# Supplementary Information

## Enhanced growth of $Nd^{3+}$:$MgGdB_5O_{10}$ laser crystal with intense multi-wavelength emissions characteristics

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**Fig. S1**. Schematic diagram of crystal growth apparatus.

**Fig. S2**. (a)View of the $B_5O_{12}$ cluster. (b) Gd/$NdO_9$ polyhedra. (c) $MgO_6$ polyhedra.

**Fig. S3.** (a) View of the B-O layer along [101] direction. (b) View of the 3D structure of **1** along [010] direction. (c) View of the M-O (M=Gd/Nd and Mg) layer along [101] direction.

**Fig. S4**. Powder XRD pattern of Nd:GMB crystal.

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**Equation S(1)**

**Equation S(2)**

**Equation S(3)**

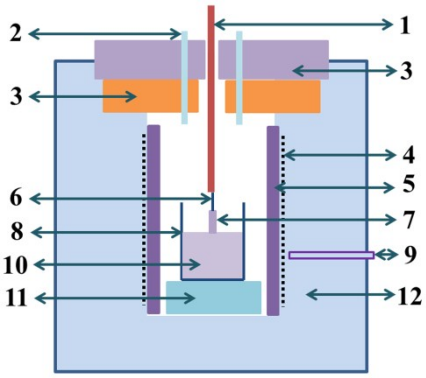


**Fig. S1**. Schematic diagram of crystal growth apparatus. (1) seed-holder, (2) watch window, (3) furnace cover (thermal insulation materials), (4) nickel-chrome heating wires, (5) $Al_2O_3$ tube, (6) platinum wires, (7) seed, (8) platinum crucible, (9) thermocouple, (10) solution, (11) thermal insulation materials (the height is based on the thermal field ), (12) thermal insulation materials.

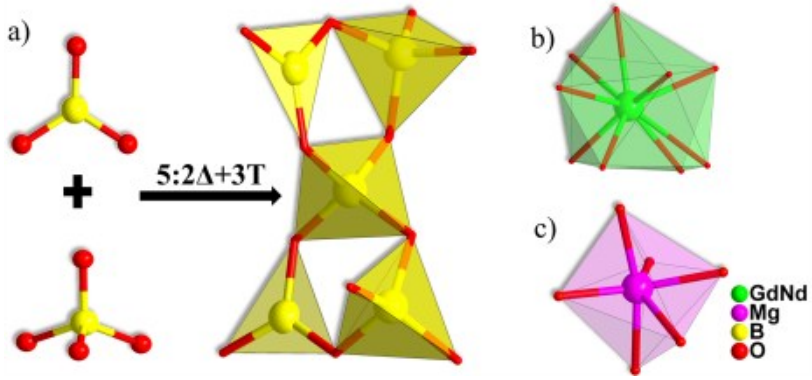


**Fig. S2**. (a)View of the $B_5O_{12}$ cluster. (b) Gd/$NdO_9$ polyhedra. (c) $MgO_6$ polyhedra.

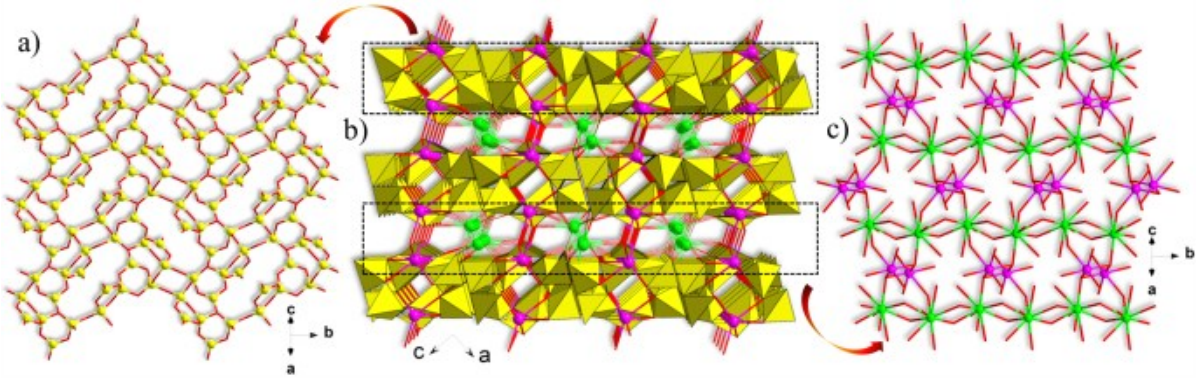


**Fig. S3.** (a) View of the B-O layer along [101] direction. (b) View of the 3D structure of **1** along [010] direction. (c) View of the M-O (M=Gd/Nd and Mg) layer along [101] direction.

