

## OPTIMIZATION OF THERMAL CONDITIONS AT CZOCHRALSKI GROWTH OF RARE-EARTH SILIKATE SINGLE CRYSTALS

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Many inorganic single crystal scintillators have been developed as gamma-ray detectors for high-energy physics, medical imaging, oil-well logging etc. Among them, inorganic single crystals such as Bi<sub>4</sub>Ge<sub>3</sub>O<sub>12</sub> (BGO), Gd<sub>2</sub>SiO<sub>5</sub> (GSO) and Lu<sub>2</sub>SiO<sub>5</sub> (LSO) are used in medical imaging equipment like PET and other radiation detectors. However, new trends in the PET scanners development dictate new requirements to scintillation materials to be considered for a mass use. Lu<sub>2x</sub>Gd<sub>2(1-x)</sub>SiO<sub>5</sub>:Ce (LGSO) is one of promising new scintillators for performance improvement in PET scanners, because substantial quantity of Lu atoms can be substituted by Gd without polymorph transition. Addition of Gd leads to decrease of radioactive background called by <sup>176</sup>Lu isotope, and to decrease of crystal cost. Rather high values of light yield [1] and energy resolution (up to 6.5 % [2]) were obtained for crystals with the same space symmetry time, as LSO (monoclinic, C2/c). Also, lower melting point of LGSO crystals (below 2000<sup>0</sup>C [3]) in comparison with LSO is one of advantages at their industrial production.

Obtaining of LGSO crystals are complicated due to polymorph transition from monoclinic lattice P2<sub>1</sub>/c (GSO) to C2/c (LSO) leading to worsening of crystal transmission and cracking of boules during growth process or at cooling of as-growth crystals.

In present work, causes of crack formation of LGSO crystals with diameter up to 50 mm and length up to 150 mm are studied using CGSim package [4]. The numerical simulation is performed in two steps: (i) a preliminary global heat transfer computation within a simplified model and (ii) a detailed conjugated analysis of the heat exchange in the crystallization zone including the crystal, the melt, the crucible, and gas region [5, 6]

CGSim Defects Module was used for stress analysis in crystal at different growth stages. The numerical algorithm used in the stress module operates with the displacement vector  $u_i$ . The axisymmetric computational domain representing the crystal is meshed using cylindrical coordinates  $\{r, \varphi, z\}$  with the temperature distribution found from the heat transfer modeling on the corresponding crystal position (stage i). The thermoelastic problem is solved using the Finite Volume Method.

Axial and radial temperature gradient inside ingot was estimated using data obtained by numerical simulation. Design defects of heat assembly were eliminated. Optimized growth regime and heat assembly construction provides decrease of probability cracks formation in LGSO crystals.

### References

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