Study on the temperature field of large-sized sapphire single crystal furnace

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Abstract. In this paper, the temperature field of large-sized (120kg, 200kg and 300kg grade) sapphire single crystal furnace was simulated. By keeping the crucible diameter ratio and the insulation system unchanged, the power consumption, axial and radial temperature gradient, solid-liquid surface shape, stress distribution and melt flow were studied. The simulation results showed that with the increase of the single crystal furnace size, the power consumption increased, the temperature field insulation effect became worse, the growth stress value increased and the stress concentration phenomenon occurred. To solve these problems, the middle and bottom insulation system should be enhanced during designing the large-sized sapphire single crystal furnace. The appropriate radial and axial temperature gradient was favorable to reduce the crystal stress and prevent the occurrence of cracking. Expanding the interface between the seed and crystal was propitious to avoid the stress accumulation phenomenon.

1. Introduction

Due to the good optical properties, stable chemical structure and strong mechanical strength of sapphire crystals, it is widely used in satellite space technology, infrared military devices, high-intensity laser window and other military fields [1–4]. Because of its lattice constant close to GaN and the growth process is mature, sapphire single crystal is widely used in SOS microelectronic circuits, LED lamp beads and other substrate industry [5, 6]. Owing to its high hardness, dielectric constant in line with the capacitive screen requirements, sapphire crystal can be used in the field of wearable equipment window [7-9]. Because of its special characteristics of the atomic level transition, titanium-doped sapphire single crystal was used in high-power laser gain media [10, 11]. With the rapid development of these industries, the growth of large-sized and high-quality sapphire single crystal has become particularly urgent [12-16]. Therefore, the temperature field study of the large-size sapphire single crystal furnace has great application value. It has been reported that 300 kg single sapphire crystal is successfully synthesized in Monocrystal Company. However, the research of large-size sapphire single crystal furnace thermal field had not been reported at present. Therefore, it had great application value that studied the large-size sapphire single crystal furnace temperature field.
In this paper, the 120 kg, 200 kg and 300 kg grade single crystal furnace temperature field have been designed and simulated. The power consumption, axial and radial temperature gradient, solid-liquid surface shape, stress distribution and flow of these three temperature fields were compared.

2. Simulation

120 kg, 200 kg and 300 kg grade temperature fields with the same of insulation system structure, material and crucible ratio of height to diameter have been designed. The temperature field structure is shown in figure 1. The middle and bottom insulation system both include the 10 layers of molybdenum screen inside and zircon outside. The temperature field diagram has been introduced into the simulation software CGSim. The power consumption, axial and radial temperature gradient, solid-liquid surface shape, stress distribution and flow of these three temperature fields have been comprehensive studied.

![Figure 1. The structure illustration of Single crystal furnace temperature field: 1 furnace shell; 2 seed bar; 3 seed chuck; 4 seed; 5 crystal; 6 melt; 7 crucible; 8 heating; 9 tungsten column; 10 tungsten column base care.](image1)

3. Results and discussion

3.1. Temperature field insulation

In order to study the thermal insulation effect of various grades (120kg, 200kg and 300kg) thermal field, 13 points marked by A', B', C', D', E', F', G', H', I', J', K', L' and M' (as shown in figure 2) are taken from the upper, middle, and bottom insulation system. The temperature of these points is measured and drawn as shown in figure 3.

![Figure 2. Schematic diagram of temperature field test.](image2)
As can be seen from figure 3, in the upper and bottom region of temperature field, the temperatures at the same position (A', B', C', M', L' and K') of the 120kg, 200 kg and 300 kg remain unchanged. However, for the same position (E', F', G', H', I' and J') of the side insulation system, the temperature of the 120 kg single crystal furnace is the lowest, followed by 200 kg and the highest is 300 kg. From the temperature curve, it can be seen that the 120 kg grade had the largest temperature gap difference between with 200 kg grade at the F' point, reaching 69.9 K, 200 kg grade had the largest temperature gap difference between with 300 kg grade at the D' point, reaching 47.34 K. Thus, as the size of the crucible increases, it can be concluded that the heat dissipation of the single crystal furnace middle insulation system increased, and more heat is taken away by the cooling water inside the furnace shell. The insulation effect of the temperature field is gradually deteriorated and the power loss of the single crystal furnace increased. Table 1 shows the power consumption, unit power consumption and maximum temperature, respectively. Not surprisingly, the 200 kg grade single crystal furnace power consumption increased 26 kw than that of 120 kg, and the 300 kg grade single crystal furnace power consumption increased 47 kw than that of 120 kg grade. These results are consistent with the results of figure 3. With the increase in crystal size, the power consumption is increase, dramatically. However, the unit power consumption decrease with increasing crystal size, which would be favorable to decrease the unit cost of sapphire products. The maximum temperature of 200 kg grade single crystal furnace is close to the 120 kg, but the maximum temperature of 300 kg grade single crystal furnace decrease 8.52 K than that of 120 kg, which would result in a decrease of the temperature gradient in the axial and radial temperature curves

![Figure 3. The temperature curve of the point taken.](image)

**Table 1.** The power consumption, unit power consumption and the maximum temperature comparison of 120kg, 200kg and 300kg single crystal furnace temperature field.

