Electronic supplementary information

Laser floating zone growth of improper geometric ferroelectric $GdInO_3$ single crystals with Z_6 topological defects

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Figure S1

As shown in Figure 1(a and b), five laser diodes (LDs) units fixed in the furnace are utilized for heating the zone, an odd number of laser beams is more effective to homogenize irradiation.[1] Maximum power of each LD is 200 W and the maximum total power is 1000 W. Generally, the ultimate temperature can reach at the central focus zone is around 2750 °C. The laser beam makes molten zone narrow and stable during crystal growth, which is good for low surface tension of melts.

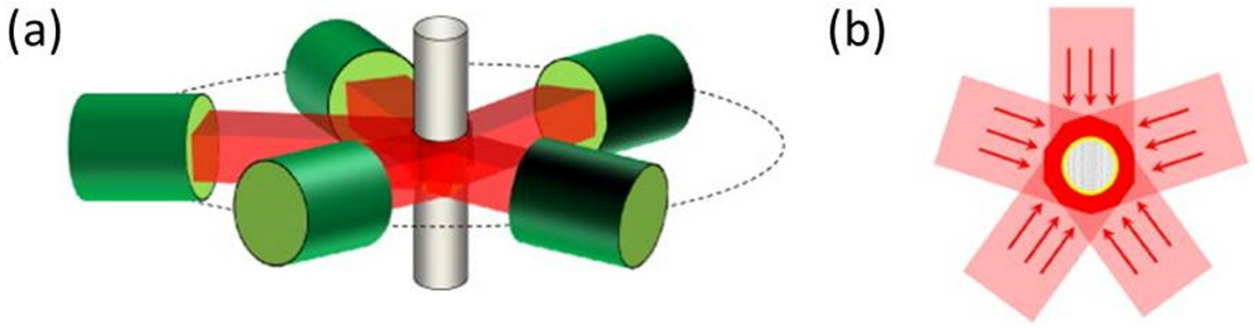

Figure S1. (a) A schematic perspective drawing of the LDFZ method. The sample is irradiated with homogeneous laser beams whose cross section is rectangular. (b) Horizontal cross section of the LFZ method.

Table S1. Refined atomic coordinates and isotropic displacement parameters for $GdInO_3$.

Atoms	Wyckoff	*x*	*y*	*z*	U_{eq}[a] (Å^2)	Occupancy
Gd1	4*b*	1/3	2/3	0.0321	0.0077 (3)	1.0
Gd2	2*a*	0	0	0	0.0050 (4)	1.0
In1	6*c*	0.3331 (6)	0	0.26881 (16)	0.00360 (19)	1.0
O1	6*c*	0.312 (3)	0	0.0986 (11)	0.0085 (16)	1.0
O2	6*c*	0.361 (3)	0	0.4351 (9)	0.011 (2)	1.0
O3	4*b*	2/3	1/3	0.2497 (14)	0.0085 (16)	1.0
O4	2*a*	0	0	0.300 (2)	0.0085 (16)	1.0

[a]U_{eq} is defined as one-third of the trace of the orthogonalized U_{ij} tensor.

Table S2. Selected bond lengths (Å) and angles (deg.) of $GdInO_3$

Gd1—O1^{i}	2.328 (10)	O1^{i}—Gd1—O1^{ii}	108.3 (3)
Gd1—O2^{iv}	2.355 (9)	O1^{i}—Gd1—O2^{iv}	78.0 (7)
Gd1—O3^{vii}	2.683 (17)	O1^{iii}—Gd1—O2^{iv}	170.0 (5)
Gd2—O1	2.322 (18)	O2^{iv}—Gd1—O2^{v}	96.5 (3)
Gd2—O2^{xi}	2.421 (17)	O1^{i}—Gd1—O3^{vii}	69.4 (3)
Gd2—O4^{xii}	2.47 (3)	O2^{iv}—Gd1—O3^{vii}	120.5 (2)
In1—O2	2.058 (12)	O1—Gd2—O1^{x}	95.1 (4)
In1—O1	2.104 (14)	O2—In1—O1	178.6 (9)
In1—O3	2.124 (3)	O2—In1—O4	84.5 (8)
In1—O4	2.144 (6)	O3—In1—O4	120.62 (10)

Symmetry codes: (i) *x*, *y*+1, *z*; (ii) -*y*, *x*-*y*, *z*; (iii) -*x*+*y*+1, -*x*+1, *z*; (iv) *y*, -*x*+*y*+1, *z*+1/2; (v) -*x*+1, -*y*+1, *z*+1/2; (vi) *x*-*y*, *x*, *z*+1/2; (vii) *y*-1, *x*, *z*; (viii) *y*, *x*+1, *z*; (ix) *y*, -*x*+*y*, *z*-1/2; (x) -*x*, -*y*, *z*-1/2; (xi) *x*-*y*, *x*, *z*-1/2; (xii) -*x*+*y*, -*x*, *z*; (xiii) -*x*, -*y*+1, *z*-1/2; (xiv) -*y*+1, -*x*, *z*-1/2; (xv) *x*, *y*-1, *z*; (xvi) *y*, *x*, *z*; (xvii) -*x*, -*y*, *z*+1/2; (xviii) -*x*+1, -*y*+1, *z*-1/2.

Reference

1 T. Ito, T. Ushiyama, Y. Yanagisawa, Y. Tomioka, I. Shindo and A. Yanase, *J. Cryst. Growth*, 2013, **363**, 264–269.