data derivation techniques are fully integrated in the system. Besides the Spinel Explorer as newly proposed interactive exploration system, we also describe the identified analysis tasks, and propose a new workflow. We evaluate the Spinel Explorer using real-life data from two locations in Argentina: the Frontal Cordillera in Central Andes and Patagonia. We describe the new findings of the geologists which would have been much more difficult to achieve using the current workflow only. Very positive feedback from geologists confirms the usefulness of the Spinel Explorer.

Index Terms—Interactive visual analysis, visualization in earth, space, and environmental sciences, coordinated and multiple views, design studies

1 Introduction

Spinel group minerals are constituents of igneous and metamorphic rocks. They are oxides, most commonly of the following chemical elements (cations): magnesium, iron, manganese, aluminium, chromium, vanadium and titanium and less frequently of zinc, nickel, copper, germanium and cobalt.

Due to the fact that they are very sensitive to the conditions prevailing during the crystallization of rocks, and due to the fact that they are very resistant to be chemically modified after the crystallization, they provide useful information regarding the geological environment in which the host rocks were formed. Therefore they constitute excellent indicators of geological environments (tectonic settings) as well as invaluable exploration tools in the search for mineral deposits of economic interest.

Geologists usually deal with rocks that are up to several thousand million years old and they currently can be found in places far away from those where they originally have been formed. By studying a particular suite of rocks, specially those with spinel group minerals, it is possible to reconstruct the tectonic setting where this suite of rocks has been formed and the history of events that affected them through the geological time. It is of uppermost importance to have indicators, such as the spinel group minerals, whose chemical composition can provide evidences about the tectonic setting where a given rock or suite of rocks have been formed. Defining the tectonic setting helps geologists to understand the geological evolution of Earth and also to locate, for example, mineral deposits.

In order to accomplish these objectives geologists use, among other criteria, the chemical composition of the spinel group minerals. The composition of these minerals allows the geologists to define compositional fields according to the tectonic settings in which the spinel group were developed. Barnes and Roeder [1] compiled a database comprising more than 26000 analyses of spinels from igneous and metamorphic rocks. The database is used to delineate and construct characteristic compositional fields for spinels of various tectonic settings and magma compositions. Manipulating and analyzing large datasets of spinel compositions is a highly time consuming process due to the fact that each mineral is composed of several chemical elements whose proportions are influenced by geologic, mineralogical, crystallographic and chemical factors. Hence the need arises to visualize the data in an easy way to compare and integrate a given dataset [8]. In this context, 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 which characterizes the tectonic setting in which they were formed.

Geoscientists often use static diagrams to support data analysis. The spinel data have some specific features. For each spinel sample there are several numeric attributes. Some of them represent ratios where groups of three or six attributes sum up to 1.0 or to 100%. This data characteristic resulted in specific plots the geoscientists use very often. They mostly plot the composition of spinels on prismatic spaces,

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which provide reasonably interpretable 3D diagrams [9] and enable the visualization of projections of datasets on the faces of the prisms. These prismatic spaces are widespread even though they are difficult to generate by hand, and therefore geologists mainly use binary and ternary plots to study prism projections and to evaluate correlations between chemical elements and/or oxides. The current workflow requires the scientists to work with different applications to produce the mentioned plots, and they are usually not interactive. Interactive visual analysis can improve the efficiency significantly.

In this design study, we introduce the Spinel Explorer - an interactive visual analysis application for spinel group minerals. The design of the Spinel Explorer and of the newly introduced interaction is a result of a careful study of geologists' tasks. The Spinel Explorer includes most of the diagrams commonly employed for analyzing spinel group minerals, including 2D binary plots, ternary plots, and 3D Spinel prism plots. Besides specific plots, conventional information visualization views are also integrated into the Spinel Explorer. All views are interactive, linked, and integrated in a coordinated multiple views setup. In addition to Spinel Explorer as interactive exploration system, we also describe the identified analysis tasks, and propose a new visual analysis workflow. We evaluate our approach using real-life data from the Frontal Cordillera in the Central Andes and from Patagonia, both in Argentina.

The contributions of the paper can be summarized as:

- A *design study* to develop an interactive tool for spinel data exploration and analysis.
- The design of *two new interactive views*, the triangle plot and the Spinel prism. The two plots often used in geology are made interactive and are linked in a coordinated multiple views setup for the first time.
- An *evaluation* of the proposed approach within the geosciences context and a report on domain experts feedback.

2 Related Work

We divide the related work into two sections. We describe previous work on plotting geological data first. Although most of the techniques are not interactive they represent the state of the art in the geologic field. An overview of related visualization techniques is also provided.

2.1 Plotting Spinel Group Minerals

It is a common practice to plot spinels on prismatic spaces, which provides a reasonable and easily interpretable 3D chart (Figure 1) [9]. Such plots are difficult to generate by hand, therefore, scientists mostly use binary and ternary plots to evaluate correlations between chemical elements or oxides. Given the lack of one application that integrates most of the diagrams commonly used for analyzing spinel group minerals, scientists typically work with different systems to generate specific diagrams, but these are usually not interactive. For example, IGPet [4], MinPet [20], MinCalc [2], GCDkit [11], etc. have been developed for better data analysis and representation. In 1990 an integrated package to analyze and visualize igneous petrology information was published for Macintosh [29]. 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 viewing angle and distinguish up to five distinct groups of spinel analyses by means of different symbols. In 2012, Ganuza et al. [8] presented a geological visualization application called SpinelViz. The application consists of an interactive 3D viewer which enables to depict and explore the Spinel prism with different datasets at the same time. SpinelViz provides the capability to manipulate, view, plot, and project data in 2D and 3D which helps the user to gain a better insight of the data distribution. The Spinel Explorer integrates the most commonly used plots in spinel exploration, integrated with other conventional plots in an interactive visual analysis framework.

2.2 Interactive Visual Analysis

Automatic analysis methods and static plots are often not sufficient as data size and complexity or analysis requirements increase. In order to effectively cope with new requirements, visual analytics offers to combine the strengths of human perception and cognition with a computational analysis [14, 15, 27]. Interactive visual analysis provides an interactive and iterative exploration and analysis framework, where the user guides the analysis [24], supported by a variety of computational analysis tools. This helps the domain expert to explore and analyze the data, and to understand complex and often hidden relationships between certain data aspects. The visual information seeking mantra - overview first, zoom and filter, then details-on-demand - as identified by Shneiderman [23], summarizes the most typical pattern in interactive visualization. Interactive visual analysis is much more than the presentation of data; it supports the user in the analysis of complex and heterogeneous datasets. Visual analytics has been successfully employed in many domains. Several authors have applied it to scientific data as well [12, 13, 17, 19]. Coordinated multiple views [21] are often employed as a proven concept in visual analysis. The main idea is to depict various dimensions using multiple views and to allow the user to interactively select (brush) subsets of the data in a view. Then all the corresponding data items in all linked views will be consistently highlighted. Although multiple views represent a very powerful methodology, interactive systems employing it have to be very carefully designed. Wang Baldonado et al. [28] describe guidelines for using multiple views. Of course, they cannot be used always, but our data, the current workflow, and the willingness of the domain experts to learn, motivated us to employ coordinated multiple views.

