Electronic Supplementary Information

Phase equilibria in the CeO_2–La_2O_3–Gd_2O_3 system at 1250 and 1500 °C

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Table S1. Phase composition and lattice parameters of the phases in the La_2O_3–Gd_2O_3 system, annealed at 1600 °C for 10 h in air (according to XRD)

Chemical composition (mol %)		Phase composition	Lattice parameters of the phases (nm)						
			<A>*			<B>			
La_2O_3	Gd_2O_3		*a*	*c*	*c/a*	*a*	*b*	*c*	*β*
100	0	<A>*	0.6523	0.3855	0,5909	–	–	–	–
95	5	<A>*	0.6517	0.3837	0.5887	–	–	–	–
90	10	<A>*	0.6496	0.3817	0.5876	–	–	–	–
85	15	<A>*	0.6491	0.3809	0.5868	–	–	–	–
80	20	<A>*	0.6478	0.3797	0.5861	–	–	–	–
75	25	<A>*	0.6468	0.3750	0.5798	–	–	–	–
65	35	<A>*	0.6458	0.3737	0.5787	–	–	–	–
60	40	<A>*+<B>	0.6447	0.3716	0.5764	1.4726	0.3632	0.9068	88.96
55	45	<A>*+<B>	0.6449	0.3710	0.5753	1.4721	0.3641	0.9052	92.46
50	50	<A>*+<B>	0.6446	0.3712	0.5758	1.4695	0.3634	0.9011	92.41
45	55	<A>*+<B>	0.6448	0.3718	0.5766	1.4671	0.3621	0.9000	92.47
40	60	<A>*+<B>	–	–	–	1.4597	0.3611	0.8968	92.55
35	65	<A>*+<B>	–	–	–	1.4573	0.3597	0.8952	92.40
30	70	<B>	–	–	–	1.4579	0.3577	0.8925	92.05
25	75	<B>	–	–	–	1.4540	0.3579	0.8914	92.50
20	80	<B>	–	–	–	1.4514	0.3573	0.8882	92.53

15	85	<B>	–	–	–	1.4543	0.3563	0.8800	92.64
10	90	<B>	–	–	–	1.4446	0.3557	0.8905	92.28
5	95	<B>	–	–	–	1.4394	0.3549	0.8800	92.73
0	100	<B>	–	–	–	1.4341	0.3566	0.8773	93.25

At given conditions (at 1600°C for 10 h in air) the hexagonal modification of A-La_2O_3 unquenchable and hexagonal modification of $La(OH)_3$ was observed instead. Designation of phases: <A*>, solid solutions based on hexagonal modification of La_2O_3; <B>, solid solutions based on monoclinic modification of Gd_2O_3

Table S2. Phase composition and lattice parameters of the phases in the La_2O_3–Gd_2O_3 system, annealed at 1500 °C for 225 h in air (according to XRD)

Chemical composition (mol %)		Phase composition	Lattice parameters of the phases (nm)						
La_2O_3	Gd_2O_3		<A>*			<B>			
			a	*c*	*c/a*	*a*	*b*	*c*	*β*
100	0	<A>*	0.6523	0.3855	0.5909	–	–	–	–
95	5	<A>*	0.6494	0.3818	0.5879	–	–	–	–
90	10	<A>*	0.6491	0.3818	0.5882	–	–	–	–
85	15	<A>*	0.6481	0.3841	0.5926	–	–	–	–
80	20	<A>*	0.6479	0.3797	0.5860	–	–	–	–
75	25	<A>*	0.6468	0.3781	0.5846	–	–	–	–
70	30	<A>*	0.6470	0.3777	0.5838	–	–	–	–
65	35	<A>* +<B>	0.6461	0.3747	0.5799	–	–	–	–
60	40	<A>* +<B>	0.6464	0.3749	0.5799	1.3635	0.3562	0.8896	90.36
55	45	<A>* +<B>	0.6460	0.3736	0.5783	1.4283	0.3556	0.8865	87.19
50	50	<A>* +<B>	0.6458	0.3746	0.5800	1.4221	0.3542	0.8856	87.85
45	55	<A>* +<B>	0.6467	0.3746	0.5792	1.4198	0.3523	0.8826	87.55
40	60	<A>* +<B>	0.6471	0.3749	0.5794	1.44642	0.3656	0.8752	91.44
35	65	<B>	–	–	–	1.4588	0.3643	0.8973	91.44
30	70	<B>	–	–	–	1.4567	0.3635	0.8954	91.51
25	75	<B>	–	–	–	1.4540	0.3621	0.8926	91.22

20	80	<B>	–	–	–	1.4492	0.3610	0.8907	91.61
10	90	<B>	–	–	–	1.3907	0.3591	0.8818	87.38
0	100	<B>	–	–	–	1.4335	0.3566	0.8813	91.85

