Supplementary Materials: Crystal growth of the R_2SiO_5 compounds (R = Dy, Ho, and Er) by the floating zone method using a laser-diode-heated furnace

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1. Crystal data for Dy_2SiO_5

Table S1. Crystal parameters refined from the room temperature single crystal X-ray diffraction data collected on a crystal piece isolated from the as-grown Dy_2SiO_5 crystal boule.

Chemical composition	Dy_2SiO_5
Origin	as-grown crystal fragment
Crystal system	Monoclinic
Space group	$I2/a$ (No. 15)
a (Å)	10.4642(2)
b (Å)	6.7498(1)
c (Å)	12.5396(3)
β (°)	102.740(2)
V (Å^3)	863.88(3)
Z	8
Radiation, wavelength	Mo Kα, λ = 0.71073 Å
Temperature (K)	298
Linear absorption coefficient (mm^{-1})	25.887
No. of reflections measured (excl. systematic absences)	14350
No. of reflections used in refinement	1152
No. of parameters refined	49
R1	0.0341
wR2	0.0692
Goodness of fit (GOF)	1.0248

Atomic site	Wyckoff position	x (Å)	y (Å)	z (Å)	U_{iso}/U_{eq} (Å^2)
Dy1	8*f*	0.80746(3)	0.37577(5)	0.64171(3)	0.01014(14)
Dy2	8*f*	0.42762(3)	0.25447(5)	0.46294(3)	0.00962(14)
Si	8*f*	0.6272(2)	0.5896(3)	0.81908(17)	0.0091(4)
O1	8*f*	0.6212(5)	0.4049(8)	0.5181(4)	0.0118(11)
O2	8*f*	0.7000(5)	0.7858(8)	0.8818(5)	0.0111(11)
O3	8*f*	0.5298(5)	0.6441(8)	0.7041(4)	0.0116(11)
O4	8*f*	0.7389(6)	0.4333(9)	0.8005(5)	0.0138(11)
O5	8*f*	0.5538(5)	0.4982(8)	0.9103(4)	0.0139(11)

Table S2. Anisotropic displacement parameters obtained for the Dy and Si sites from the room temperature single crystal X-ray diffraction data collected on a crystal piece isolated from the as-grown Dy_2SiO_5 crystal boule.

Atomic site	U_{11} (Å^2)	U_{22} (Å^2)	U_{33} (Å^2)	U_{12} (Å^2)	U_{13} (Å^2)	U_{23} (Å^2)
Dy1	0.0098(2)	0.0113(2)	0.0094(2)	0.00033(12)	0.00227(13)	0.00141(12)
Dy2	0.0097(2)	0.0099(2)	0.0096(2)	0.00046(12)	0.00274(14)	0.00098(12)
Si	0.0082(9)	0.0102(10)	0.0089(9)	-0.0008(7)	0.0019(7)	0.0008(7)

Table S3. Characteristics of the polyhedra formed around the Dy and Si, obtained from the room temperature single crystal X-ray diffraction data collected on a crystal piece isolated from the as-grown Dy_2SiO_5 crystal boule. Data were obtained from VESTA software.

	$Dy1O_6$	$Dy2O_7$	SiO_4
Average bond length (Å)	2.2819	2.3720	1.6289
Polyhedral volume (Å^3)	14.7349	19.0315	2.2041
Distortion index (bond length)	0.00973	0.02984	0.00459
Quadratic elongation	1.0497	-	1.0042
Bond angle variance (deg.^{2})	175.8383	-	17.4776
Effective coordination number	5.9569	6.4942	3.9953
Bond valence sum	2.925	3.097	3.949

$Dy1O_6$		$Dy2O_7$		SiO_4	
Bond	Bond length (Å)	Bond	Bond length (Å)	Bond	Bond length (Å)
Dy1-O1	2.215(5)	Dy2-O1	2.235(6)	Si-O3	1.614(5)
Dy1-O3	2.289(5)	Dy2-O5	2.328(6)	Si-O4	1.629(7)
Dy1-O4	2.294(7)	Dy2-O3	2.338(6)	Si-O5	1.633(7)
Dy1-O4	2.295(7)	Dy2-O5	2.339(6)	Si-O2	1.640(6)
Dy1-O1	2.296(6)	Dy2-O1	2.379(6)		
Dy1-O2	2.302(6)	Dy2-O2	2.384(5)		
		Dy2-O2	2.601(7)		

Table S4. Crystal parameters refined from the room temperature single crystal X-ray diffraction data collected on a crystal piece isolated from the Dy_2SiO_5 crystal fragment annealed in air, at 950 °C, for 30 days.

