

Introducing gradient Er ions and oxygen defects into SrCoO₃ for regulating structure, electrical and magnetic transport properties

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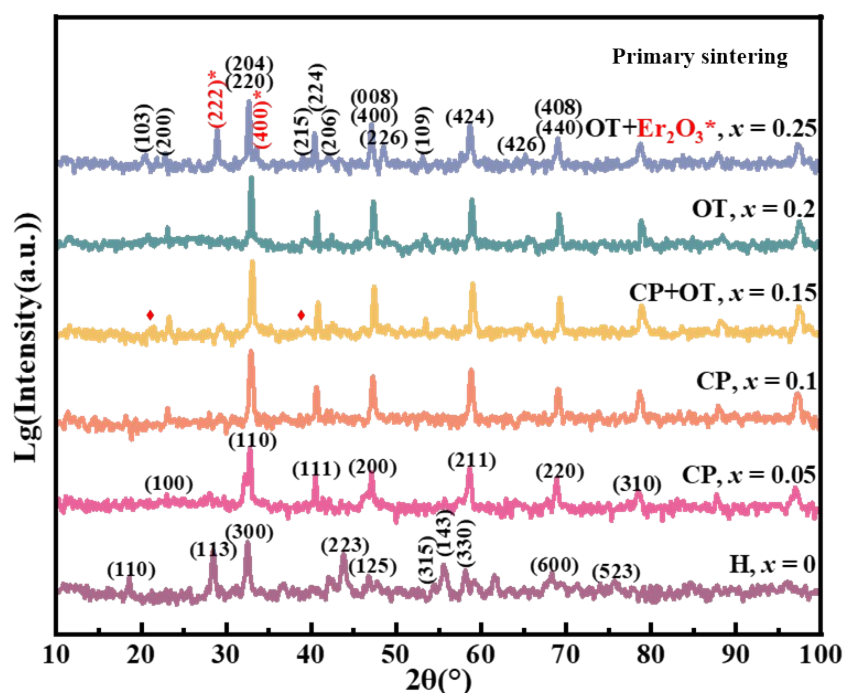


Fig.1. (a) XRD patterns of primary sintering Sr_{1-x}Er_xCoO_{3-δ} (x = 0~0.25) polycrystals.

Table 1. Phase structures, lattice constants, space groups and densities of Sr_{1-x}Er_xCoO_{3-δ} (x = 0~0.25) polycrystals.

Samples	Phase structure	Lattice constant		Space group	Density P /g·cm ⁻³
		a /Å	c /Å		
x = 0	H	9.5035	12.3966	R32	4.608
x = 0.05	CP	3.8508	—	Pm $\bar{3}$ m	4.793
x = 0.1	CP	3.8459	—	Pm $\bar{3}$ m	4.903
x = 0.15	CP+T	3.8382/7.6241	—/15.3711	Pm $\bar{3}$ m/+I4/mmm	4.887
x = 0.2	OT	7.6155	15.3501	I4/mmm	4.762
x = 0.25	OT	7.6246	15.3241	I4/mmm	5.002

Table 2. Atomic parameters following the conclusion of the Rietveld refinement in H, CP and OT.

Samples	Phase	Atoms	Site	x	y	z	Occ
$x = 0$ H		Sr ₁	9d	0.3206	0	0	1
		Sr ₂	9e	0.6447	0	0.5	1
		Co ₁	3b	0	0	0.5	1
		Co ₂	6c	0	0	0.095	1
		Co ₃	6c	0	0	0.299	1
		O ₁	9d	0.8466	0	0	1
		O ₂	18f	0.4959	0.6746	0.4789	1
		O ₃	18f	0.8419	-0.0229	0.6116	1
$x = 0.1$ CP		Sr	1a	0	0	0	0.9
		Co	1b	0.5	0.5	0.5	1
		O	3c	0.5	0.5	0	0.88
		Er	1a	0	0	0	0.1
0.2 OT		Er	4e	0	0	0.13608	0.833
		Sr ₁	4e	0	0	0.62844	1
		Sr ₂	8g	0	0.5	0.12942	1
		Co ₁	8h	0.24221	0.24221	0	1
		Co ₂	8f	0.25	0.25	0.25	1
		O ₁	16m	0.24068	0.24068	0.10956	1
		O ₂	8i	0.51830	0	0	0.232
		O ₃	8i	0.33085	0	0	0.148
		O ₄	8j	0.23815	0.5	0	1
	O ₅	16n	0	0.24904	0.25853	1	

