TECHNICAL NOTE

Three-dimensional visualization of ternary prisms (T-prism): Development of a spreadsheet-based tool for Earth and material sciences

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T-prism is a Microsoft-Excel-based tool that visualizes ternary space diagrams (i.e., ternary prisms) in three-dimensional (3D) space. This tool allows us to examine the overall features of a dataset in both three- and two-dimensional spaces by altering the viewing angles. T-prism involves two algorithms that coordinate the transformation and rotation of diagrams in a virtual 3D space. This paper describes a new and simple coordinate transformation from a ternary space diagram (i.e., ternary prisms) to an XYZ orthogonal system. Coordinates of a point of interest in the ternary space diagram, expressed using the proportions of three components of a basal triangle (r , l , and t , where $r + l + t = 100$) and an additional variable (h), are converted into coordinates in the orthogonal system as follows: $x = (r + 100 - l)/2$, $y = \sqrt{3}/2t$, and $z = fh$. Here, f represents the correction factor used to appropriately express the length of an axis perpendicular to the basal ternary diagram. T-prism is particularly suitable for visualizing phase relations in multicomponent systems, the physical properties of materials, and compositional variations in solid solutions. Hence, the tool is applicable to a broad variety of research and teaching fields, including Earth science, material science, and physical chemistry.

Keywords: Ternary prism, Three-dimensional visualization, Coordinate transformation, Phase diagram

INTRODUCTION

Ternary space diagrams are variably referred to as ternary prisms, triangular prisms, ternary phase diagrams, three-dimensional (3D) ternary plots, and ternary space models. These diagrams are widely used in a variety of fields (e.g., Earth science, physical chemistry, and material sciences for metal alloys and ceramics) to express the relationships among four variables. A well-known example of the ternary prism is the phase diagram for a three-component system, wherein the basal triangle represents the proportions of three components, and an axis perpendicular to the triangle often shows the temperature. The diagram can also depict physical and thermodynamic properties in three-component systems (Thurston, 1877) and chemical variations in solid solutions (e.g., spinel group minerals; Haggerty, 1991). Consequently, ternary prisms are suitable for representing the relationships of four var-

iables when temperature, pressure, or physical properties are included as independent variables. Such relationships are not well expressed by a tetrahedral plot.

The ternary prism has often been demonstrated by a handmade 3D model in the late 1800s to early 1900s. Thurston (1877) demonstrated the cohesive strength of alloys for a Cu–Zn–Sn system using a plaster model. Similarly, Rankin (1915) visualized liquidus surfaces for a CaO–Al₂O₃–SiO₂ system using a plaster model. These solid models qualitatively revealed the general relationships between variables but are unsuitable for a detailed quantitative analysis.

For quantitative examinations, ternary prisms are typically projected onto triangular two-dimensional (2D) plots. Projection methods of ternary phase diagrams were established within two decades of the publication of Gibbs' phase rules and his thermodynamic considerations for heterogeneous systems (Gibbs, 1876, 1878). For example, both the solvus curve and tie lines of co-existing phases were expressed on a triangular plot for Sn–Pb–Zn alloys by Wright et al. (1890), following the suggestions

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of G.G. Stokes. In addition, other important information such as liquidus surface, phase boundaries (including cotectics), direction of temperature change, isothermal lines, and alkemade lines (van Rijn van Alkemade, 1893) were projected onto a right-angled isosceles triangle by Roozeboom (1893). Roozeboom (1894) further modified the shape of the triangle to project the phase relations onto an equilateral triangle. Additional improvements were realized by Bancroft, who introduced grid lines within a triangular plot and prepared the original graphs accordingly (Bancroft, 1897a; Howarth, 1996). Further, Bancroft (1897a, 1897b) proposed that a triangular ternary phase diagram should be combined with three orthogonal binary phase diagrams. This diagram is typically used to simplify triangular plots by eliminating isothermal lines (e.g., Bowen, 1914). In summary, the conversion of 3D ternary prisms to 2D ternary plots was established successfully in the 1890s.

Currently, we can plot large volumes of data on 3D diagrams using personal computers. Computer visualizations can be used easily to change the dimensions of diagrams by changing the viewing angle, thereby enabling the quantitative investigations of data features in 3D diagrams, and subsequently the quantitative examinations of these features through 2D projection. In this context, computer visualization could be an effective tool, especially in educational settings, to assist students in the quantitative reading of ternary phase diagrams. However, while many plotting programs such as TERNPLOT (Marshall, 1996), CSpace (Torres-Roldan et al., 2000), Tri-plot (Graham and Midgley, 2000), PetroGraph (Petrelli et al., 2005), GCDkit (Janoušek et al., 2006), and t-Igpet (Carr and Gazel, 2017) are available for 2D triangle plots, those for 3D ternary prisms remain scarce. At this stage, only Ganuza et al. (2014) have created a free program for visualizing compositional variations in spinel group minerals on a ternary prism. Indeed, some commercial applications such as ORIGIN® (OriginLab) and Mathematica® (Wolfram Research) allow a user to obtain 3D ternary prisms by inputting a specific command or by clicking a button without any mathematical knowledge. However, these commercial applications are not always accessible owing to financial barriers and limited educational/research resources. Moreover, the mathematics of the visualizations are often hidden in the background in these commercial applications.

