A Three-dimensional Topological Model of Ternary Phase Diagram

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Abstract. In order to obtain a visualization of the complex internal structure of ternary phase diagram, the paper realized a three-dimensional topology model of ternary phase diagram with the designed data structure and improved algorithm, under the guidance of relevant theories of computer graphics. The purpose of the model is mainly to analyze the relationship between each phase region of a ternary phase diagram. The model not only obtain isothermal section graph at any temperature, but also extract a particular phase region in which users are interested.

1. Introduction

The phase diagram can reflect many important content with our industrial production and scientific research. Therefore, the study of phase diagram is of important practical significance. The traditional ternary phase diagram is mainly expressed by plane projection, isothermal section, vertical section and other plane figures. The ternary phase diagram figured by the thermodynamic calculation software not only needs to go through a series of complex computations, but also stays on the plane figure [1]. Thus it is necessary to establish a three-dimensional model of ternary phase diagram. The visualization of three-dimensional phase diagram can help people understand the complex internal structure of ternary phase diagram intuitively.

The spatial model of ternary phase diagram is described as a special kind of three prisms, which is shown in Figure 1. The equilateral triangle ΔABC of the bottom represents the concentration information of the three constituent elements. Each point in the equilateral triangle can be represented by the relative content of the three elements. The sides of the prism are the relevant three binary phase diagrams A-B, B-C, A-C, the height which is vertical to the bottom of ΔABC represents the temperature.

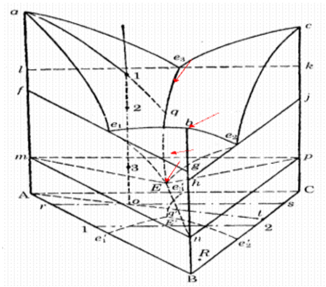


Figure 1. Space model of ternary phase diagram

2. Modeling Approch

The modeling methods of ternary phase diagram mainly use multivariate linear regression methods [2,3] to obtain a three-dimensional phase diagram, the spatial model made from which is barely satisfactory. As the rapid development of computer graphics, the Bezier method for phase diagram expression is proposed [4]. However the method is confined to the liquidus surface of ternary phase for three-dimensional reconstruction. According to the designed data structure and improved algorithm, the line frame model was adopted to realize a three-dimensional topology model of ternary phase diagram in this paper. Not only the model improves the drawing efficiency of isothermal section of phase diagrams, but also can be established easily.

2.1. Phase Diagram Selection

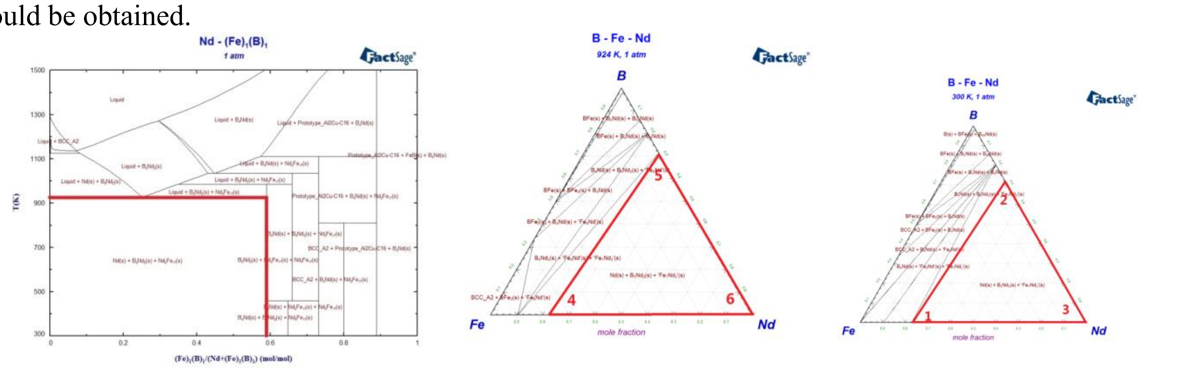
As a new type of alloy with permanent magnetic properties the ternary phase diagram B-Fe-Nd can be processed simply and has low price. It has captured great attention both at home and abroad [5]. So the ternary phase diagram B-Fe-Nd is selected as the research object.