Chemical composition	Dy_2SiO_5
Origin	annealed crystal fragment
Crystal system	Monoclinic
Space group	*I*2/*a* (No. 15)
a (Å)	10.4617(3)
b (Å)	6.7484(2)
c (Å)	12.5382(3)
β (°)	102.748(3)
V (Å^3)	863.37(4)
Z	8
Radiation, wavelength	Mo Kα, λ = 0.71073 Å
Temperature (K)	298
Linear absorption coefficient (mm^{-1})	25.902
No. of reflections measured (excl. systematic absences)	9051
No. of reflections used in refinement	1113
No. of parameters refined	49
R1	0.0342
wR2	0.0656
Goodness of fit (GOF)	1.0130

Atomic site	Wyckoff position	*x* (Å)	*y* (Å)	*z* (Å)	U_{iso}/U_{eq} (Å^2)
Dy1	8*f*	0.19259(3)	0.37579(5)	0.35828(3)	0.00991(14)
Dy2	8*f*	0.57236(3)	0.25451(5)	0.53703(3)	0.00936(14)
Si	8*f*	0.3729(2)	0.5896(3)	0.18066(16)	0.0087(4)
O1	8*f*	0.3793(5)	0.4057(8)	0.4818(4)	0.0105(11)
O2	8*f*	0.3003(5)	0.7862(8)	0.1178(4)	0.0098(11)
O3	8*f*	0.4692(5)	0.6444(8)	0.2957(4)	0.0115(11)
O4	8*f*	0.4463(5)	0.4983(8)	0.0903(4)	0.0133(11)
O5	8*f*	0.2613(6)	0.4340(8)	0.1998(5)	0.0134(11)

Table S5. Anisotropic displacement parameters obtained for the Dy and Si sites from the room temperature single crystal X-ray diffraction data collected on a crystal piece isolated from the Dy_2SiO_5 crystal fragment annealed in air, at 950 °C, for 30 days.

Atomic site	U_{11} (Å^2)	U_{22} (Å^2)	U_{33} (Å^2)	U_{12} (Å^2)	U_{13} (Å^2)	U_{23} (Å^2)
Dy1	0.0092(2)	0.0114(2)	0.0090(2)	-0.00033(13)	0.00181(14)	-0.00152(13)
Dy2	0.0088(2)	0.0100(2)	0.0094(2)	-0.00060(12)	0.00220(14)	-0.00090(12)
Si	0.0086(10)	0.0099(9)	0.0075(9)	0.0003(7)	0.0017(8)	-0.0007(7)

Table S6. Characteristics of the polyhedra formed around the Dy and Si, obtained from the room temperature single crystal X-ray diffraction data collected on a crystal piece isolated from the as-grown Dy_2SiO_5 crystal boule. Data were obtained from VESTA software.

	$Dy1O_6$	$Dy2O_7$	SiO_4
Average bond length (Å)	2.2847	2.3705	1.6254
Polyhedral volume (Å^3)	14.7837	18.9915	2.1905
Distortion index (bond length)	0.00974	0.02891	0.00536
Quadratic elongation	1.0500	-	1.0041
Bond angle variance (deg.^{2})	176.6457	-	17.0882
Effective coordination number	5.9570	6.5037	3.9932
Bond valence sum	3.074	2.934	3.986

$Dy1O_6$		$Dy2O_7$		SiO_4	
Bond	Bond length (Å)	Bond	Bond length (Å)	Bond	Bond length (Å)
Dy1-O1	2.218(5)	Dy2-O1	2.232(6)	Si-O3	1.610(5)
Dy1-O5	2.291(7)	Dy2-O4	2.332(6)	Si-O4	1.624(7)
Dy1-O3	2.299(5)	Dy2-O3	2.336(6)	Si-O5	1.627(7)
Dy1-O5	2.300(6)	Dy2-O4	2.342(6)	Si-O2	1.641(6)
Dy1-O2	2.300(6)	Dy2-O1	2.371(6)		
Dy1-O1	2.301(6)	Dy2-O2	2.386(5)		
		Dy2-O2	2.594(6)		

2. Crystal data for Ho_2SiO_5

Table S7. Crystal parameters refined from the room temperature single crystal X-ray diffraction data collected on a crystal piece isolated from the as-grown Ho_2SiO_5 crystal boule.