There are many interactive visualization systems available. Some of them represent general purpose tools (Xmdv Tool [22], GGobi [26], or Polaris [25], for example), and some have been developed for specific data and domains. VisMon [3], e.g., deals with fishery data, and SimVis [5] has been designed for simulation data. As we focus on the spinel minerals data none of the existing tools could have been employed directly. According to the best of our knowledge the state of the art tools do not support triangle plots and Spinel prism views. These plots are so specific that they do not appear in other tools. The newly developed Spinel Explorer supports iterative composite brushing and on-the-fly data derivation [16]. Some other tools, SimVis, for example, support a feature definition language [5] to create composite brushes. Many researchers exploit brushing as firstly described by Martin and Ward [18]. We paid special attention to interaction when proposing new views. Brushing in new views is carefully designed to support data semantics. Instead of a common rectangular brush we use a triangular brush. The triangular brush makes no sense in a scatterplot or other standard views. Such differences, originating from specific data and tasks, make a systematic comparison with the state of the art tools rather complicated. Instead we focus on a comparison with the standard workflow of domain experts. The Spinel Explorer employs basic principles of visual analytics and coordinated multiple views. The addition of two new interactive views and the accompanying interaction makes it a unique exploration and analysis tool for spinel data.

3 Domain Background - Spinel Group

Spinel group minerals are constituents of igneous rocks, particularly mafic and ultramafic as well as metamorphic rocks. They crystallize over a wide range of pressure and temperature conditions in different tectonic settings. They are relatively refractory and resistant to alteration compared with other high-temperature igneous minerals such as olivine and pyroxene [1]. Therefore their composition provides reliable and valuable information regarding the geologic conditions under which their hosting rocks crystallized. They constitute tectonic tracers because the information they provide contributes to decipher past tectonic settings. When the pure end-member chromite concentrates in layers, for example, the rock is called chromitite. The chromitite rocks are of great economic importance because they are the source of chromium (Cr) which is used in metallurgy, alloys, paintings, etc. Spinels are frequently associated to rocks carrying economic concen-

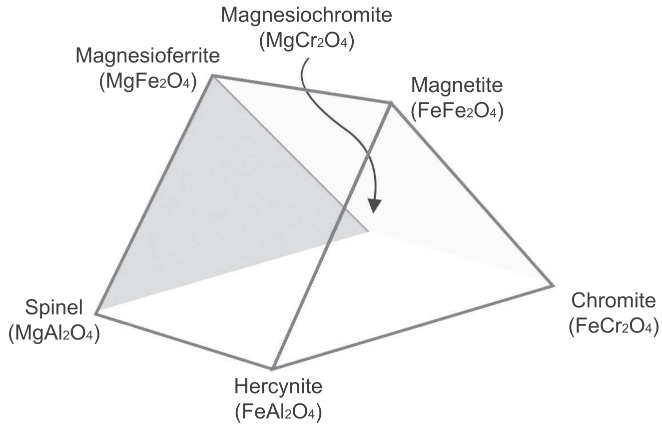

Fig. 1. The Magnetite Prism - an example of a commonly used Spinel prism. The Spinel prism is a prismatic space whose vertices correspond to the end-members of the compositional space. All points inside the prism represent various compositions of the six end-members at the vertices.

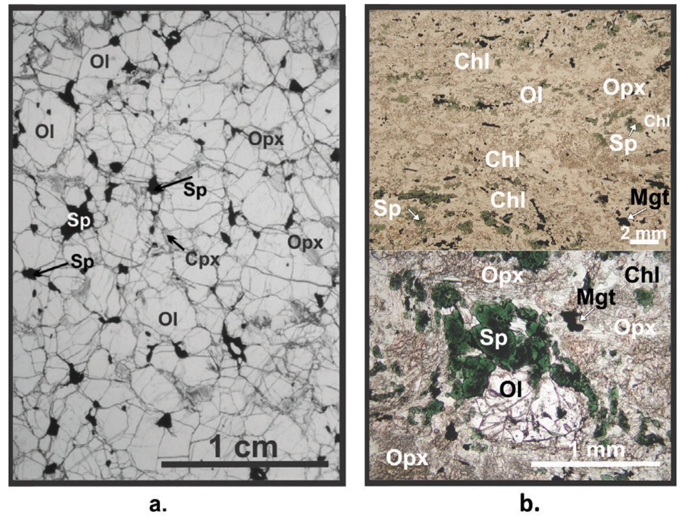

Fig. 2. Thin sections obtained from slabs of represetative rock samples. **a.** Thin section of lithospheric mantle xenolith. This rock is a Harzburgite with the following mineralogy: olivine (Ol), orthopyroxene (Opx), spinel (Sp) and clinopyroxene (Cpx). **b.** Thin section of a metaperidotite from an ophiolite type geological setting with the following mineralogy: olivine (Ol), orthopyroxene (Opx), spinel (Sp), magnetite (Mgt) and chlorite (Chl).

trations of copper, nickel, cobalt, platinum group minerals, and diamonds, among others. As such, they are a helpful guide in the exploration of deposits which are the source of minerals used in a wide spectrum of industries. These rocks are indicative of particular past tectonic settings, as well.

The spinel group minerals are oxides represented by the following standard chemical formula: $X^{2+}Y_2^{3+}O_4$ where X represents bivalent cations and Y represents trivalent or tetravalent cations. The composition of whatever combination of spinel elements can be expressed with the proportions of each end-member in the solid solution. The chemical composition of a particular end-member is always pure, which means that the proportion of all the other end-members of the solid solution must be zero. Spinel group minerals constitute a solid solution with 22 end-members which are arranged into five subgroups [7].

From all end-members, only eight are commonly used for representation on chemical diagrams. Magnetite and Ulvöspinel prisms, which are generally referred to as Spinel prism, are examples of such diagrams. These are triangular prisms where each vertex represents one end-member. Depending on the ratios of the elements in a mineral, the mineral is plotted at a specific position inside the prism (or on the border for minerals that do not consist of all end-members). The Magnetite prism is used to plot the chemical compositions of the solid solution integrated by Hercynite-Spinel-Magnesioferrite-Magnetite-Magnesiochromite-Chromite end-members. The Ulvöspinel prism is used to plot the chemical compositions for the solid solution represented by Hercynite-Spinel-Ulvöspinel-Qandilite-Magnesiochromite-Chromite end-members. The ratios of end-elements in each sample will sum up to 1.0. Of course, it is possible that some of the ratios are 0.0. In extreme cases where all but one element have ratios 0.0 the mineral is plotted at a vertex of a triangular prism. Figure 1 shows the Magnetite prism.