2.2. Data Source

FactSage is one of the largest fully integrated database computing systems in chemical thermodynamics in the world. With FactSage users can calculate the conditions for multiphase, multicomponent equilibria, with a wide variety of tabular and graphical output modes, which is under a large range of constraints. For example, general N-component phase diagram sections can be easily generated with a wide choice of axis variables. FactSage has several hundred industrial, governmental and academic users in materials science, pyrometallurgy, hydrometallurgy and other different fields. It is used internationally in graduate and undergraduate teaching and research. It can provide users with more authorized accurate data.

As shown in Figure 2(a), the vertical section calculated by Factsage was shaped when the ratio of element Fe and element B is equal to 1:1. Vertical sections reflect the topological relations between different phase regions. Since each phase region is a closed set, so we treat the single phase region as the body element to collect, then select corresponding phase boundary face, phase boundary edge and vertices at the single phase region. The phase region Nd(s)+B5Nd2(s)+Nd5Fe17(s) numbered as 1 will be an example to introduce.

A line separating the two phase regions on the vertical section is extending into a plane or a curved surface in space. As shown in Figure 2(a), the phase boundary temperature of phase NO.1 are 924K and 300K. In order to intercept the phase boundary faces of the phase, FactSage is used to calculate the isothermal section of 300K and 924K, as shown in Figure 2(b)&(c). Through isothermal section, the phase boundary faces and vertices 1,2,3,4,5,6 component concentration information of phase NO.1 could be obtained.



(a) (b) (c)

Figure 2. (a) Vertical section; (b) Isothermal section at temperature 924K; (c) Isothermal section at temperature 300K

2.3. 3D Coordinate Transformation
The composition of ternary phase diagram is usually expressed as an equilateral triangle, which is called the concentration triangle. Any point within a concentration triangle can be expressed as a percentage of the concentration of three components. After the steps mentioned above, the component concentration information of six vertices of phase NO.1 can be figured out. However, to describe the ternary phase diagram in three-dimensional rectangular coordinate system, it's necessary to convert the data in concentration triangle into Cartesian Coordinate System (CCS). Because the meaning of temperature in the coordinate system is the same as that of CCS, we only need to convert the coordinates of the component concentration into CCS. As shown in Figure 3, point A is the origin of CCS. If the length of the equilateral triangle is l, and the composition of the point Q is (B, C), the relationship between the point Q(x,y) in CCS and the composition of the point Q (B, C) satisfies equation 1.

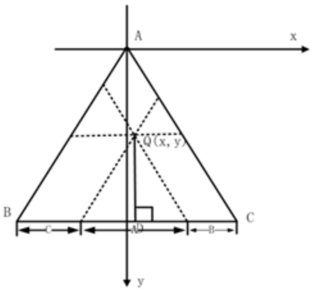


Figure 3. Coordinate transformation.

$$\begin{cases} A = l - B - C \\ x = C + A/2 - l/2 \\ y = \sqrt{3}/2(l - A) \end{cases} \tag{1}$$