This paper presents a new and simple procedure of coordinate transformation from a ternary space diagram to an XYZ orthogonal system, and a visualization tool for ternary prisms called T-prism. T-prism is a spreadsheet-based tool that visualizes the ternary prism in a 3D virtual space. Microsoft Excel is typically used in education and

research, and thus no significant barriers exist for T-prism, even in the classroom. T-prism operates by copying data into designated cells in a spreadsheet. The viewing angle is changed by modifying the values of two cells or by using mouse clicks. We do not use any programming language or ActiveX Control in the spreadsheet; therefore, machine dependence does not exist and compatibility with both Mac and Windows is enabled. The algorithms and architecture of the spreadsheet are simple, and allow users to introduce new functions by themselves. The Microsoft Excel file containing T-prism and the T-prism architecture description are available in Supplementary Materials SA and SB (Supplementary Materials SA and SB are available online from <https://doi.org/10.2465/jmps.181214>), respectively.

COORDINATE TRANSFORMATION

Shimura and Kemp (2015) described coordinate transformation from a tetrahedral system to an orthogonal coordinate system. This procedure has been expanded to the ternary prism herein (Fig. 1). Figure 1 depicts a ternary prism using an orthogonal coordinate system. A basal triangle of the ternary prism is situated on the XY plane, whereas the vertical axis of the prism corresponds to the Z-axis direction. Here, the apexes of the triangle are referred to as top (T), left (L), and right (R), where apex L conforms to the origin of the XY orthogonal coordinate system. Furthermore, the side length of the equilateral triangle is set to 100. Thus, coordinates (x , y) of apexes T, L, and R are expressed as $(50, \frac{\sqrt{3}}{2} \times 100)$, $(0, 0)$, and $(0, 100)$, respectively. Similarly, coordinates (x , y) of the point of interest (point P in Fig. 1) are expressed as follows, using the mixing ratios of t , l , and r (here, $t + l + r = 100$):

$$x = (r + 100 - l)/2 \quad (1)$$

and

$$y = \frac{\sqrt{3}}{2} t \quad (2).$$

In contrast to coordinates (x , y), the z -coordinate of point P is not simply derived from the coordinate transformation described by Shimura and Kemp (2015). This is because the unit system of the Z-axis is not comparable with that of the basal triangle (Fig. 1). For example, a point on the basal triangular plane (t , l , and r ratios, or x and y) is described by the proportions of three variables normalized to 100%; however, the height of the ternary prism is described by a raw value (e.g., temperature).

Figure 1. Geometrical relationship between the ternary prisms and the XYZ orthogonal system. Here, t , l , and r are the mixing ratios ($t + l + r = 100$) of the end members T, L, and R, respectively; h denotes the height; f is the correction factor for the side-surface shape (see Eqs. 3, 4, and 5 in the text).

Thus, the values on the Z -axis change independently against the other three variables representing the basal triangle, thus modifying the aspect ratio of the prism during rotation in 3D space.

To maintain the shape of the ternary prisms in a virtual 3D space, we introduced two parameters: absolute aspect ratio (A_a) and visual aspect ratio (A_v) that allow us to express the X -, Y -, and Z -axes in the same unit system. The absolute aspect ratio (A_a) is calculated from the height data, for example, the temperature range of the ternary prism:

$$A_a = (h_{\max} - h_{\min})/S \quad (3),$$

where $h_{\max}$ and $h_{\min}$ are the maximum and minimum values of the height of the ternary prism, respectively, and S is the length of the basal triangle (typically, $S = 100$).

The visual aspect ratio (A_v) is defined as follows:

$$A_v = H/S \quad (4),$$

where H is the height of the ternary prism in a virtual 3D space. Because S is the length of the basal triangle in a virtual 3D space, A_v indicates the visual shape of the side surface. For example, $A_v = 1$ corresponds to a square and $A_v = 2$ indicates a rectangle with a length that is twice the

width.

Using parameters A_a and A_v , the correction factor (f) is defined as follows:

$$f = A_v/A_a \quad (5).$$

Subsequently, the z -coordinate of point P is expressed as

$$z = fh \quad (6),$$

where h is the raw value (e.g., temperature) of point P.