3.1 Spinel Group Data

The spinel datasets analyzed in this paper are from two different types of tectonic settings from Argentina: ophiolites from the Frontal Cordillera in the Central Andes and lithospheric mantle xenoliths from Patagonia. The data collection process is similar for both datasets. Polished thin sections are obtained from slabs of representative rock samples collected in the field. These thin sections (see Figure 2) are composed of crystals of the minerals to be analyzed. The chemical analyses of the mineral phases present in the thin sections are carried out using an electron microprobe with a scanning electron microscope incorporated. The electron microprobe gives the concentration of the 11 major chemical elements expressed as oxides (TiO_2, Al_2O_3, Cr_2O_3, V_2O_3, FeO, MnO, MgO, CaO, ZnO, NiO and CuO). In each thin section, all of the mineral crystals under examination are analyzed. For each measured point in a single crystal the concentrations of the major chemical elements are obtained. The number of analyzed points depends on the size of the crystals which can vary between few micrometers up to centimetres in most of the rock samples and on the inhomogeneous chemical composition of the crystals. These chemical inhomogeneities are very important to be analyzed since they give information related to variations in the conditions at the time the minerals crystallized.

With the obtained concentration of each major element, the EMG 3.0 software [6] provides the following results:

- The normalization of the oxides includes discrimination of Fe^{2+} and Fe^{3+}.
- Their atomic proportion per formula unit (p.f.u.), that is:
  atoms of element/formula of mineral = moles of element/mole of mineral formula.
- The 16 end-members of the spinel group ($MgAl_2O_4$ (Spinel), $FeAl_2O_4$ (Hercynite), etc.).
- The proportions of the spinel group end-members in the Magnetite and Ulvöspinel prisms.

The chemical analyses of the ophiolites samples were carried out using a Jeol SEM 6310 electron microprobe at the Institute of Earth Sciences, Mineralogy and Petrology section, Karl-Franzens University of Graz, Austria, using a LINK ISIS energy dispersive system (EDS) and a MICROSPEC wavelength dispersive system (WDS). The chemical analyses of the mantle xenoliths samples were carried out using a Cameca SX100 electron microprobe at the Department of Lithospheric Research, University of Vienna, Austria.

The above described procedure resulted in two datasets we used in this design study. The first dataset has 114 records. Each record corresponds to the chemical composition of an analyzed point of xenoliths samples. The second dataset consists of 58 records. Each record corresponds to an analyzed point of ophiolites samples. Both datasets have 60 attributes including the values of the oxides, the cations and the end-members composing the analyzed point. Of these 60 attributes, 12 can be combined into groups of six which sum up to 1.0, another 12 can be combined into groups of three where members sum up to 1.0.

3.2 Analysis Goals and Current Workflow

Once the data is collected the geologists studying the spinel group minerals have two key objectives to determine:

- The tectonic setting based on the chemical composition of the spinel group minerals dataset.
- The geological processes linked with the compositional variation of the spinel group minerals dataset.

The data represent a multidimensional dataset with some specific characteristics – there are groups of three and of six attributes that sum up to 1.0. The conventional analysis, which is currently the state of the art in the field, carefully examines many binary and ternary plots. Scatterplots (binary plots) are commonly used in the chemical studies of spinel group minerals to show the relationship between the cations assumed to be in the octahedral site of the crystalline framework (Y) against those which are expected to be in the tetrahedral site (X), according to the structural formula XY_2O_4. Scatterplots with the representation of the cation proportion in the Y site versus the cation proportion in the X site are one of the classic visualization diagrams used for chemical studies of spinel group minerals. They show the chemical variations in the dataset and they also represent the lateral faces of the Magnetite or Ulvöspinel prisms.

Triangle plots (sometimes also referred to as ternary plots) are diagrams used to plot groups of three elements ($Y(Cr)$, $Y(Al)$ and $Y(Fe)$ or $Y(Ti)$) which sum up to 1.0. They are analogue to Spinel prisms, but only for three end-members.

Collections of static visualizations provide a general idea about the chemical behavior of the dataset and the groups and subgroups formed in the different tested diagrams. From each plot, compositional trends are observed and analyzed in order to determine the chemical behavior of each group and subgroup. According to the crystallization conditions of the spinel group minerals and the geological context in which the spinel crystals are formed, it is possible to explain the observed chemical trends and the groups and subgroups identified in the scatterplots and triangle plots considered. Interestingly, all the plots typically used in the analysis are static. They are also generated employing different tools, and printouts or screenshots are then used in the analysis. This motivated the development of the interactive Spinel Explorer.

4 Interactive Spinel Explorer

When developing Spinel Explorer we wanted to have a unified system for the exploration of spinel minerals . Since scatterplots, triangle plots and Spinel prisms are well known and established visual representations in the geology domain, they represent the basis of the system. In addition, we included parallel coordinates [10], histograms, and statistics overviews. All views are linked. The Spinel Explorer makes it possible to efficiently visualize 2D diagrams, the Magnetite and the Ulvöspinel prims at the same time. Figure 3 shows a screenshot from an analysis session where most of the available views were used. All views are linked and support interactive selections. The whole system provides iterative composite brushing. An arbitrary number of brushes can be combined using Boolean operations in such a way that each new brush is combined with the current state. This makes it possible to drill-down (using logical AND and DIFF operations) or to broaden the current selection (using logical OR).

As all views besides the interactive triangle plot and the interactive Spinel prism are standard in the visualization literature, we will describe the two new views and the supported interactions next.

4.1 Interactive Triangle Plot

A triangle plot is a barycentric depiction of three variables (see Figure 4). The proportions of the three variables plotted always sum up to some constant that is represented as 1.0 or 100%. It is most often used in geologic studies to show the relative compositions of soils and rocks, but it can be more generally applied to any system of three variables. It is commonly used in physical chemistry, petrology, mineralogy, metallurgy, and other physical sciences to show the compositions of systems made up of three components. As detailed in the previous section, the triangle plots are very useful for spinel group mineral analysis, as they represent the chemical exchange between the cations in the octahedral site (Y). They also represent the triangular faces of the Magnetite and Ulvöspinel prisms.

