



# Mechanical, thermal and spectral characteristics of Nd<sup>3+</sup>:Sr<sub>6</sub>YSc(BO<sub>3</sub>)<sub>6</sub> crystal



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## ABSTRACT

A crystal of Nd<sup>3+</sup>:Sr<sub>6</sub>YSc(BO<sub>3</sub>)<sub>6</sub> was grown successfully by the top-seeded solution growth method. The average laser-induced damage thresholds are 1.76 GW/cm<sup>2</sup> for (001) face and 1.47 GW/cm<sup>2</sup> for (100) face at 1064 nm radiation, respectively. The average Vickers hardness of (100) and (001) faces are 629 and 545 N/mm<sup>2</sup>, respectively. The thermal expansion coefficients are  $12.3 \times 10^{-6} \text{ K}^{-1}$  along *a*-axis and  $9.39 \times 10^{-6} \text{ K}^{-1}$  along *c*-axis, respectively. The thermal conductivity is about 2.3 W/m K at room temperature. The polarized spectral properties were investigated in detail. Based on the Judd–Ofelt theory, the intensity parameters were obtained. The results show that Nd<sup>3+</sup>:Sr<sub>6</sub>YSc(BO<sub>3</sub>)<sub>6</sub> crystal is a potential laser crystal.

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## 1. Introduction

With the rapid development of diode-pumped solid-state lasers, research on high efficient diode-pumped materials become more and more important. Nd<sup>3+</sup>:YAG and Nd<sup>3+</sup>:YVO<sub>4</sub> are commercially available laser crystals, but limited to low Nd<sup>3+</sup> ( $\approx 1$  at.%) doping concentration and narrow absorption bands near the diode output wavelength of 808 nm.

The borate crystals are a type of excellent laser gain media [1–6], most of them have good spectral and thermal properties. Sr<sub>3</sub>Y(BO<sub>3</sub>)<sub>3</sub> crystal is one of them, it is isostructural with Sr<sub>3</sub>Sc(BO<sub>3</sub>)<sub>3</sub>, which crystallizes in the R $\bar{3}$  (No. 148) structure [7]. The Yb-doped Sr<sub>3</sub>Y(BO<sub>3</sub>)<sub>3</sub> crystal has broad emission bandwidth, in the actual state of the art, one of the broadest for an Yb-doped crystal. A 69 femtosecond pulse laser with 80 mW average power had been produced [2]. But a drawback with the Yb:Sr<sub>3</sub>Y(BO<sub>3</sub>)<sub>3</sub> crystal is its brittleness, which limited its application. The Stack family with formula A<sub>6</sub>MM'(BO<sub>3</sub>)<sub>6</sub>, where A = Sr, Ba, Pb, or Ln (lanthanide) and M, M' = +2, +3, or +4 metal cations belongs to the trigonal system with space group R $\bar{3}$ , is derived from the structure of the compound Sr<sub>3</sub>Sc(BO<sub>3</sub>)<sub>3</sub>. Its structure can be simply described as: the metal-centered octahedra (MO<sub>6</sub> and M'O<sub>6</sub>) linked by BO<sub>3</sub> groups to form chains, these chains are connected together

by the 9-coordinate Sr atoms to form a 3D framework. The MO<sub>6</sub> octahedron is larger and trigonally elongated and shares vertexes with the 9-fold site, while the M'O<sub>6</sub> is trigonally compressed and shares its triangular faces with the 9-fold site. When A = Sr atom, M = M' = Sc atom, A<sub>6</sub>MM'(BO<sub>3</sub>)<sub>6</sub> corresponds to Sr<sub>3</sub>Sc(BO<sub>3</sub>)<sub>3</sub> compound, on the other hand, when M = Y and M' = Sc, Sr<sub>6</sub>YSc(BO<sub>3</sub>)<sub>6</sub> compound is formed [8–10]. In A<sub>6</sub>MM'(BO<sub>3</sub>)<sub>6</sub> compounds, the large ion usually occupies the M site, whereas the small ion prefers to occupy the M' position. However, in some cases, they can statistically occupy the same site, which leads to a partial disordered structure. For example, in Sr<sub>6</sub>HoSc(BO<sub>3</sub>)<sub>6</sub>, the occupancy of M site is 89% Ho and 11% Sc atoms, whereas the occupancy of M' site is 93% Sc and 7% Ho atoms [8]. It is generally believed that the disordered structure would result in the broad absorption and emission bandwidth of laser crystals, which will be beneficial to diode pumping and production of ultrashort pulses. Moreover, as the ionic radius of Sc<sup>3+</sup> is about 20% smaller than that of Y<sup>3+</sup>, which will make the crystal structure of Sr<sub>6</sub>YSc(BO<sub>3</sub>)<sub>6</sub> more compact than that of Sr<sub>3</sub>Y(BO<sub>3</sub>)<sub>3</sub>, this may improve the thermal and mechanical strength of the material.