* At given conditions (at 1600°C for 10 h in air) the hexagonal modification of A-La_2O_3 unquenchable and hexagonal modification of $La(OH)_3$ was observed instead. Designation of phases: <A*>, solid solutions based on hexagonal modification of La_2O_3; <B>, solid solutions based on monoclinic modification of Gd_2O_3;

Table S3. Phase composition and lattice parameters of the phases in the La_2O_3–Gd_2O_3 system, annealed at 1100 °C for 9820 h in air (according to XRD)

Chemical composition (mol %)		Phase composition	Lattice parameters of the phases (nm)						
La_2O_3	Gd_2O_3		<A>*			<B>			
			a	*c*	*c/a*	*a*	*b*	*c*	*β*
100	0	<A>*	0.6523	0.3855	0.5909	–	–	–	–
95	5	<A>*	0.6497	0.3835	0.5903	–	–	–	–
90	10	<A>*	0.6492	0.3825	0.5892	–	–	–	–
85	15	<A>*	0.6489	0.3815	0.5879	–	–	–	–
80	20	<A>* + <B>	0.6494	0.3797	0.5854	–	–	–	–
75	25	<A>* + <B>	0.6497	0.3788	0.5837	1.4331	0.5119	0.8581	115.57
70	30	<A>* + <B>	0.6477	0.3781	0.5838	1.6157	0.6423	0.8653	126.97
65	35	<A>* + <B>	0.6488	0.3808	0.5884	1.6675	0.6784	0.8644	129.37
60	40	<B>	–	–	–	1.4704	0.3548	0.9137	88.96
55	45	<B>	–	–	–	1.4672	0.3627	0.9076	90.58
45	55	<B>	–	–	–	–	–	–	–
40	60	<B>	–	–	–	1.4052	0.3651	0.8946	87.18
35	65	<B>	–	–	–	1.4077	0.3644	0.8944	87.49
30	70	<B>	–	–	–	1.3986	0.3627	0.8892	87.66
25	75	<B>	–	–	–	1.3981	0.3619	0.8870	87.72
20	80	<B> + <C>	–	–	–	1.3940	0.3606	0.8844	87.45
15	85	<B> + <C>	–	–	–	1.3919	0.3598	0.8827	87.48
10	90	<B> + <C>	–	–	–	1.3907	0.3591	0.8818	87.38

5	95	<B> + <C> *a* = 1.0816	–	–	–	1.4340	0.3430	0.8926	88.82
0	100	<C> *a* = 1.0777	–	–	–	–	–	–	–

At given conditions (at 1600°C for 10 h in air) the hexagonal modification of A-La_2O_3 unquenchable and hexagonal modification of $La(OH)_3$ was observed instead. Designation of phases: <A*>, solid solutions based on hexagonal modification of La_2O_3; <B>, solid solutions based on monoclinic modification of Gd_2O_3 <C>, solid solutions based on cubic modification of Gd_2O_3

Table S4 Phase composition and lattice parameters of CeO_2–La_2O_3–Gd_2O_3 samples annealed at 1500 °C for 130 h (according to XRD and scanning electron microscopy)

Chemical composition, mol%			Phase composition and lattice parameters of the phases a (nm) by XRD data	Lattice parameter of phases, nm	
CeO_2	La_2O_3	Gd_2O_3		<C>	<F>
1	2	3	4	5	6
Section CeO_2 – (50 mol % La_2O_3 – 50 mol % Gd_2O_3)					
5	47.5	47.5	<F>+<B>+<A*> (*a* = 0.6395, *c* = 0.3744)	–	0.5516
10	45	45	<F>+<B>+<A*> (*a* = 0.6444, *c* = 0.3708)	–	0.5515
15	42.5	42.5	<F>+<B>+<A*> (*a* = 0.6437, *c* = 0.3699)	–	0.5514
20	40	40	<F>+<B>+<A*> (*a* = 0.6419, *c* = 0.3710)	–	0.5509
25	37.5	37.5	<F>+<B>+<A*>	–	0.5516
30	35	35	<F>+<B>+<A*>	–	0.5516
35	32.5	32.5	<F>+<B>	–	0.5512
40	30	30	<F>+<B>+<C>	1.1020	0.5510
45	27.5	27.5	<F>+<B>+<C>	1.1019	0.5509
50	25	25	<F>+<B>+<C>	1.1021	0.5510
55	22.5	22.5	<F>+<C>	1.0998	0.5508
60	20	20	<F>+<C>	1.0992	0.5504
65	17.5	17.5	<F>	–	0.5493
70	15	15	<F>	–	0.5483
75	12.5	12.5	<F>	–	0.5477
80	10	10	<F>	–	0.5466
85	7.5	7.5	<F>	–	0.5451
90	5	5	<F>	–	0.5439
95	2.5	2.5	<F>	–	0.5425
100	0	0	<F>	–	0.5409
Section La_2O_3 – (50 mol % CeO_2– mol % Gd_2O_3)					
50	0	50	<F> + <C>	1.0836	0.5418
47.5	5	47.5	<F> + <C>	1.0868	0.5434
45	10	45	<F> + <C>	1.0888	0.5446
42.5	15	42.5	<F> + <C>	1.0930	0.5465