When drawing triangle plots it is usual to show a grid as well. In contrast to a scatterplot, or a conventional line chart, where the grid is rectangular, the grid is arranged in a triangular fashion (see Figure 4). Each line in the grid represents positions having a constant ratio of one component. The grid lines thus represent iso-lines. Figure 4 illustrates a triangle plot and four characteristic points are shown. Point A has a $Y(Fe)$ value of 100% and the values of $Y(Cr)$ and $Y(Al)$ are equal to 0%. All points along the BC line have an $Y(Fe)$ of 70%. Point B has no $Y(Al)$ component, and point C has no $Y(Cr)$. Point D has no $Y(Fe)$ and contains 70% of $Y(Cr)$ and 30% of $Y(Al)$. Figure 5a shows a technically possible rectangular brush which is very hard to describe semantically. Just as the grid in the triangle plot cannot be rectangular, a rectangular brush makes not much sense in our case. It could be used to select an isolated group of points, but it cannot be interpreted. In the case of a scatterplot we could easily interpret it as a cross section of two intervals. Using the same analogy here we need a triangle brush. The triangle brush is also shown in the figure. Now, it is easy to interpret what is brushed. Intervals I1, I2, and I3 define the selection. Figure 5b shows a triangle grid brush. The user specifies a triangle of the grid and all points inside are selected. This is easy to interpret, the brush shown selects points where $Y(Fe)$ is between 0% and 10%, $Y(Al)$ is between 70% and 80%, and $Y(Cr)$ is between 20% and 30%. The user can combine several grid triangles in a single brush. Finally, Figure 5c, shows a selection on an axis. All points having a certain range of $Y(Cr)$ are selected. Boolean combinations of such selections can be used for drill-down. In this way, semantically meaningful brushes like *"A between 20% and 30%, B between 30% and 40%, and C between 30% and 50%"* can be created. Composite brushing allows the user to broaden intervals in this case, and grid refinement can be employed if smaller intervals have to be selected. The plot is linked with all other views in the system.

4.2 Spinel Prism

The Spinel prism is a prismatic space whose vertices correspond to end-members of the compositional space. All points inside the prism represents various compositions of the six end-members at the vertices.

As we described above, it is a common practice to plot spinels on the Magnetite and Ulvöspinel prisms, as they provide a reasonable and easily interpretable 3D chart [9]. Ganuza et al. [8] developed the first interactive Spinel prism. However, their prism is not integrated in a multiple coordinated views system, and it supports only limited filtering of the data.

Spinel Explorer has an integrated interactive Spinel prism that allows the user to plot a dataset within a prismatic space. This enables to select which variables are associated with each vertex of the prism to generate the Magnetite and the Ulvöspinel prisms, and any other prismatic space that can be constructed from the data. In addition to displaying data in 3D prismatic space, the Spinel Explorer depicts the projection of the data on the faces of the prism, offering brushing on the projections. The prism is unfolded prior to projection and the faces are shown below the 3D prism. The 3D prism can be freely rotated. Concerning selection, the same rules as for the triangle plots apply here. Rectangular brushes make sense on rectangular sides of the prism, and triangle brushes on the prism bases. Figure 6 shows an interactive prism consisting of a 3D view and 2D projections of the unfolded prism. Note that each point is projected three times. A point is always projected onto the base, and it is projected to the closest lateral and triangular sides of the prism. As a consequence, if the user selects one point in a projection, the same point in the other projections of the same plot will be highlighted although being outside the brush.

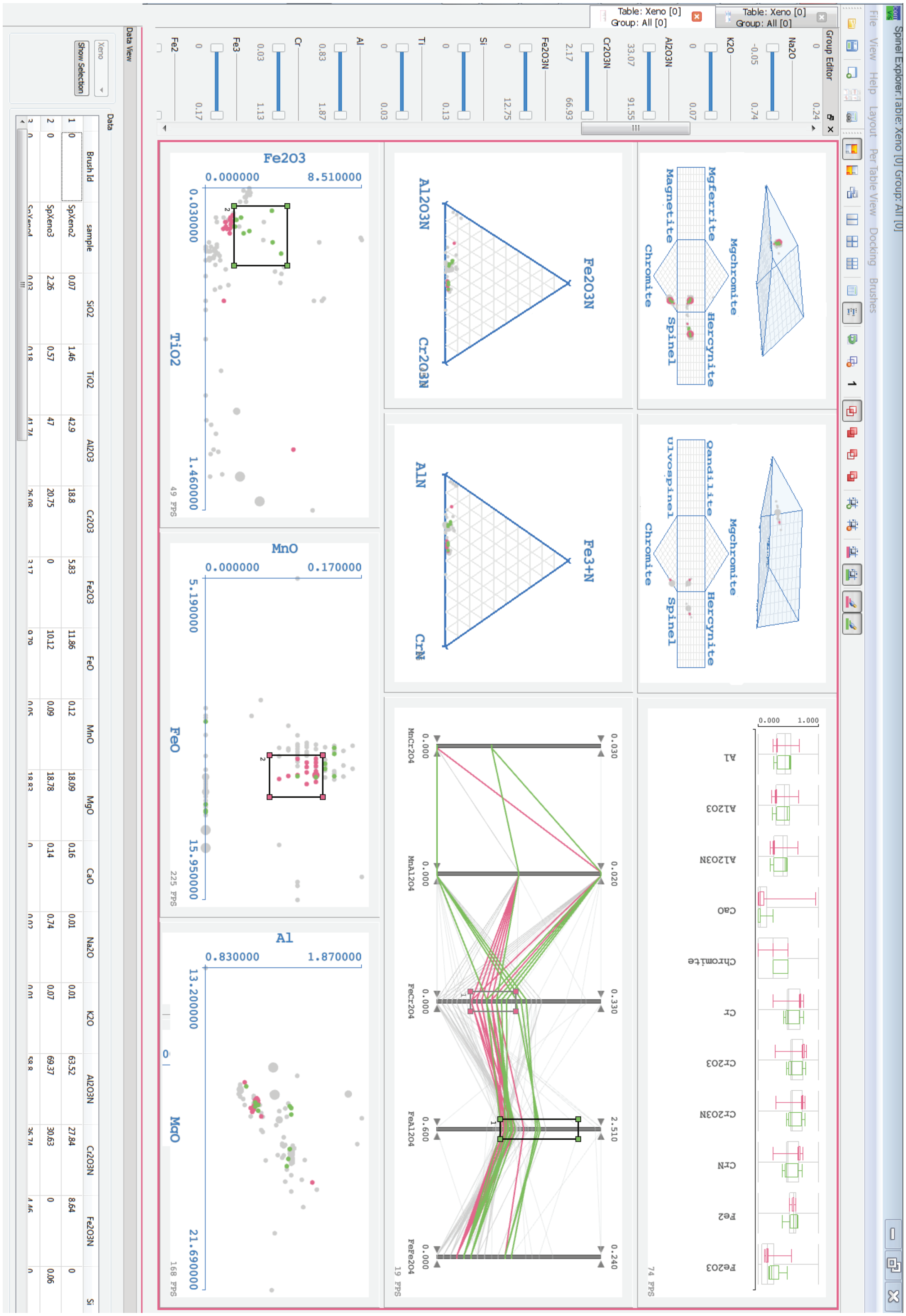

Fig. 3. A screenshot from an analysis session where Spinel prisms, triangle plots, parallel coordinates, scatterplots, and box-plot views for statistics were used. Two composite brushes are active (red and green). The data pane on the left can be used for filtering, all details are shown on demand in a table.