Nd<sup>3+</sup> doped Sr<sub>6</sub>YSc(BO<sub>3</sub>)<sub>6</sub> crystal had been grown by the Czochralski method [11]. However, the thermal properties and polarized spectroscopic characteristics of the crystal have not been investigated, and they are very important for evaluating laser performances and designing of laser device. Therefore, in this paper, we report the growth, mechanical, thermal and polarized spectroscopic characteristics of Nd<sup>3+</sup>:Sr<sub>6</sub>YSc(BO<sub>3</sub>)<sub>6</sub> crystal.

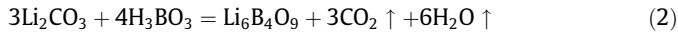
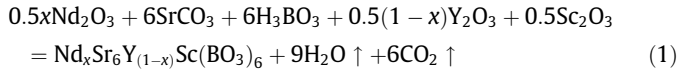
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## 2. Experimental procedure

It is well known that the crystallographic orientation of the crystal grown by the top-seeded solution growth (TSSG) method is usually easier to be determined than that of the crystal grown by the Czochralski method. Therefore, the TSSG method with a flux of  $\text{Li}_6\text{B}_4\text{O}_9$  was used to grow the  $\text{Nd}^{3+}:\text{Sr}_6\text{YSc}(\text{BO}_3)_6$  crystal.

The starting materials of 80 at.%  $\text{Nd}^{3+}:\text{Sr}_6\text{YSc}(\text{BO}_3)_6$  and 20 at.%  $\text{Li}_6\text{B}_4\text{O}_9$  were weighed according to the following chemical reaction equations:



The raw chemicals used were  $\text{Nd}_2\text{O}_3$ ,  $\text{SrCO}_3$ ,  $\text{Y}_2\text{O}_3$ ,  $\text{Sc}_2\text{O}_3$ ,  $\text{Li}_2\text{CO}_3$  and  $\text{H}_3\text{BO}_3$  with a purity of 99.99%. The weighed materials with 8 at.%  $\text{Nd}_2\text{O}_3$  were mixed and put into a platinum crucible of  $\phi$  60 × 50 mm, then the crucible was placed into a vertical tubular furnace with a nickel–chrome wire as the heating element. The mixture was melt and kept at 30 °C above the saturation temperature (about 950 °C) for 2 days to make the solution melt completely and homogeneously. After the saturation temperature was exactly determined by repeated seeding trials, the growing seed was contacted the melt at 1 °C above the saturation temperature for half an hour to dissolve the outer surface of the seed. The crystal was grown at a cooling rate of 1–2 °C/day and a rotating rate of 10 rpm. When the growth process ended, the crystal was drawn out of the melt surface and cooled to room temperature at an annealing rate of 20 °C/h.

To identify the grown crystal, the data of X-ray powder diffraction (XRD) of the crystal was collected on a *D/max-rA* type diffractometer with  $\text{Cu K}\alpha$  radiation in the continuous scanning mode in the range of 10–70°, with a step of 0.02° and a scan speed of 5°/min at room temperature.

Laser-induced damage threshold testing is a good method for quantifying the amount of electromagnetic radiation an optical component can withstand. Two polished samples of  $\text{Nd}^{3+}:\text{Sr}_6\text{YSc}(\text{BO}_3)_6$  crystal with (001) and (100) faces were used to the measurement. The damage thresholds were measured in three different parts of each piece of samples. The hardness of  $\text{Nd}^{3+}:\text{Sr}_6\text{YSc}(\text{BO}_3)_6$  crystal was determined using a 401MVA™ Vickers-microhardometer. Two slices of (100) and (001) face were used, five points were collected for each slice.

