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The Charge Components Proportions Influence On The Second Phase Emergence Probability, During Czochralski Process YAG MC Growth.

Gurenko Sergey Alekseevich[1]*, Sinelnikov Boris Mihaylovich[4], Nagdalian Andrey Ashotovich[1], Krivenko Dmitry Valentinovich[2], Povetkin Sergey Nikolaevich[1], Ziruk Irina Vladimirovna[2], Rodin Igor Alekseevich[3], and Trushov Pavel Andreevich[1].

[1]Noth Caucasus Federal University, Stavropol, Russia.
[2]Saratov State University named after NI Vavilov, Saratov, Russia.
[3]Kuban State Agrarian University, Krasnodar, Russia.
[4]Exiton Ltd, Stavropol, Russia.

ABSTRACT

The causes of the second phase inclusions in YAG:Nd crystals are considered. The optimal ratio of the initial components of the raw material was found experimentally. The found composition provides the minimum probability of formation of the second phase inclusions in the conditions of fluctuation of technological parameters.
Keywords: YAG MC, crystals, probability

Corresponding author

INTRODUCTION

The current rapid laser technology development leads to increasing demands for the lasers components quality. In particular, the active elements, from which their basis is composed of [1]. Their most important features are: optical homogeneity, impurity dispersion equitability, the foreign inclusions absence [2]. The crystals grown with the modern technology, contain a large number of the second phase inclusions. While sometimes, it leads to the good products output factor decrease, in other cases it causes lasing properties deterioration, since the inclusions dissipate the emission (rays).

METHODS AND MATERIALS

According to the phase chart [3] (see Figure 1), the optimal growth conditions for the optical yttrium-aluminum garnet monocrystal (YAG MC) are the pulling from the melt composition: weight 43% Al_2O_3 and weight 57% Y_2O_3. For the doped YAG crystal: Nd^{3+}, where the stoichiometric ratio is calculated according to the equation:

$$Y_{3(1-x)}Nd_{3x}Al_5O_{12} = (1-x)\cdot Y_3Al_5O_{12} + x\cdot Nd_3Al_5O_{12} \tag{1}$$

$$x = \frac{C(Nd^{3+})}{k\cdot 100\%},$$

for which x is the neodymium atoms proportion, C(Nd3+) is the neodymium concentration in atomic percent, k is the inclusion dispersion ratio. For concentration of Nd^{3+} =1.1 at.%, x=0,061.

While growing monocrystals with the Czochralski process, a diffusion layer emerges in the near of the crystallization front [4], where the mass transfer occurs between between the crystal and the main melt bulk. There is no convective melt mixing in the diffusion layer. If the melt composition differs from the growing crystal composition, then the excessive component is separated to the main melt bulk during the crystallization process before the crystallization front from the crystallized bulk. The crystallization front pushes off the Nd_2O_3, as the distribution ratio between the melt and the crystal is different from 1 (for yttrium aluminum garnet it is equal to 0.18). Another excessive component might be Y_2O_3 or Al_2O_3. If the crystallization rate is equal to f, then the crystallized bulk per time unit the volume will be equal $f\cdot S$. By multiplying this bulk by the pushed off excessive component concentration $\frac{dC(x)}{d\text{v}}$, we get the excessive component stream, pushed of by the growing crystal into the melt bulk before the crystallization front: $j_{\hat{e}\eth} = f\frac{d\tilde{N}^p(x)\cdot S}{dx\cdot S} = f\frac{dC^p(x)}{dx}$ [5]. The distance x is measured from the moving crystallization front. In the near of the crystallization front emerges the most prominent deviation in the melt composition. The magnitude of this deviation will depend on the following factors:

1) The crystallization rate.
2) The excessive component concentration in the main melt bulk
3) The diffusion layer thickness (depends on the crystallization front shape, the crystal rotational speed, the melt hydrodynamics, the crystallization front temperature gradient), crystal diameter, the crystal rotational speed.
4) The melt components diffusion rate. If the excessive component concentration (Y_2O_3 or Al_2O_3) begins to exceeds the critical point (compositions 6 or 9 correspondingly), the second phase crystallization takes place (see Figure 1).

The real fact is that the crystal growth rate is not constant, due to pulling mechanism unevenness, the heating and cooling system parameters variability [6] (the crystallization rate changes can be traced by crystal's waists – local diameter changes). Thus it is obligatory to set the technological parameters to prevent the allowed deviations in the machinery workflow affect the crystal quality, i.e. keep the melt bulk contained in the 1 and 2 areas (Figure 1).

RESULTS AND DISCUSSION

The first stage of the research was to grow YAG MC: Nd^{3+}, using stoichiometric stock composition. The top part of the grown crystals does not contain any inclusions, in the the cylindrical part, however, perovskite phase inclusions have started to emerge ($Y_2O_3 \cdot Al_2O_3$). The number of inclusions increases towards the bottom of the crystal and in places of the waists emergence (see Figure 2). The cause for the perovskite inclusions emergence is the change in melt composition due to the uneven evaporation of its components – Al_2O_3 has higher vapor pressure.

At the second stage of the research a series of experiments with the addition of aluminum oxide excess in order to compensate for evaporative losses was conducted (Table 1).