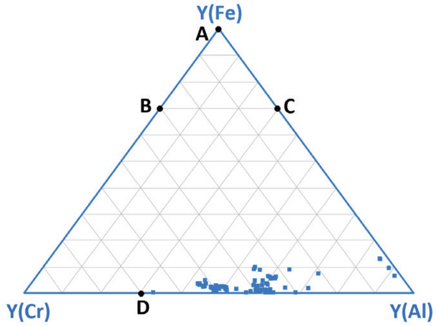

Fig. 4. The triangle plot is used to depict attributes which sum up to 1.0 or 100%. Point A consists of $Y(Fe)$ only; all points on the BC line have 70% of $Y(Fe)$. Point B has no $Y(Al)$, and point C has no $Y(Cr)$. Point D has no $Y(Fe)$, and has 70% of $Y(Cr)$ and 30% of $Y(Al)$.

4.3 Standard Views and Corresponding Interactions

Besides the two new views we extensively use scatterplots, parallel coordinates, and statistics views in the analysis. A scatterplot depicts two dimensions and can be used to easily detect correlations between two attributes. Our scatterplot supports a rectangular brush – the user can draw a rectangle and all points inside the rectangle are selected. The rectangle is easy to interpret, and its size corresponds to the two ranges of the depicted attributes. Figure 3 shows three scatterplots in the bottom row. Two of them have brushes. The parallel coordinates view shows several attributes simultaneously. The main idea is to use one vertical axis per attribute, and then the values of a record are connected using a polyline. Although the domain experts were not familiar with the view at the beginning, they quickly learned how to use it, and employed it extensively afterwards. The user can select ranges on individual axes. Figure 3 shows a parallel coordinates view with two brushes in the middle row. Finally, as geologists are used to box-plots we included a statistics view as well. It shows box-plots for selected dimensions. Besides an overall view, the values for a brushed subset are shown as well. Figure 3 illustrates an example in the top row.

5 Case Study - Interactive Visual Analysis of Spinel Group Minerals

We evaluate the Spinel Explorer in two case studies conducted with geologists. The overall feedback of domain experts was very positive. For the first time they were able to do the analysis in a unified framework. Linking and brushing (a novel concept for them) was very appreciated, and extensively used during the study. The Spinel Explorer makes it possible to simultaneously visualize triangle plots, Spinel prisms, scatterplots, and other diagrams. The addition of statistics in the form of interactive box-plots also increase the quality of the analysis. In their current workflow, geologists use several tools for plotting, another tool for statistical evaluation, and then compare all results manually.

5.1 Case 1: Determination of the Tectonic Setting of a Spinel Group Mineral Dataset Based on the Chemical Composition

This case study is based on the dataset corresponding to the lithospheric mantle xenoliths from Patagonia. The goal was to determine the tectonic settings of a set of spinel group minerals. The tectonic settings are determined by comparison with the spinel database gathered and systematized by Barnes and Roeder [1]. If the tectonic setting is assumed to be known domain experts can look up the corresponding mineral distributions roughly delimited by contours in the plot and the examined samples can be compared (see Figures 7 and 8). There is no automatic comparison method available, comparison is always done manually. The definition of a metric which could be used for an automatic comparison or, at least, as a guidance, represents a major challenge and will be covered in future work.

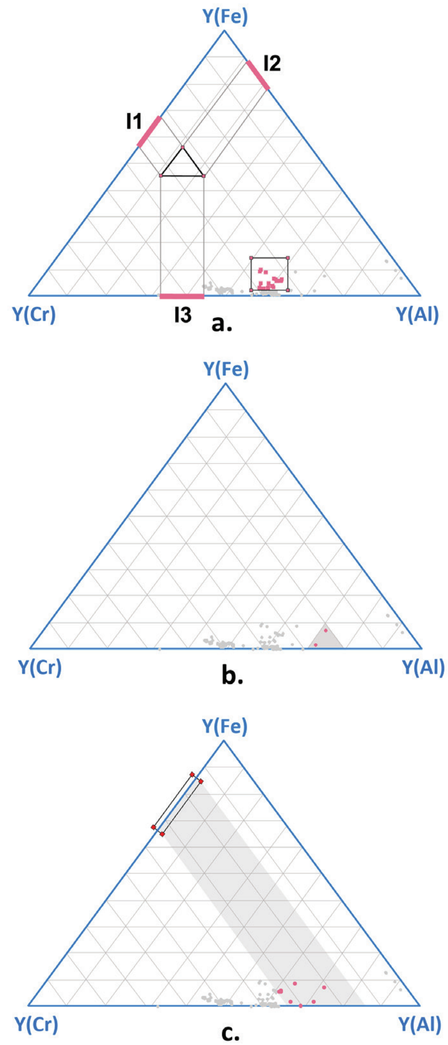

Fig. 5. A triangle plot and supported interaction. **a.** Brushing in the triangle plot enables the selection of points. A rectangular brush is technically possible but almost imposible to interpret (or to describe verbally). A triangle brush can be easily described. **b.** Another selection mechanism allows the user to select grid triangles. **c.** The axis brush selects an interval on an axis, and the corresponding area in the triangle plot. All brushes can be combined using Boolean operations.

At the beginning of our analysis, the geologists assume the rock's tectonic setting. They are aware of the geologic context and the regional environment where the rock was collected in the field. The geologists compare scatterplots of samples with scatterplots from the database. As the number of scatterplots combining the possible attributes of the samples is large, even for small data, we decide which scatterplots will be used. The domain experts call the chosen attributes control parameters.