Chemical composition	Ho_2SiO_5
Origin	as-grown crystal fragment
Crystal system	Monoclinic
Space group	*I*2/*a* (No. 15)
a (Å)	10.4156(2)
b (Å)	6.7273(1)
c (Å)	12.5019(3)
β (°)	102.630(2)
V (Å^3)	854.80(3)
Z	8
Radiation, wavelength	Mo Kα, $\lambda = 0.71073$ Å
Temperature (K)	298
Linear absorption coefficient (mm^{-1})	27.706
No. of reflections measured (excl. systematic absences)	10695
No. of reflections used in refinement	1129
No. of parameters refined	49
R1	0.0294
wR2	0.0648
Goodness of fit (GOF)	1.0116

Atomic site	Wyckoff position	*x* (Å)	*y* (Å)	*z* (Å)	U_{iso}/U_{eq} (Å^2)
Ho1	8*f*	0.19327(3)	0.62397(4)	0.35845(2)	0.00947(13)
Ho2	8*f*	0.57198(3)	0.74517(4)	0.53708(2)	0.00907(13)
Si	8*f*	0.37353(18)	0.4098(3)	0.18132(15)	0.0085(4)
O1	8*f*	0.3792(5)	0.5956(7)	0.4817(4)	0.0106(9)
O2	8*f*	0.2994(5)	0.2135(7)	0.1181(4)	0.0098(9)
O3	8*f*	0.4710(5)	0.3551(7)	0.2962(4)	0.0103(9)
O4	8*f*	0.4472(5)	0.4999(7)	0.0900(4)	0.0134(10)
O5	8*f*	0.2616(5)	0.5669(8)	0.2004(4)	0.0130(10)

Table S8. Anisotropic displacement parameters obtained for the Ho and Si sites from the room temperature single crystal X-ray diffraction data collected on a crystal piece isolated from the as-grown Ho_2SiO_5 crystal boule.

Atomic site	U_{11} (Å^2)	U_{22} (Å^2)	U_{33} (Å^2)	U_{12} (Å^2)	U_{13} (Å^2)	U_{23} (Å^2)
Ho1	0.00913(18)	0.01037(19)	0.00891(19)	0.00041(10)	0.00195(12)	0.00127(10)
Ho2	0.00905(18)	0.00903(19)	0.00921(19)	0.00049(10)	0.00216(13)	0.00079(10)
Si	0.0091(8)	0.0089(8)	0.0075(9)	-0.0011(6)	0.0017(7)	-0.0002(6)

Table S9. Characteristics of the polyhedra formed around the Ho and Si, obtained from the room temperature single crystal X-ray diffraction data collected on a crystal piece isolated from the as-grown Ho_2SiO_5 crystal boule. Data were obtained from VESTA software.

	$Ho1O_6$	$Ho2O_7$	SiO_4
Average bond length (Å)	2.2714	2.3617	1.6268
Polyhedral volume ($Å^3$)	14.5290	18.7935	2.1950
Distortion index (bond length)	0.00994	0.03090	0.00560
Quadratic elongation	1.0498	-	1.0044
Bond angle variance ($deg.^2$)	175.6121	-	18.2862
Effective coordination number	5.9537	6.4507	3.9927
Bond valence sum	3.078	2.910	3.972

$Ho1O_6$		$Ho2O_7$		SiO_4	
Bond	Bond length (Å)	Bond	Bond length (Å)	Bond	Bond length (Å)
Ho1-O1	2.204(5)	Ho2-O1	2.217(5)	Si-O3	1.610(5)
Ho1-O5	2.274(6)	Ho2-O4	2.316(5)	Si-O4	1.626(6)
Ho1-O3	2.280(5)	Ho2-O3	2.325(6)	Si-O5	1.629(6)
Ho1-O2	2.288(5)	Ho2-O4	2.333(6)	Si-O2	1.643(6)
Ho1-O5	2.289(6)	Ho2-O1	2.371(5)		
Ho1-O1	2.293(6)	Ho2-O2	2.373(5)		
		Ho2-O2	2.596(6)		

3. Crystal data for Er_2SiO_5

Table S10. Crystal parameters refined from the room temperature single crystal X-ray diffraction data collected on a crystal piece isolated from the as-grown Er_2SiO_5 crystal boule.