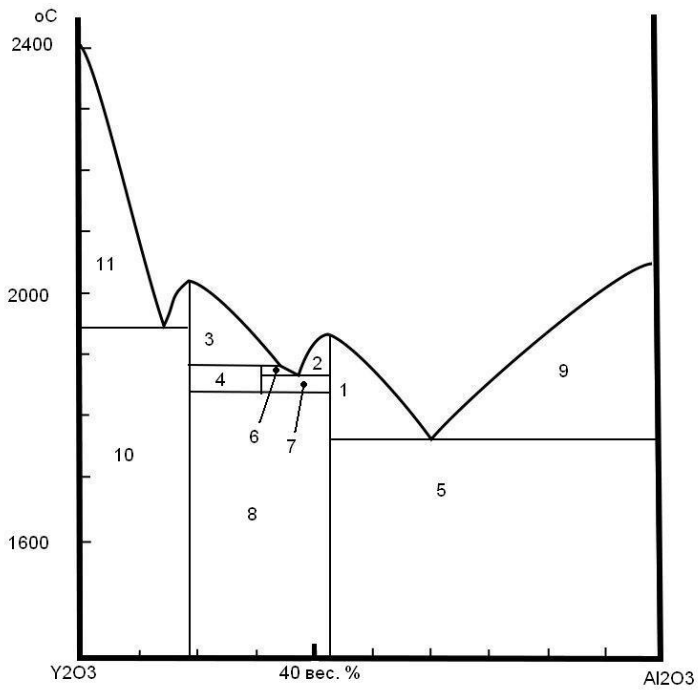

Figure 1: System state chart Al_2O_3-Y_2O_3:

(1,2) $Y_3Al_5O_{12}$ (YAG) + Liq, (3) $2Y_2O_3 \cdot Al_2O_3$+Liq, (4) $2Y_2O_3 \cdot Al_2O_3$ + $Y_2O_3 \cdot Al_2O_3$,(5) $Y_3Al_5O_{12}$ (YAG) + Al_2O_3, (6) $Y_2O_3 \cdot Al_2O_3$+Ж, (7) $Y_2O_3 \cdot Al_2O_3$ + $Y_3Al_5O_{12}$(YAG), (8) $2Y_2O_3 \cdot Al_2O_3$ + $Y_3Al_5O_{12}$(YAG)

Table 1: A series of processes with different number of excess Al_2O_3

Process #	aluminum oxide excess, weight. %	Crystal description
1	3	60mm of the top part of the crystal contains inclusions of Al_2O_3 phase in the form of vapor
2	2	40mm of the top part of the crystal contains inclusions of Al_2O_3 phase in the form of vapor
3	1	No inclusions
4	1	No inclusions
5	1	No inclusions
6	0.7	A pervoskite narrow inclusions zone near the waist
7	0.5	Dispersed inclusions

The addition of 2 and 3 % aluminum oxide to the charge causes the Al_2O_3 inclusions zone emergence in the form of vapor in top part of the crystals. The further crystal growth is pure, due ti the aluminum oxide vaporization during the growth process, which leads to the yttrium oxide ratio increase and composition drift from area 9 to area 1 of the phase chart (see Figure 1).

In processes with 0.5% of excess ratio, emerge the dispersed perovskite inclusions .

When setting 0.7-1 weight the aluminum oxide excess % crystals contain the minimal number of inclusions.

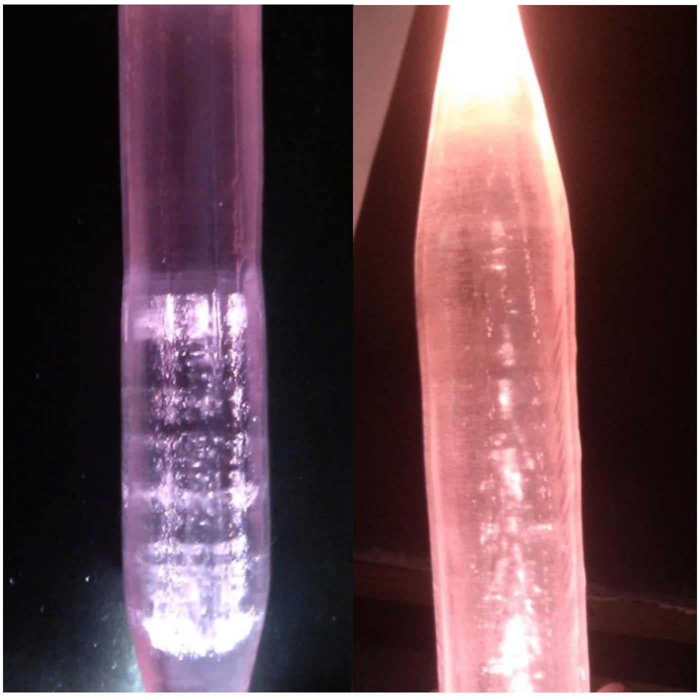

Figure 2: The perovskite inclusions number increase in the bottom of the crystal.

CONCLUSION

The research has found the stock charge components proportions, which enables to grow YAG MC: Nd^{3+} with the minimal number of the second phase inclusions. It enabled to increase the production output efficiency per crystal. Also the theoretical grounds for the inclusions emergence process were found.

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