40	20	40	<F> + <C> + <B>	1.0960	0.5478
35	30	35	<F> + <C> + <B>	1.0959	0.5479

Table 4 Continued

1	2	3	4	5	6
32.5	35	32.5	<F> + <B>	–	0.5502
30	40	30	<F> + <B> + <A*>	–	0.5526
			(*a* = 0.6432, *c* = 0.3769)		
27.5	45	27.5	<F> + <B> + <A*>	–	0.5526
			(*a* = 0.6438, *c* = 0.3768)		
25	50	25	<F>+<B>+<A*>	–	0.5531
			(*a* = 0.6469, *c* = 0.3759)		
22.5	55	22.5	<F>+<B>+<A*>	–	0.5528
			(*a* = 0.6473, *c* = 0.3784)		
20	60	20	<F>+<B>+<A*>	–	0.5525
			(*a* = 0.6499, *c* = 0.3775)		
17.5	65	17.5	<F>+<A*>	–	0.5546
			(*a* = 0.6493, *c* = 0.3775)		
12.5	75	12.5	<F>+<A*>	–	0.5556
			(*a* = 0.6493, *c* = 0.3775)		
10	80	10	<F>+<A*>	–	0.5571
			(*a* = 0.6524, *c* = 0.3810)		
7.5	85	7.5	<F>+<A*>	–	0.5579
			(*a* = 0.6524, *c* = 0.3810)		
5	90	5	<A*>	–	–
			(*a* = 0.6534, *c* = 0.3820)		
2.5	95	2.5	<A*>	–	–
			(*a* = 0.6536, *c* = 0.3822)		
			Iso-concentration line 15 mol % CeO_2		
15	10	75	<C>+<B>	1.0865	–
15	15	70	<C>+<B>	1.0891	–
15	20	65	<F>+<C>+<B>	1.0915	0.5482
15	25	60	<F>+<C>+<B>	1.0918	0.5480
15	30	55	<F>+<C>+<B>	1.0912	0.5481
15	35	50	<F>+<B>	–	0.5488
15	40	45	<F>+<A*>+<B>	–	0.5494
15	45	40	<F>+<A*>+<B>	–	0.5498
15	50	35	<F>+<A*>+<B>	–	0.5493
15	55	30	<F>+<A*>+<B>	–	0.5498
			(*a* = 0.6524, *c* = 0.3810)		
15	60	25	<F>+<A*>+<B>	–	0.5500
			(*a* = 0.6456, *c* = 0.3773)		
15	65	20	<F>+<A*>+<B>	–	0.5496
			(*a* = 0.6477, *c* = 0.3781)		

15	70	15	<A*>+<F> (*a* = 0.6477, *c* = 0.3802)	–	0.5505

Table 4 Continued

1	2	3	4	5	6
15	75	10	<A*>+<F> (*a* = 0.6506, *c* = 0.3799)	–	0.5510
15	80	5	<A*>+<F> (*a* = 0.6525, *c* = 0.3799)	–	0.5516
			Iso-concentration line 45 mol % CeO_2		
45	5	50	<F> + <C>	1.0868	0.5434
45	10	45	<F> + <C>	1.0902	0.5451
45	15	40	<F> + <C>	1.0938	0.5469
45	25	30	<F>+<C>+<B>	1.1159	0.5499
45	30	25	<F>+<C>+<B>	1.1057	0.5494
45	35	20	<F>+<B>+<A*>	–	0.5532
45	40	15	<F>+<B>+<A*>	–	0.5535
45	45	10	<F> + <A*>	–	0.5563

At given conditions (at 1500°C for 130 h in air) the hexagonal modification of A-La_2O_3 unquenchable and hexagonal modification of $La(OH)_3$ was observed instead. Designation of phases: <A>, solid solutions based on hexagonal modification of La_2O_3; <F>, solid solutions based on cubic modification with fluorite-type structure of CeO_2; <C>, solid solutions based on cubic modification of Gd_2O_3; <B>, solid solutions based on monoclinic modification of Gd_2O_3

Table S5 – Phase composition and lattice parameters of CeO_2–La_2O_3–Gd_2O_3 samples annealed at 1250 °C for 6200 h (according to XRD)