The analyst configures the Spinel Explorer to show the control parameters in several scatterplots, triangle plots and Spinel prisms. Chemical parameters are depicted using mainly scatterplots and triangle plots. Initially, scatterplots are used to depict $Y(Fe)$ vs. $X(Fe)$ and $Cr/(Cr+Al)$ vs. $X(Fe)$. They are chosen since they represent the projections on the rectangular faces of the Magnetite prism. The $Y(Al)$-$Y(Fe)$-$Y(Cr)$ triangle plot represents the projection on the triangular faces of the prism. Another diagram that we specify is the

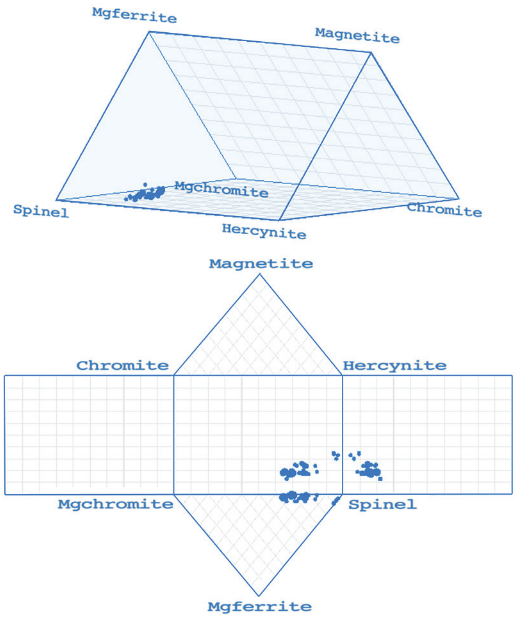

Fig. 6. The Spinel prism as implemented in the Spinel Explorer. The 3D view can be arbitrarily rotated, and the user can brush in the projections. The prism is unfolded prior to projection. Each point is projected three times: to the base, and to the triangle and lateral rectangle which are closer to the position of the point. A rectangular brush is supported in the three rectangles and a triangle brush in the two triangles.

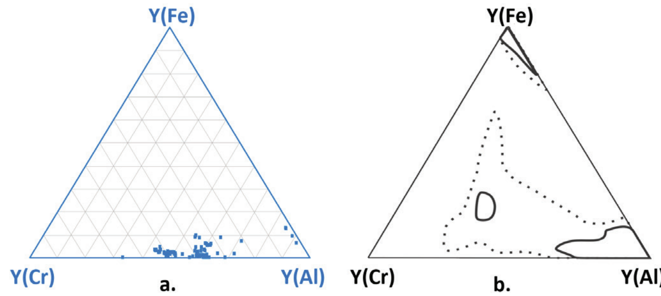

Fig. 7. Matching the triangular face of the prism **a.** with the compositional field for lithospheric mantle xenoliths **b.** delimited contour fields based on Barnes and Roeder [1].

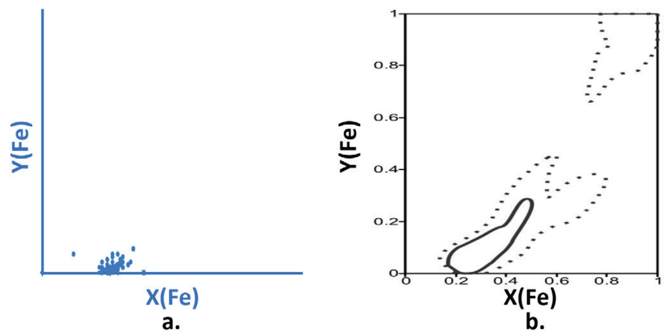

Fig. 8. Matching rectangular faces of the prism **a.** with the compositional field for lithospheric mantle xenoliths **b.** delimited contour lines based on Barnes and Roeder [1].

scatterplot showing FeO vs. MgO (see Figure 9). We expect to have a negative trend evidencing the exchange between the considered elements in this case. Sometimes we expect different trends or points in certain areas of the scatterplot, depending on the target spinel from the database. In Figure 9 we can see two subgroups G1 and G2 with negative trends plus one subgroup G3 with a constant trend. This last subgroup was an unexpected finding and led to a further exploration. Composite rectangular brushes over the unfolded prisms were used to brush the output trend and the Spinel prism diagrams revealed that data in the G1 and the G2 groups comprise mineral compositions that correspond to two different compositional fields (the Magnetite and the Ulvöspinel prisms) and that group G3 was an artifact (see Figure 10). The Spinel Explorer, employing coordinated multiple views and the ability to view the 3D Spinel prism, made it possible to detect a major inconsistency in the data. To choose the appropriate prism we used additional views, such as the $Y(Ti)$ vs. $X(Fe)$ scatterplot and the $Y(Al)$-$Y(Ti)$-$Y(Cr)$ triangle plot.

If a certain dataset matches with the compositional field for some of the tectonic settings defined by Barnes and Roeder [1] in all these diagrams and there is consistency in the results, then it is possible to determine the tectonic setting of the rocks. The obtained tectonic setting must also be consistent with the geological field context. In Figure 8 a diagram from the database along with the corresponding Spinel Explorer scatterplot is shown. The marked area in the database diagram indicates the area where the points of lithospheric mantle xenoliths should be. All of our points fall into the desired area, so we can conclude that our sample indeed belongs to lithospheric mantle xenoliths. The Spinel Explorer currently supports loading annotated static images of Barnes and Roeder [1]. Otherwise data which is not annotated can be loaded. We display our views next to the database diagrams in order to visually inspect them. We plan to convert the database data in the future so that we can depict our data and the Barnes and Roeder [1] annotated data in the same diagram. Using the Spinel Explorer, even without automatic comparison, enables to show all projections next to the database data, saving a significant amount of time.

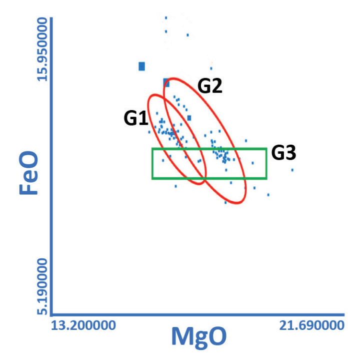

Fig. 9. A scatterplot showing MgO and FeO. We expected negative trends in the scatterplot as we assume a certain mineral composition. Groups G1 and G2 correspond to our expectations, while G3 represents an unexpected finding. Further investigation confirmed that the initial assumption was wrong for G3.

