Supporting Information

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Controlling growth of BBO crystals

Pt crucible: $\phi 90 \times 80$ mm, the density of BBO: $\rho = 3.85$ g/cm^3

Starting materials: BBO and NaF are 4.9503 mol (1103.6575g) and 2.5507 mol, respectively, the total quantity is 7.501 mol.

I) Assuming the diameter of target crystal is 7 cm ($R_s = 3.5$ cm) and ignoring the volatilization of NaF during the crystal growth, we can get the following results according to the deduced formulas:

The weight of as-grown BBO crystal: $W_{BBO} = \pi R_s^2 h\rho = 3.14 \times 3.5^2 \times 3.85h = 148.0903h$

namely, $n_{BBO} = 148.0903h / 222.95$.

So, x mol% = NaF mol% = $\{2.5507/[(4.9503 - n_{BBO}) + 2.5507]\} \times 100\%$

The slope of liquidus AB: $m = 0.0045x^2 - 0.2906x - 2.460 = x(0.0045x - 0.2906) - 2.460$

The daily temperature decrease: $\Delta T = 0.00159 \times 3.5^2 \times mx^2 v / 7.501$

When the crystal thickness h = 2.0 cm, the total temperature decrease $\Delta T_{all} = 902.35 - 851.10 = 51.25$℃, the crystallization yield will reach 26.8% (namely, $1.3285 \times 100\%/4.9503$) which is higher than that of the average value (25%), so the crystal thickness is hard to grow thicker continually. It is necessary to increase the weight of melt and use large crucible or controlling the diameter of BBO less than 7 cm.

II) Suppose $R_s = 3.0$ cm, then $W_{BBO} = 108.801h$, $n_{BBO} = 108.801h/222.95$, NaF mol% = $\{2.5507/[(4.9503 - n_{BBO}) + 2.5507]\} \times 100\%$, $m = 0.0045x^2 - 0.2906x - 2.460 = x(0.0045x - 0.2906) - 2.460$, $\Delta T = 0.00159 \times 3.0^2 \times mx^2 v / 7.501$.

When the crystal thickness h = 2.4 cm, the $\Delta T_{all} = 44.22$℃, the crystallization yield will reach 23.7% which is less than that of the average value (25%); When h = 2.6 cm, $\Delta T_{all} = 44.22$℃, the crystallization yield will reach 25.6%, which means the crystal thickness is hard to grow thicker.