Chemical composition	Er_2SiO_5
Origin	as-grown crystal fragment
Crystal system	Monoclinic
Space group	*I*2/*a* (No. 15)
a (Å)	10.3690(3)
b (Å)	6.7028(2)
c (Å)	12.4640(3)
β (°)	102.533(3)
V (Å^3)	845.62(4)
Z	8
Radiation, wavelength	Mo Kα, $\lambda = 0.71073$ Å
Temperature (K)	298
Linear absorption coefficient (mm^{-1})	29.709
No. of reflections measured (excl. systematic absences)	8808
No. of reflections used in refinement	1092
No. of parameters refined	49
R1	0.0392
wR2	0.0790
Goodness of fit (GOF)	1.0149

Atomic site	Wyckoff position	*x* (Å)	*y* (Å)	*z* (Å)	U_{iso}/U_{eq} (Å^2)
Er1	8*f*	0.80609(4)	0.62370(6)	0.64137(3)	0.01011(16)
Er2	8*f*	0.42845(4)	0.74490(6)	0.46292(3)	0.00969(16)
Si	8*f*	0.6258(2)	0.4092(4)	0.8185(2)	0.0099(5)
O1	8*f*	0.6206(6)	0.5961(10)	0.5180(5)	0.0112(13)
O2	8*f*	0.5274(6)	0.3549(9)	0.7030(5)	0.0082(12)
O3	8*f*	0.7018(6)	0.2148(10)	0.8819(5)	0.0102(13)
O4	8*f*	0.5516(6)	0.4977(10)	0.9107(5)	0.0124(13)
O5	8*f*	0.7377(6)	0.5685(10)	0.7992(5)	0.0132(13)

Table S11. Anisotropic displacement parameters obtained for the Er and Si sites from the room temperature single crystal X-ray diffraction data collected on a crystal piece isolated from the as-grown Er_2SiO_5 crystal boule.

Atomic site	U_{11} (Å^2)	U_{22} (Å^2)	U_{33} (Å^2)	U_{12} (Å^2)	U_{13} (Å^2)	U_{23} (Å^2)
Er1	0.0094(2)	0.0115(3)	0.0093(2)	-0.00032(15)	0.00177(16)	-0.00115(15)
Er2	0.0091(2)	0.0101(3)	0.0099(2)	-0.00048(14)	0.00220(16)	-0.00091(14)
Si	0.0083(11)	0.0128(13)	0.0081(11)	0.0007(9)	0.0008(9)	-0.0005(9)

Table S12. Characteristics of the polyhedra formed around the Er and Si, obtained from the room temperature single crystal X-ray diffraction data collected on a crystal piece isolated from the as-grown Er_2SiO_5 crystal boule. Data were obtained using VESTA software.

	$Er1O_6$	$Er2O_7$	SiO_4
Average bond length (Å)	2.2596	2.3491	1.6275
Polyhedral volume ($Å^3$)	14.2959	18.5039	2.1962
Distortion index (bond length)	0.00965	0.03284	0.00386
Quadratic elongation	1.0502	-	1.0049
Bond angle variance ($deg.^2$)	176.9839	-	20.1620
Effective coordination number	5.9541	6.3967	3.9969
Bond valence sum	3.067	2.917	3.963

$Er1O_6$		$Er2O_7$		SiO_4	
Bond	Bond length (Å)	Bond	Bond length (Å)	Bond	Bond length (Å)
Er1-O1	2.194(6)	Er2-O1	2.200(7)	Si-O2	1.615(7)
Er1-O2	2.261(6)	Er2-O4	2.292(7)	Si-O4	1.627(8)
Er1-O5	2.262(7)	Er2-O2	2.312(7)	Si-O5	1.633(8)
Er1-O5	2.271(7)	Er2-O4	2.322(7)	Si-O3	1.635(7)
Er1-O1	2.283(7)	Er2-O3	2.357(6)		
Er1-O3	2.287(7)	Er2-O1	2.365(7)		
		Er2-O3	2.596(7)		