From Eqs. (1), (2), and (6), point P on the ternary prism (Fig. 1) is expressed by the following equation:

$$(x, y, z) = \left(\frac{r + 100 - l}{2}, \frac{\sqrt{3}}{2} t, fh \right) \quad (7).$$

ROTATION IN 3D SPACE

The rotation of a ternary prism can be described by rearranging the procedure detailed in the appendix of Shimura and Kemp (2015). Here, the center of rotation is set to the geometric center of the prism ($50, \frac{\sqrt{3}}{6} \times 100, \frac{h_{\max} - h_{\min}}{2} \times f$); therefore, the original position of the ternary prism (x, y, z) shifts to the new coordinates (x_0, y_0, z_0) for rotation as follows:

$$x_0 = x - 50 \quad (8a),$$

$$y_0 = y - \frac{\sqrt{3}}{6} \times 100 \quad (8b),$$

and

$$z_0 = z - \frac{h_{\max} - h_{\min}}{2} \times f \quad (8c).$$

Here, the rotation angles around the X -, Y -, and Z -axes are referred to as α , β , and γ , respectively (Fig. 2). However, only two angles are necessary to express the diagram's orientation: the rotation angle γ ($0 \leq \gamma \leq 360^\circ$) and the dip angle of the observer, d ($0 \leq d \leq 90^\circ$; Fig. 2). From these angles, the rotation of the ternary prism can be calculated using the Euler angle equation. After a γ -rotation, the coordinates ($x_\gamma, y_\gamma, z_\gamma$) are as follows:

$$x_\gamma = x_0 \cos \gamma - y_0 \sin \gamma \quad (9a),$$

$$y_\gamma = x_0 \sin \gamma + y_0 \cos \gamma \quad (9b),$$

and

$$z_\gamma = z_0 \quad (9c).$$

Figure 2. Ternary prism in the right-handed orthogonal coordinate system. G is the center of mass of a triangular prism and d is the observer dip angle relative to the horizontal surface.

Furthermore, the coordinates after changing the observer dip angle (x_d, y_d, z_d) are as follows:

$$x_d = x_\gamma \quad (10a),$$

$$y_d = y_\gamma \cos d - z_\gamma \sin d \quad (10b),$$

and

$$z_d = y_\gamma \sin d + z_\gamma \cos d \quad (10c).$$

Defining the horizontal axis and longitudinal axis of a computer screen as x_p and z_p , the 3D position (x_d, y_d, z_d) can be plotted onto a 2D surface as a ‘parallel projection’:

$$(x_p, z_p) = (x_d, z_d) \quad (11).$$

By this projection, we can observe a ternary prism as a virtual 3D graphic on a spreadsheet (e.g., Excel) and other graph drawing applications.

APPLICATION EXAMPLES

Phase relations in the ternary feldspar system

Feldspar is the most typical solid-solution mineral on the Earth’s crust. Figure 3 shows the hypothetical phase relations of ternary feldspar at 100 kPa. The basal triangle of the ternary prism represents the proportion of the three end-member components of feldspar: anorthite (An, $\text{CaAl}_2\text{Si}_2\text{O}_8$), albite (Ab, $\text{NaAlSi}_3\text{O}_8$), and orthoclase (Or, KAlSi_3O_8), while the vertical axis represents the temperature. The plot data were obtained using a thermody-

Figure 3. Isometric projection showing compositions of ternary feldspar at 100 kPa. Vertical axis represents temperature ($^{\circ}\text{C}$), whereas basal equilateral triangle represents the proportions of the three components of feldspar: albite (Ab), anorthite (An), and orthoclase (Or). The diamond and solid circle symbols represent feldspar on the solidus and solvus, respectively. It is noteworthy that the Or-rich side shows the metastable phase relations, where leucite is of the liquidus phase. Starting compositions used in the calculation of phase relations are listed in the ‘starting composition’ cells in Supplementary Material SC. Color version is available online from <https://doi.org/10.2465/jmps.181214>.

namic software package rhyolite-MELTS ver. 1.0.1 (Gualda et al., 2012) for 84 different starting compositions listed in Supplementary Material SC (Supplementary Material SC is available online from <https://doi.org/10.2465/jmps.181214>). The thermodynamic software reasonably simulates the phase relations for silicic magmas, although it overestimates the temperatures by $\sim 40^{\circ}\text{C}$ (Gardner et al., 2014). Figure 3 captures the general features of phase relations for ternary feldspar; however, the Or-rich side shows metastable relations, where leucite is of the liquidus phase (Waldbaum and Thompson, 1969).