2.4. Data Structure Constructing
A series of discrete space points are obtained by means of three-dimensional coordinate transformation. It's necessary to build up a high efficient data structure to organize these discrete points in space. Thus users can quickly access the phase boundary faces, phase boundary edges and vertices of each phase region. The winged-edge data structure is a typical data structure. The structure is well adapted for the representation of a convex polyhedron. In the ternary phase diagram system B-Fe-Nd, the shape of solid phase regions are most convex polyhedron. Secondly, the winged-edge structure clearly describes the geometric and topological features of the faces, edges and vertices of three or more intersecting surfaces. Based on and starting from the edges, it can retrieve the two adjacent surfaces and four adjacent edges of the edge's starting point, as well as the edge's own attributes. In order to simplify the winged-edge structure, an improvement is made to draw the whole body with the right adjacent surface of the winged-edge structure [6,7].

```
DATA structure of the four tables {
        Data object: S, F, E, P;
        S represents the voxel, F represents the face structure, E represents the edge structure, P
represents the point set;
        Data relationship: R={SFR,FER,EPR};
        SFR={<s, f>|s∈ S, f∈ F; represents face f in s};
        FER={<f, e>|f∈ F, e∈ E; represents edge e in f};
        EPR={<e, p>|e∈ E, p∈ P; represents point p in e};
}
```

Storage mode of winged-edge data structure:
(1)Voxel structure

```
class solid
{
Id solid; /*the number of phase region*/
Face *sface; /*the face number contained in the phase region*/
}
```

The voxel structure is the upper layer of the whole data structure. The phase boundary faces, phase boundary edges, vertices and other elements that constitute the polyhedron can be found by traversing the voxel structure.

(2)Face structure

```
class face
{
Id facenum; /*the number of the face */
 Edge edgeid; /*the edge number contained in the face*/
Int flag; /*a flag of whether to be traversed*/
}
```

Face structure contains the face number, edge number contained in the face and the flag of whether to be traversed. If the flag is 1, it has been traversed.

(3)Edge structure

```
class edge
{
Id edgeid; /*the number of edge*/
Int PS; /* Initial vertex*/
Int PE; /* End vertex*/
Id facenum; /* Right adjacent surface*/
}
```

Edge structure includes the edge number edgeid, starting point PS, ending point PE and adjacent right face facenum.

(4)Vertex set

```
class point
{
id point; /*the number of vertex*/
Int x, y, z; /* vertex coordinates*/
}
```

Vertex set includes the number of vertex and the coordinate of the vertex(x, y, z).

According to the above data structure, the phase region NO.1 is stored in the computer as shown in Table 1.

Table 1. Four tables structure of phase region NO.1

Voxel structure	
Solid	Face num
1	1,2,3,4,5

Face structure		
facenum	Flag	edgeid
1	0	1,2,3
2	0	4,5,6,7
3	0	8,9,10,11
4	0	12,13,14,15
5	0	16,17,18

Vertex set			
point	X	Y	Z
1	-27	50	300

Edge structure			
edgeid	PS	PE	facenum
1	1	2	2
2	2	3	3
3	3	1	4
4	2	1	1
5	1	4	4
6	4	5	5
7	5	2	3
8	3	2	1
9	2	5	2
10	5	6	3
11	6	3	4
12	1	3	1
13	3	6	3

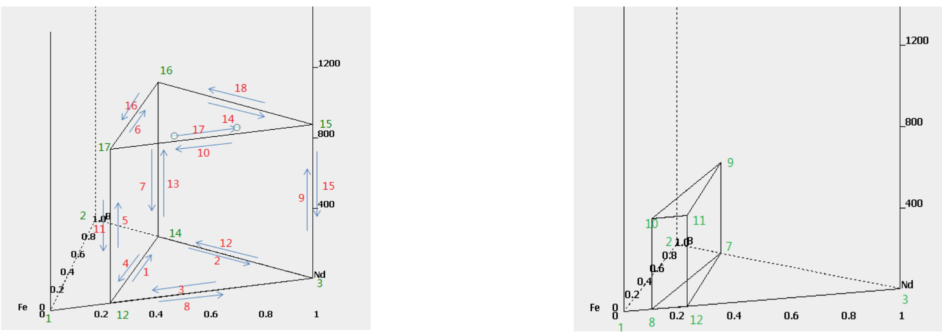
2	14.5	14.5	300		14	6	4	5
3	50	86.6	300		15	4	1	2
4	-27	50	924		16	5	4	2
5	14.5	14.5	924		17	4	6	4
6	50	86.6	924		18	6	5	3

2.5. Transformation from the World Coordinate System (WCS)to the Screen Coordinate System (SCS)
Currently, we have obtained the three-dimensional coordinates of phase region in WCS and organized the discrete coordinate points using the designed data structure. However in order to output the three-dimensional phase diagrams on computer screen, the conversion from WCS to SCS will be involved in. Detailed conversion processes are shown in Figure 4.