5.2 Case 2: Study of the Geological Processes Possibly Linked with the Compositional Variation Observed in the Spinel Group Minerals Dataset

In this case we use a dataset corresponding to an ophiolite tectonic setting from the Frontal Cordillera of the Central Andes, Argentina. This dataset has been chosen because it clearly shows different compositional groups related with diverse geological processes. The task here is to identify different processes. The processes involved in the geological history of a spinel dataset are difficult to detect. This is due to the fact that a detailed study of the geological, petrological, and mineralogical aspects of the rocks with spinel minerals must be previously done. The goal is to have a clearer idea about the context in which the rocks under study are being considered. Once the detailed study has been conducted, similarities of subgroups can be explored,

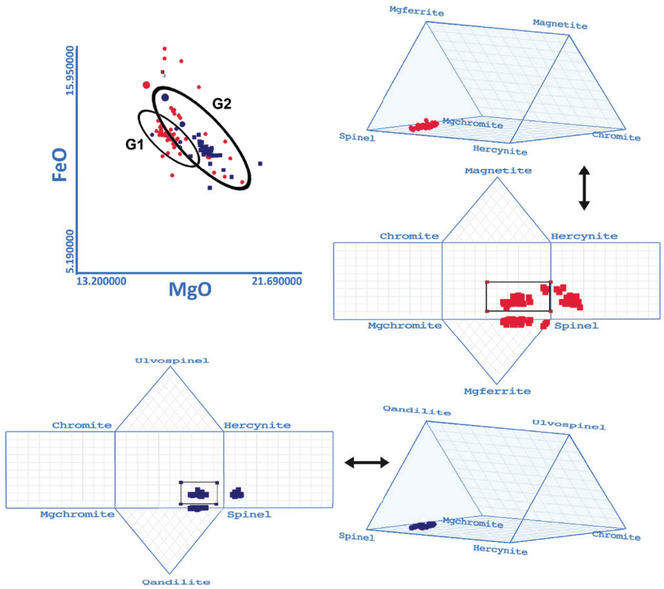

Fig. 10. A more detailed investigation of the unexpected finding in Figure 9 confirmed that the G1 and the G2 groups comprise mineral compositions that correspond to two different compositional fields (the Magnetite and the Ulvöspinel prisms). Blue points correspond to mineral compositions belonging to the Ulvöspinel prism and red points correspond to mineral compositions belonging to the Magnetite prism.

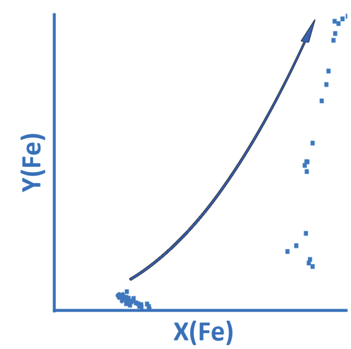

Fig. 11. Trend detection on a scatterplot. Scatterplot $X(Fe)$ vs $Y(Fe)$ with samples of spinel group minerals of the ophiolites tectonic setting from the Frontal Cordillera. The diagram shows a compositional trend with samples trending towards enrichment of the magnetite component.

again manually in the current state of the art workflows.

We start the analysis using a similar setup as in the first case study. A scatterplot showing $X(Fe)$ vs. $Y(Fe)$, reveals a trend (see Figure 11). This trend indicates that the dataset evolves to the Magnetite composition. We plot the data on the Magnetite prism to verify this (see Figure 12). The plot confirms what we expected. We can also see that data are grouped into different sectors of the prismatic space, reinforcing the idea that we could be facing compositionally different data subsets.

In order to further pursue this hypothesis we use additional views. By displaying scatterplots, triangle plots, Magnetite prism views, and parallel coordinates simultaneously (see Figure 13), the geologists confirm that the dataset comprises three main compositional groups. In order to do so, we use three brushes, each in a different color. There can be multiple composite brushes in the Spinel Explorer in order to support comparisons. We brush the Al-rich-group (magenta), the Cr-rich-group (blue), and the Al-poor-group with a strong variation in the

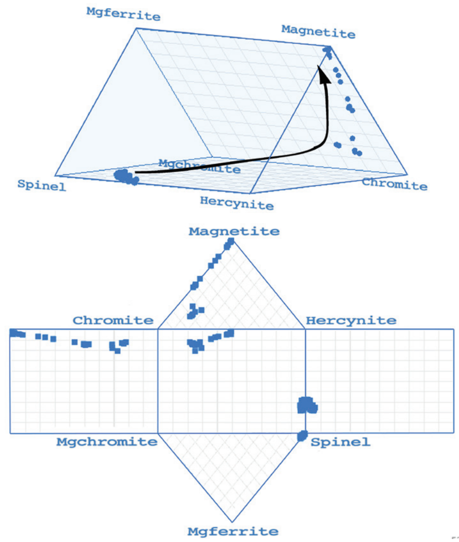

Fig. 12. Plotting the end-members of the spinel group mineral from ophiolites on the Magnetite prism to verify the compositional trend detected using a 2D scatterplot.

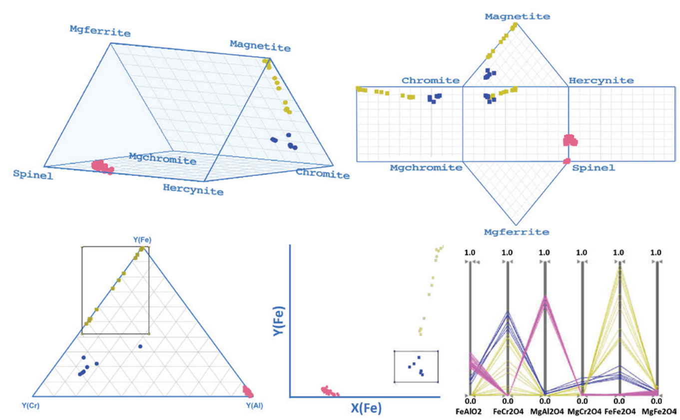

Fig. 13. By displaying scatterplots, triangle plots, Magnetite prism views and parallel coordinates diagrams simultaneously, the geologists confirm that the dataset is composed of three main compositional groups: the Cr-rich-subgroup (blue), the Al-rich-subgroup (magenta) and the Al-poor subgroup (yellow) with a strong variation in the $Y(Fe)$ ratio.

$Y(Fe)$ ratio (yellow), each with its own brush. We needed two brushes to compose the yellow brush (low Al and strong variation in the $Y(Fe)$ ratio). Figure 13 shows the described views. All diagrams consistently show three groups. Furthermore, by plotting the data in the Magnetite prism we can see that they are grouped into different sectors of the prismatic space. This strengthens the notion that we could be facing compositionally different data subsets. These three groups are related with the geological process that affected the studied rocks. The Cr-rich group represents the magmatic composition of the spinel minerals. The Al-rich group represents metamorphosed spinels in conditions of very high temperature. The Al-poor group with the strong variation in the Y(Fe) ratio represents metamorphic crystals which preserves the compositional variation during the metamorphic process with decreasing temperature.

It is important to emphasize that the use of the Spinel Explorer in this exploration was crucial. Until now it was not possible to visually detect this kind of compositionally different subsets at the same time. Furthermore a detailed study of the geological, petrological, and mineralogical aspects of the rocks must be previously done to have a clearer idea about the context in which the rocks under study are being considered. This is a long, complex, and error-prone process. Employing the Spinel Explorer, and its linking and brushing features, as well as specially tailored views (the triangle plot and the Spinel prism) enables to carry out this task in a very intuitive way and in half an hour.