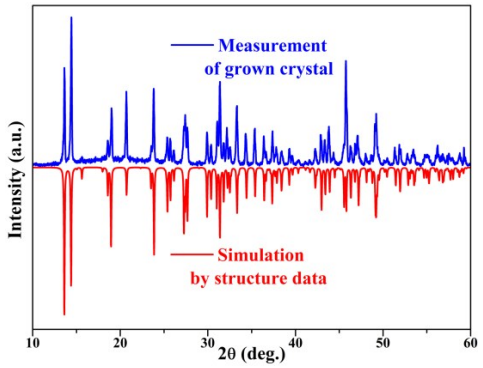


**Fig. S4**. Powder XRD pattern of Nd:GMB crystal.

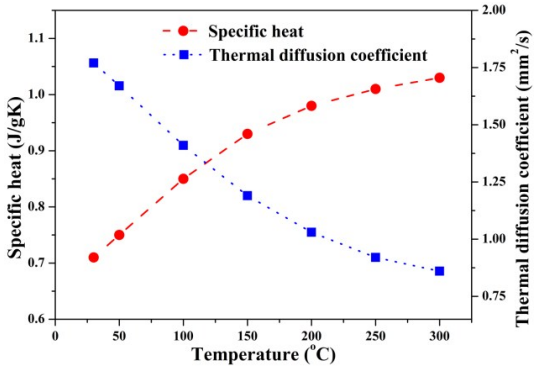


**Fig. S5**. Specific heat and thermal diffusion coefficent of Nd:GMB crystal.

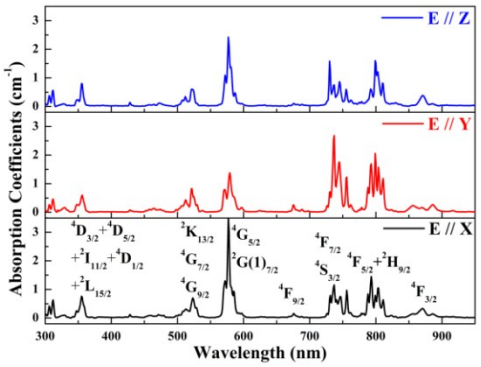


**Fig. S6**. Polarized absorption coefficients of Nd:GMB crystal.

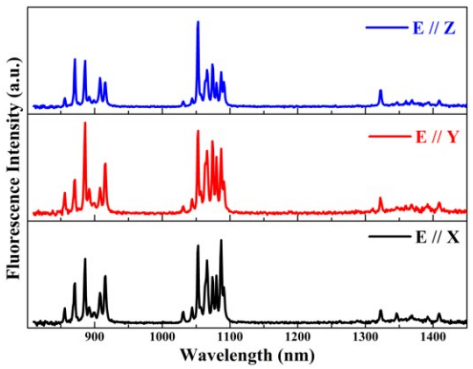


**Fig. S7**. Polarized fluorescence spectra of Nd:GMB crystal.

**Table S1.** Atomic coordinates and equivalent isotropic displacement parameters of Nd:GMB crystal.

| Atom | *x*/a | *y*/b | *z*/c | *U*(eq)[Å$^2$]* |
|---|---|---|---|---|
| Gd(1) | 8148(1) | 1872(1) | 7634(1) | 5(1) |
| Nd(1) | 8148(1) | 1872(1) | 7634(1) | 5(1) |
| Mg(1) | 3959(3) | 4101(3) | 8745(2) | 7(1) |
| B(1) | 10662(9) | 3122(8) | 5875(8) | 6(1) |
| B(2) | 2214(8) | 321(9) | 9474(7) | 7(1) |
| B(3) | 9843(9) | -1715(8) | 8920(8) | 4(1) |
| B(4) | 6551(8) | -969(9) | 4999(7) | 6(1) |
| B(5) | 10842(8) | 5775(9) | 7373(7) | 7(1) |
| O(10) | 7368(5) | -452(6) | 6189(5) | 8(1) |
| O(9) | 5329(6) | 2147(6) | 7352(5) | 6(1) |
| O(8) | 3174(5) | 1518(6) | 8706(5) | 6(1) |
| O(7) | 8259(5) | -1050(6) | 9149(4) | 6(1) |
| O(6) | 10857(5) | -267(5) | 8524(5) | 7(1) |
| O(5) | 6854(5) | 1290(6) | 10082(4) | 6(1) |
| O(4) | 9593(5) | 2746(6) | 9833(4) | 6(1) |
| O(3) | 3165(5) | 356(6) | 6322(5) | 6(1) |
| O(2) | 10085(5) | 4140(6) | 6916(5) | 7(1) |
| O(1) | 9976(5) | 1491(6) | 5729(5) | 6(1) |

* *U*(eq) is defined as one-third of the trace of the orthogonalized $U_{ij}$ tensor.