As detailed in Figure 3, a concave-upward solidus is intersected by a dome-like solvus at approximately 1000–1100 $^{\circ}\text{C}$, thus yielding an arcuate intersection opening towards the An–Or join. The arcuate intersections govern the compositions of the co-existing plagioclase and alkali feldspar, while the melt lies on a cotectic line. In contrast, under subsolidus conditions, the compositions of two co-existing feldspars are constrained by a miscibility gap that expands toward the lower temperatures. Figure 3 also depicts the morphology of the solvus, in which the critical curve (ridge lines of the solvus) extends from $\text{Ab}_{66}\text{Or}_{34}$ to the Ab–Or join toward $\text{Ab}_{56}\text{Or}_{30}\text{An}_{14}$ through

Figure 4. Feldspar compositions for different temperature ranges at 100 kPa. The diamond and solid circle symbols represent feldspar on the solidus and solvus, respectively. Color version is available online from <https://doi.org/10.2465/jmps.181214>.

$\text{Ab}_{67}\text{Or}_{31}\text{An}_2$. The feldspar compositions governed by the solidus and solvus are well examined using the 3D prism generated by T-prism. Furthermore, the feldspar compositions can be examined quantitatively on the 2D projection when the viewing angle is changed (Fig. 4). These procedures show the extent to which feldspar compositions change systematically with temperature. A similar approach is applicable to other mineral groups (e.g., pyroxenes). Thus, examining the ternary prism from different viewing angles is effective for understanding phase relations in multicomponent systems and is the basis of solvus geothermometers (e.g., two-feldspar thermometers; Stormer, 1975; Brown and Parsons, 1981; Putirka, 2008; Benisek et al., 2015).

Phase equilibria in a four-component system

Combining the ternary prism and tetrahedral plots is recommended. Shimura and Kemp (2015) provided the algorithms of a tetrahedral four-component system to an XYZ-orthogonal coordinate axis system and presented a Microsoft Excel spreadsheet for the tetrahedral plot (see Deposit item of Shimura and Kemp, 2015). Cucci-niello (2016) presented a similar but partially updated spreadsheet tool based on the coordinate transformation of Shimura and Kemp (2015). It is noteworthy that these tools are easy to use with the T-prism developed in this study because both the ternary prism and tetrahedral plot can be viewed on the spreadsheet. An example is described below.

Equilibrium crystallization under 300 MPa was simulated using rhyolite-METLS ver. 1.0.1 (Gualda et al.,

Figure 5. Visualization of phase relations for a hydrous granitoid system at 300 MPa. Tetrahedral plot shows compositions of melt (M), plagioclase (PL), alkali feldspar (Afs), and quartz (Qz). Coexisting phases are represented by tie-lines. An, Ab, and Or represent anorthite, albite, and orthoclase, respectively. Color version is available online from <https://doi.org/10.2465/jmps.181214>.

2012) for a hypothetical hydrous granitoid melt ($\text{Qz}_{16}\text{Or}_{32}\text{Ab}_{32}\text{An}_{20}$) with 3 wt% H_2O . Supplementary Material SD (Supplementary Material SD is available online from <https://doi.org/10.2465/jmps.181214>) lists the composition and abundance of each phase. We plotted the resulting melt compositions on a tetrahedral plot (Fig. 5) and ternary prism (Fig. 6) for the temperature range of 1021–733 °C, as well as for three coexisting mineral phases, i.e., plagioclase (1019 °C), alkali feldspar (823 °C), and quartz (739 °C) begin to precipitate in that order. The evolved melt was saturated with water at 747 °C immediately before the onset of quartz precipitation. After quartz saturation, the amount of melt decreased rapidly and crystallization was nearly completed at approximately 733 °C. T-prism allows for the further investigation of the compositional changes in feldspar against temperature (Fig. 6). Labradorite plagioclase ($\text{Ab}_{39}\text{An}_{59}\text{Or}_2$) at liquidus temperature (1019 °C) changes its composition toward andesine with decreasing temperature. Subsequently, alkali feldspar ($\text{Ab}_3\text{An}_{25}\text{Or}_{73}$) begins to precipitate with andesine plagioclase ($\text{Ab}_{39}\text{An}_{55}\text{Or}_6$) at 823 °C, where the melt reaches a cotectic surface. With decreasing temperature, the two feldspars further change their compositions along the intersection of the solidus and solvus surfaces until the melt is consumed. Combining the ternary prism and tetrahedral plots may assist undergraduate students in Earth and material sciences to effectively understand the multicomponent phase relations and

Figure 6. T-prism visualization showing feldspar and melt compositions against temperature (°C). Abbreviations are identical to those in Figure 5. Color version is available online from <https://doi.org/10.2465/jmps.181214>.

mineral assemblages in rock samples in both 3D and 2D sections. A similar approach is applicable to other quaternary systems, such as the diopside-forsterite-anorthite-albite system.

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SUPPLEMENTARY MATERIALS

Color version of Figures 3–6 and Supplementary Materials SA–SD are available online from <https://doi.org/10.2465/jmps.181214>.

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