Figure 4. Conversion processes

The coordinate system where three-dimensional phase diagram locate is WCS, which is defined using right-handed coordinate system [8]. While Viewing Coordinate System (VCS) is a coordinate system, which a view point and projection plane can be defined. And by standing on such view point, the three-dimensional objects can be projected to projection plane. SCS is a coordinate system where the diagram on projection plane is displayed on screen. WCS, VCS and SCS are correlated with each other. VCS is evolved on the basis of WCS. The object displayed in SCS is the projection of three-dimensional object in projection plane of VCS.

2.6. Display a single phase region
After the steps mentioned above, the visual expression of the phase region could be displayed on the computer screen intuitively. Currently, the existing written phase diagram data or some phase diagram calculation software such as FactSage and Pandat can’t present the specific form of a single phase region. However based on the data structure defined above, it is easy to realize the reconstruction of a single phase region. The voxel structure as the root node store the number of phase regions, which is equal to the index data and guide us to extract patch set displayed in the phase regions. It isn't hard to obtain the information of edge structure of all the patch sets in the phase region by searching the number of patch set in face structure. Accordingly, all the information of vertices can be get according to the edge structure. Then the result of phase region NO.1 Nd(s)+B5Nd2(s)+Nd5Fe17(s) and region NO.5 B4Nd(s)+Nd2Fe17(s)+Nd5Fe17(s) was listed in Figure 5(a)&(b).



(a) (b)

Figure 5. (a) Phase region Nd(s)+B5Nd2(s)+Nd5Fe17(s); (b) Phase region B4Nd(s)+Nd2Fe17(s)+Nd5Fe17(s)

3. Discussion

According to the method proposed in this paper, the three-dimensional topological model of any ternary phase diagram can be realized through a small amount of data and the isothermal section of model is drawn. And the writer extracts the single-phase region in which users interested. The visualization of ternary phase diagram help people to understand the complex internal structure of ternary phase diagram.

4. Conclusion

Based on the concept from whole to part, the paper firstly divided the whole system into different phase regions, and then restored all phase regions with well-designed data structure and algorithm, finally combined all phase regions into a whole body. Thus the topological model of ternary phase diagram B-Fe-Nd was realized, shown in Figure 6. Regarding this system, it can also obtain the isothermal section diagram of a random temperature. See the isothermal section diagram at 900K in Figure 7.

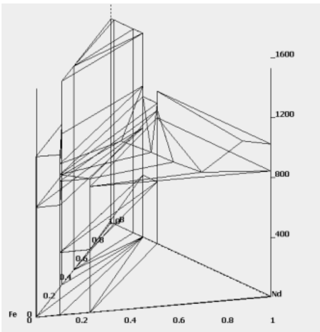


Figure 6. Topological model of the ternary phase diagram B-Fe-Nd.

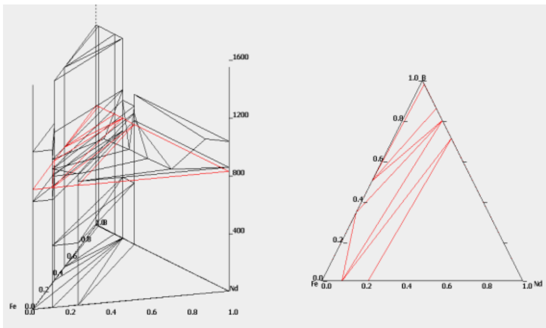


Figure 7. Isothermal section diagram at temperature 924K.

Acknowledgments

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