5.3 User Feedback

The Spinel Explorer has been developed in a close collaboration with geology experts. They also coauthor the paper. The primary target group for the Spinel Explorer are geology researchers.

We studied their workflow at the beginning and noticed how they use several tools and spend a lot of time configuring them and comparing different plots. When we initially showed them possibilities of coordinated multiple views they were very enthusiastic on the one hand, but they also were a little bit hesitant to use *”such a complicated system”*, as one of them pointed out. We soon realized that we had to implement their standard plots, and they soon adopted linking and brushing. They also accepted parallel coordinates very soon. They have never seen them before, but they really liked the idea of showing many dimensions at once.

The Spinel Explorer at its current state represents a major advantage compared to the conventional workflow that geologists used before. The conventional workflow for a chemical composition study involves three main 2D diagrams to represent the chemical mixture of spinel group minerals. These are the triangle plot $Y(Al)$-$Y(Fe)$-$Y(Cr)$ which represents the projections of the data on the triangular faces of the Spinel prism and the scatterplots $Y(Fe)$ vs. $X(Fe)$ and $Cr/(Cr+Al)$ vs. $X(Fe)$, which represent the projections of the data on the rectangular faces of the Spinel prism (see Figure 14). The 3D plot is complicated to create and it is used at a later stage of the analysis. We were somewhat reluctant concerning the inclusion of a 3D view but geologists insisted.

The 3D Spinel prism view provided by the Spinel Explorer allows the user the representation of the chemical compositions within the prismatic space. This makes it possible to show the compositions of the spinel crystals in the chemical system of the solid solutions represented by the six end-members in the vertices of the Spinel prism. One of the geologists mentioned *”It is amazing how easy we can create 3D prisms now, and how efficiently we can drill down using iterative brushes and linked views”*. This makes it much easier to understand the inherently 3D chemical variations related to an entire chemical system. However, the 2D views are still needed. After several iterations and interviews with the geologists, the Spinel prism view includes the unfolded prism which shows the two triangle plots and the three scatterplots typically used in the literature.

The 3D prism is also used to differentiate between spinel group minerals with $Fe_2O_3 > 2TiO_2$ belonging to the Magnetite prism and those with $Fe_2O_3 < 2TiO_2$ belonging to the Ulvöspinel prism. This distinction is not visible on a standard TiO_2 vs. $Y(Fe)$ scatterplot.

Geologists also consider that the contours of the tectonic fields should not be especified using only the classical scatterplots and triangle plots but they should be redefined in 3D diagrams in the future for a better understanding of the compared dataset. The interpretations would be difficult at the beginning because geologists are used to work with spinel compositions only in 2D diagrams. Therefore, even if the representation of the chemical data is easily interpreted if plotted in the Spinel prism (3D diagram), 2D diagrams are still necessary since they are used to compare new data with those in the literature. After one of the first sessions with the Spinel prism view one of the geologists said: *”We either use 3D or 2D views, and because of a tedious switching and data exchange between various tools we’ve never had exploration and analysis possibilities offered by the Spinel Explorer”*.

As mentioned above the geologists liked the parallel coordinates at the end. Although they were not used to parallel coordinates, this technique turned out to be a very useful tool to visualize the chemical data of the spinel group minerals. This specially holds for the analysis of the proportions of the eight commonly used end-members. Besides this, geologists have begun to explore relationships between the 22 end-members and found the parallel coordinates view very promising because they allow comparisons of the proportions of each end-member in only one diagram as well as the interpretation of geochemical variations in a given group of rock types. *”I really like the possibility to show many end-members at once. The solution seems really simple, and yet, I never thought something like this would be possible”*, one of the geologists said. The parallel coordinates are not known in the geology community. Due to the very positive feedback we have got from domain experts we do believe that parallel coordinates have a good potential in the geology domain. They might be beneficial specially for those who are aiming at a deeper understanding of the mineral chemistry systems. Since many of the minerals in nature integrate complex solid solutions between different end-members, parallel coordinates represent a convenient way to show the proportions of each end-member involved in the solid solution.

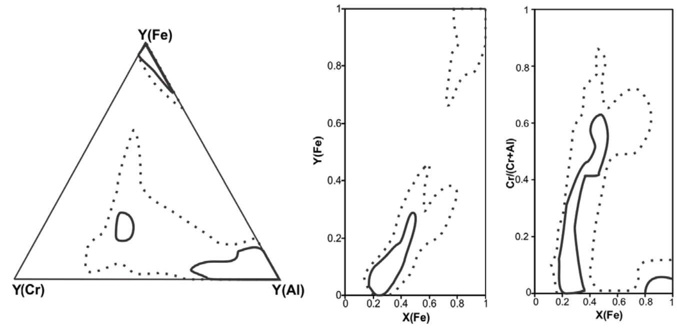

Fig. 14. Barnes and Roeder [1] compositional fields illustrated in the 2D diagrams used to represent the chemical composition of spinel group minerals of xenoliths in basalts.

We were surprised how quickly geologists got used to the parallel coordinates, the coordinated multiple views, and the introduced interactive plots. They are used to work with many diagrams, which certainly helped in adopting to the new technology. They were also willing to learn, and did not give up even with the first preliminary prototypes of the Spinel Explorer. All involved researchers from both domains (visualization and geology) enjoyed collaborating with each other. Our collaboration does not end with this paper. We are currently improving the system and preparing a comprehensive case study.

6 Conclusions and Future Work

Geologists analyze the spinel group minerals in order to understand Earth’s history, and to identify regions where mineral deposits might be of economic interest. The current state of the art includes a tedious use of several tools and complex and error-prone manual comparison of different plots and tables. We introduce the Spinel Explorer, a unified visual analytics framework for geological data. The Spinel Explorer employs coordinated multiple views, and, for the first time, an interactive triangle plot and interactive Spinel prism plot. These two plots are an important part of geologists’ workflow. The geologists can now take advantage of them in an interactive system. Their feedback on interaction and integration into a unified framework was very positive. According to the first informal evaluation, they can carry out tasks in just a few hours that previously required several weeks. They used mostly static diagrams and arranged them manually. They are much more efficient now, but, what is even more important, they can solve analysis tasks which were more difficult before. Multiple composite brushes, e.g., make comparisons fast and intuitive.

The domain experts are enthusiastic about future improvements. Besides a formal evaluation, we also plan to add a support for semi-automatic comparisons with the standard database [1]. A visual analytics functionality seems to be the first choice for such a comparison.

Acknowledgments

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