**Table S2.** Selected bond lengths (Å) of Nd:GMB crystal.

| | | | |
|---|---|---|---|
| Gd/Nd-O(10) | 2.296(4) | B(1)-O(5)#6 | 1.371(9) |
| Gd/Nd-O(10)#1 | 2.357(4) | B(2)-O(8) | 1.443(8) |
| Gd/Nd-O(9) | 2.428(5) | B(2)-O(7)#7 | 1.480(8) |
| Gd/Nd-O(4) | 2.436(4) | B(2)-O(6)#8 | 1.494(7) |
| Gd/Nd-O(1) | 2.457(5) | B(2)-O(5)#7 | 1.503(7) |
| Gd/Nd-O(2) | 2.506(4) | B(3)-O(6) | 1.459(8) |
| Gd/Nd-O(7)#1 | 2.549(4) | B(3)-O(4)#9 | 1.464(7) |
| Gd/Nd-O(7) | 2.625(4) | B(3)-O(9)#4 | 1.471(8) |
| Gd/Nd-O(5) | 2.640(4) | B(3)-O(7) | 1.476(8) |
| Mg(1)-O(3)#2 | 2.052(5) | B(4)-O(10) | 1.342(7) |
| Mg(1)-O(1)#3 | 2.060(5) | B(4)-O(3)#5 | 1.357(8) |
| Mg(1)-O(8) | 2.065(5) | B(4)-O(4)#4 | 1.396(8) |
| Mg(1)-O(1)#1 | 2.072(5) | B(5)-O(2) | 1.450(7) |
| Mg(1)-O(6)#1 | 2.193(5) | B(5)-O(8)#1 | 1.464(8) |
| Mg(1)-O(9) | 2.331(6) | B(5)-O(9)#1 | 1.477(8) |
| B(1)-O(2) | 1.357(9) | B(5)-O(3)#1 | 1.485(7) |
| B(1)-O(1) | 1.370(7) | | |

Symmetry codes: (#1) -x+3/2,y+1/2,-z+3/2; (#2) -x+1/2,y+1/2,-z+3/2; (#3) x-1/2,-y+1/2,z+1/2; (#4) -x+3/2,y-1/2,-z+3/2; (#5) -x+1,-y,-z+1; (#6) x+1/2,-y+1/2,z-1/2; (#7) -x+1,-y,-z+2; (#8) x-1,y,z; (#9) -x+2,-y,-z+2.

**Table S3**. Experimental and calculated line strength parameters of Nd:GMB crystal.

| J'-manifold | *E//X* | | | *E//Y* | | | *E//Z* | | |
|---|---|---|---|---|---|---|---|---|---|
| | $\bar{\lambda}_{abs}$ (nm) | $S_{exp}$ ($10^{-20}cm^2$) | $S_{cal}$ ($10^{-20}cm^2$) | $\bar{\lambda}_{abs}$ (nm) | $S_{exp}$ ($10^{-20}cm^2$) | $S_{cal}$ ($10^{-20}cm^2$) | $\bar{\lambda}_{abs}$ (nm) | $S_{exp}$ ($10^{-20}cm^2$) | $S_{cal}$ ($10^{-20}cm^2$) |
| $^4F_{3/2}$ | 869.4 | 1.332 | 1.460 | 873.3 | 1.558 | 1.492 | 872.5 | 1.135 | 1.160 |
| $^4F_{5/2}$, $^2H_{9/2}$ | 798.5 | 4.025 | 4.105 | 799.7 | 6.235 | 6.486 | 801.7 | 3.472 | 3.643 |
| $^4F_{7/2}$, $^4S_{3/2}$ | 742.7 | 3.873 | 3.850 | 742.5 | 7.404 | 7.254 | 740.6 | 3.713 | 3.611 |
| $^4F_{9/2}$ | 677.5 | 0.278 | 0.280 | 680.6 | 0.460 | 0.485 | 680.8 | 0.265 | 0.256 |
| $^4G_{5/2}$, $^2G(1)_{7/2}$ | 578.3 | 8.575 | 8.592 | 579.2 | 5.052 | 5.064 | 578.6 | 6.321 | 6.334 |
| $^2K_{13/2}$, $^4G_{7/2}$,$^4G_{9/2}$ | 519.1 | 2.425 | 2.158 | 518.3 | 2.579 | 2.361 | 517.9 | 1.911 | 1.748 |
| $^4D_{3/2}$,$^4D_{5/2}$,$^2I_{11/2}$,$^4D_{1/2}$,$^2L_{15/2}$ | 354.1 | 3.125 | 3.125 | 354.2 | 2.768 | 2.799 | 354.3 | 2.442 | 2.418 |
| RMSEΔS | $0.1543\times10^{-20}cm^2$, 3.7% | | | $0.1857\times10^{-20}cm^2$, 4.2% | | | $0.1301\times10^{-20}cm^2$, 3.9% | | |

**Equation S(1):**

$$A_r\left[(S'L')J',(S''L'')J''\right]=\frac{n\left(n^2+2\right)^2}{9}\times\frac{64\pi^2e^2}{3h\left(2J'+1\right)\bar{\lambda}^3}\times\sum_{\lambda=2,4,6}\Omega_\lambda\left|\left\langle(S'L')J'\left\|U^{(\lambda)}\right\|(S''L'')J''\right\rangle\right|^2$$

**Equation S(2):**

$$\tau_r=\frac{1}{\sum_{S'',L'',J''}A_r\left[(S',L')J';(S'',L'')J''\right]}$$

**Equation S(3):**

$$\beta_r\left[(S',L')J';(S'',L'')J''\right]=\frac{A_r\left[(S',L')J';(S'',L'')J''\right]}{\sum_{S'',L'',J''}A_r\left[(S',L')J';(S'',L'')J''\right]}$$