Chemical composition, mol%			Phase composition and lattice parameters of the phases a (nm) by XRD data	Lattice parameter of phases, nm	
CeO_2	La_2O_3	Gd_2O_3		<C>	<F>
1	2	3	4	5	6
			Section CeO_2–(50 mol % La_2O_3–50 mol % Gd_2O_3)		
5	47.5	47.5	<F>+<A>+<B>	–	0.5545
10	45	45	<F>+<B>	–	0.5542
15	42.5	42.5	<F>+<B>+<C>	1.1071	0.5534
20	40	40	<F>+<B>+<C>	1.1073	0.5536
25	37.5	37.5	<F>+<B>+<C>	1.1070	0.5538
30	35	35	<F>+<B>+<C>	1.1066	0.5533

35	32.5	32.5	<F>+<B>+<C>	1.1074	0.5537
40	30	30	<F>+<B>+<C>	1.1071	0.5536
45	27.5	27.5	<F>+<C>	1.1062	0.5531
50	25	25	<F>+<C>	1.1058	0.5527
55	22.5	22.5	<F>+<C>	1.1055	0.5516
60	20	20	<F>	–	0.5498
65	17.5	17.5	<F>	–	0.5493
70	15	15	<F>	–	0.5481
75	12.5	12.5	<F>	–	0.5470
80	10	10	<F>	–	0.5450
85	7.5	7.5	<F>	–	0.5446
90	5	5	<F>	–	0.5436
95	2.5	2.5	<F>	–	0.5419
100	0	0	<F>	–	0.5409
			Section La_2O_3–(50 mol % CeO_2–50 mol % Gd_2O_3)		
50	0	50	<F> + <C>	1.0865	0.5433
47.5	5	47.5	<F> + <C>	1.0869	0.5435
45	10	45	<F> + <C>	1.0898	0.5449
42.5	15	42.5	<F> + <C>	1.0936	0.5467
40	20	40	<F> + <C>	1.0999	0.5499
37.5	25	37.5	<F> + <C> + <B>	1.1039	0.5520

Table 5 Continued

1	2	3	4	5	6
35	30	35	<F> + <C> + <B>	1.1040	0.5515
32.5	35	32.5	<F> + <C> + <B>	1.1038	0.5522
30	40	30	<F> + <C> + <B>	1.1037	0.5518
27.5	45	27.5	<F> + <B>	–	0.5528
25	50	25	<F>+<B>+<A*>	–	0.5536
			(*a* = 0.6471, *c* = 0.3782)		
20	60	20	<F>+<B>+<A*>	–	0.5535
			(*a* = 0.6473, *c* = 0.3784)		
15	70	15	<F>+<B>+<A*>	–	0.5537
			(*a* = 0.6475, *c* = 0.3786)		
10	80	10	<F>+<B>+<A*>	–	0.5536
			(*a* = 0.6473, *c* = 0.3784)		
7.5	85	7.5	<F>+<A*>	–	0.5542
			(*a* = 0.6524, *c* = 0.3810)		
5	90	5	<A*>(*a* = 0.6534, *c* = 0.3820)	–	–

2.5	95	2.5	<A*> *a* = 0.6536, *c* = 0.3822)	–	–
			Iso-concentration line 15 mol % CeO_2		
15	0	85	<C>	1.0830	–
15	5	80	<C>	1.0838	–
15	10	75	< C > + < B >	1.0850	–
15	15	70	< C > + < B >	1.0872	–
15	20	65	< F >+< C > + < B >	1.0891	0.5520
15	25	60	< F >+< C > + < B >	1.0892	0.5522
15	30	55	< F >+< C > + < B >	1.0899	0.5518
15	35	50	< F >+< C > + < B >	1.0910	0.5521
15	40	45	< F >+< C > + < B >	1.0898	0.5520
15	45	40	< F >+ < B >	–	0.5530
15	50	35	< F >+< B> + < A >	–	0.5535
			(*a* = 0.6477, *c* = 0.3781)		
15	60	25	< F >+< B> + < A >	–	0.5537
			(*a* = 0.6477, *c* = 0.3802)		
15	75	10	< F >+< B> + < A >	–	0.5534
			(*a* = 0.6479, *c* = 0.3800)		
15	80	5	< F > + < A >	–	0.5540
			(*a* = 0.6523, *c* = 0.3797)		

At given conditions (at 1250°C for 620 h in air) the hexagonal modification of A-La_2O_3 unquenchable and hexagonal modification of $La(OH)_3$ was observed instead. Designation of phases: <A>, solid solutions based on hexagonal modification of La_2O_3; <F>, solid solutions based on cubic modification with fluorite-type structure of CeO_2; <C>, solid solutions based on cubic modification of Gd_2O_3; <B>, solid solutions based on monoclinic modification of Gd_2O_3