For a good laser crystal, high thermal conductivity and a small thermal expansion coefficient are needed to diffuse enough heat rapidly and to maintain the morphology of the crystal. Besides, they are also the significant factors in crystal growth and applications.  $\text{Nd}^{3+}:\text{Sr}_6\text{YSc}(\text{BO}_3)_6$  crystal belongs to trigonal system, there are only two independent thermal feature's orientations. Two samples with dimensions of  $\phi$  2.5 × 13.8 mm<sup>3</sup> and  $\phi$  2.5 × 12.8 mm<sup>3</sup> were cut along *c*- and *a*-axis for the measurement of thermal expansion, respectively. The thermal expansion was measured by a thermal dilatometer (DIL 402PC) in the range of 30–750 °C at a heating rate of 5 K/min. The thermal conductivity of  $\text{Nd}^{3+}:\text{Sr}_6\text{YSc}(\text{BO}_3)_6$  crystal was measured using a Laser Flash Apparatus (Netzsch LFA 457, Germany). A sample of  $\text{Nd}^{3+}:\text{Sr}_6\text{YSc}(\text{BO}_3)_6$  crystal with dimensions of 10 × 10 × 2 mm<sup>3</sup> was used. Before the measurement, both of the front and back faces of the specimen were coated with a thin layer of graphite to prevent the laser beam pass through the specimen directly.

A sample of  $\text{Nd}^{3+}:\text{Sr}_6\text{YSc}(\text{BO}_3)_6$  crystal with dimensions of 8 × 6 × 1 mm<sup>3</sup> was cut along the [001] direction from the as-grown crystal and polished, applied to the spectroscopic measurements. The polarized absorption spectra were measured using a

Perkin–Elmer UV–vis–NIR spectrometer (Lambda-900) in the range of 350–1000 nm at room temperature. The polarized fluorescence spectra and fluorescence lifetime at room temperature were



Fig. 1. The grown  $\text{Nd}^{3+}:\text{Sr}_6\text{YSc}(\text{BO}_3)_6$  crystal.

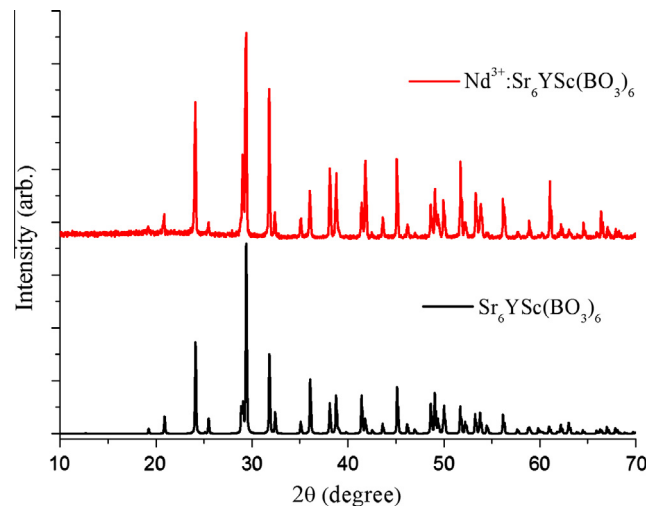


Fig. 2. XRD of  $\text{Nd}^{3+}:\text{Sr}_6\text{YSc}(\text{BO}_3)_6$  and  $\text{Sr}_6\text{YSc}(\text{BO}_3)_6$  crystal.

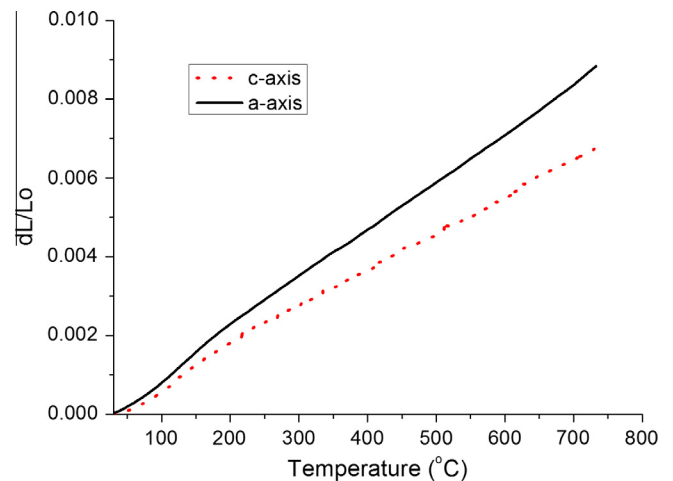


Fig. 3. Thermal expansion of  $\text{Nd}^{3+}:\text{Sr}_6\text{YSc}(\text{BO}_3)_6$  crystal.

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