|            | 120kg  | 200kg  | 300kg  |
|------------|--------|--------|--------|
| power consumption (kw) | 71.675 | 97.0344| 117.948|
| unit power consumption (kw/kg) | 0.5973 | 0.4851 | 0.39316|
| maximum temperature (K) | 2555.1 | 2555.97| 2546.58|

3.2. **Axial and radial temperature gradients**

In order to verify the axial and radial temperature gradient of 120 kg, 200 kg and 300 kg single crystal furnace, the axial and radial temperature curves are plotted. The measured curve position is shown in figure 4. The measurement of the axial temperature curve is from point A to point B and the radial temperature curve is from point C to point D.
Figure 4. The measurement illustration of axial and radial temperature curve. (Point A to point B for the axial temperature curve measurement; Point C to point D for the radial temperature curve measurement).

Figure 5 shows the radial temperature gradient of 120 kg, 200 kg and 300 kg single crystal furnace. These three temperature curves are similar to each other. The starting point C of these curves is almost coincident. With the increasing of the distance from C to the D, the temperature curve began to appear differences. All the corresponding point temperatures of the 120 kg are the highest, the 200 kg is followed and the 300 kg is minimum. Due to the different crucible size, the ending position of these radial temperature curves is different. The simulation results indicate that the radial temperature gradient of 120 kg, 200 kg and 300 kg are 0.16436 K/mm, 0.14990 K/mm and 0.10389 K/mm, respectively. With the crucible size increase, the radial temperature gradient decrease.

Figure 6 shows the axial temperature gradient of 120 kg, 200 kg and 300 kg single crystal furnace. It can be seen that the three curves coincide at the starting point A. With the increase of distance from point starting A, the temperature curve began to differ. All the corresponding point temperatures of the 120 kg also are the highest, the 200 kg is followed and the 300 kg is minimum. However, due to the different crucible size, the ending position of these axial temperature curves is also different. The simulation results show that axial temperature gradient of 120 kg, 200 kg and 300 kg respectively are 0.45622 K/mm, 0.39511 K/mm and 0.33707 K/mm, respectively. As the size of the single crystal furnace increases, the axial temperature gradient decrease. By keeping in mind the decrease of radial and axial temperature gradient, let's look at the maximum temperature (Table 1). The maximum temperature of 200 kg grade single crystal furnace is close to the 120 kg, but the maximum temperature of 300 kg decrease 8.52 K than that of 120 kg. These result in the decrease of unit power dissipation and the axial temperature gradient, with the size of the sapphire single crystal size increasing.

![Figure 4](image1.png)

![Figure 5](image2.png)
3.3. Solid-liquid surface shape and stress distribution

The change of radial and axial temperature gradient would cause the growth angle of solid-liquid surface and crystal internal stress to change. It is important to analyse the shape of the solid-liquid surface and its stress distribution. Figure 7 shows that Solid-liquid surface shape and stress distribution of 120 kg, 200 kg and 300 kg. With the increase of crystal size, the growth angle between the solid and liquid surface increase, this inevitably led to the change of the stress distribution inside the crystal and the stress value.

It is well known that the maximum stress distribution of the crystal is at the junction of the seed and crystal and the junction of the crystal and melt. From the crystal local stress amplification diagram (figure 7 right), it can be seen that no stress enrichment phenomenon occurs at the junction of seed and crystal for 120 kg grade temperature field. With the increase of crystal size, the stress enrichment phenomenon appears and becomes serious. Very serious stress enrichment is observed when the crystal size reaches 300 kg grade. Therefore, the cracking probability of the 300 kg grade single crystal becomes larger during the process of crystal growth. Expanding the interface between the seed and crystal was propitious to smooth the junction of the angle and avoid the stress accumulation phenomenon.

3.4. The melt flow conditions

Figure 8 shows that the melt flow condition of 120 kg, 200 kg and 300 kg single crystal furnace. The liquid flow of these three temperature fields is similar, only one liquid vortex exists. However, with
the increase of the crucible size, the density of liquid flow line decrease. These results indicate that the flow rate gradually slowed down. This is due to the decrease of the melt internal temperature and the expansion of the crucible.

![Figure 8](image)

**Figure 8.** The melt flow conditions: (a) 120 kg; (b) 200 kg and (c) 300 kg.

4. **Conclusions**
In this paper, the power consumption, axial and radial temperature gradient, solid-liquid surface shape, stress distribution and melt flow of 120 kg, 200 kg and 300 kg grade single-crystal furnace have been studied. The simulation results show that with the increase of the single crystal furnace size, the power consumption increase, the temperature field insulation effect become worse, the growth stress value increase and the stress enrichment phenomenon occurs. Therefore, during the design process of large-size sapphire single crystal furnace, the middle and bottom insulation system, insulation effect should be enhanced. The appropriate radial and axial temperature gradient can effectively reduce the crystal stress and prevent the occurrence of cracking. During seeding process, expanding the interface between the seed and the crystal can slow down the angle between the seed and the crystal and avoid the stress accumulation phenomenon.

**Acknowledgment**
This work was financed by Shenzhen Strategic Emerging Industry Development Special Fund of Knowledge (JCYJ20150525092941038, JCYJ20150525092940969)

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