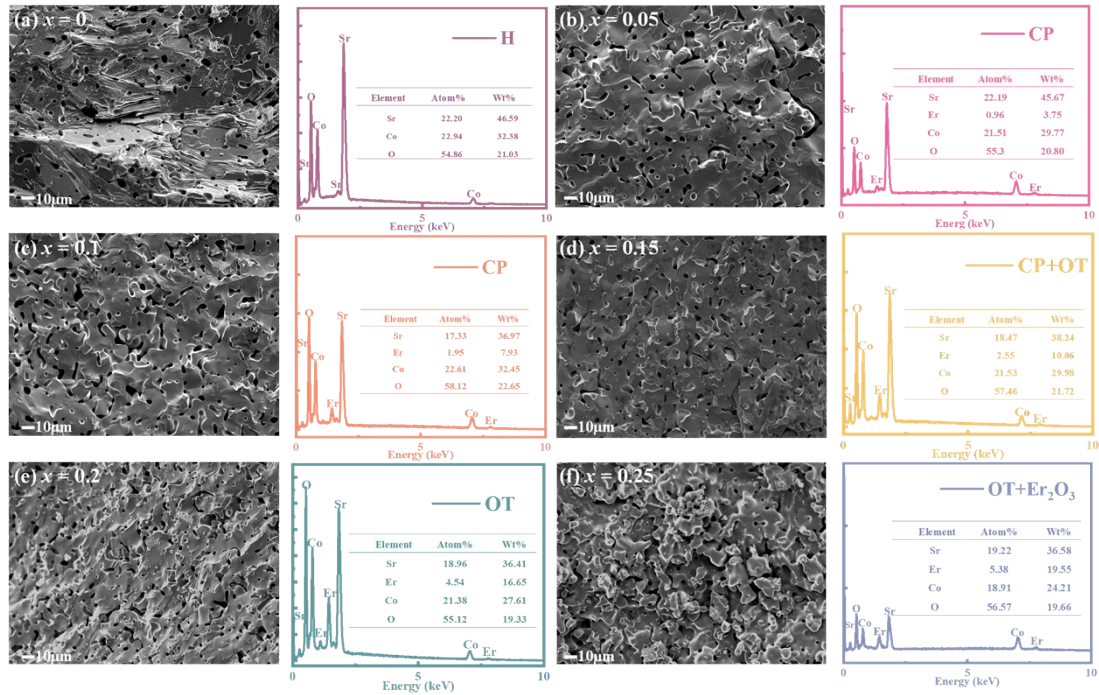


Figure 2. Cross-section micromorphology and EDS of $\text{Sr}_{1-x}\text{Er}_x\text{CoO}_{3-\delta}$ ($x = 0\sim 0.25$) polycrystals.

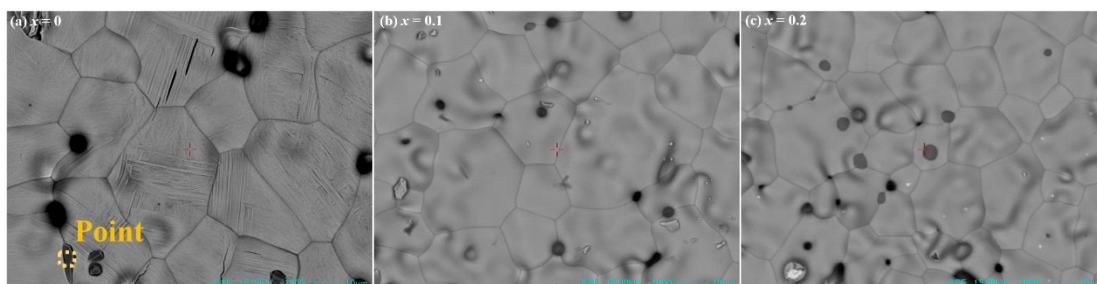


Figure 3. Surface micromorphology images of $\text{Sr}_{1-x}\text{Er}_x\text{CoO}_{3-\delta}$ ($x = 0, 0.15, 0.2$) polycrystals.

Table 3. Surface elements analysis of $\text{Sr}_{1-x}\text{Er}_x\text{CoO}_{3-\delta}$ ($x = 0, 0.15, 0.2$) polycrystals.

Samples	Elements	Line	Mass/%	Normalized Mass/%	Mol/%
$x = 0$ ($\text{Sr}_6\text{Co}_5\text{O}_{15}$)	O	K_a	20.899	20.9	55.151
	Co	K_a	28.710	28.709	20.568
	Sr	L_a	50.391	50.391	24.281
$x = 0.1$ ($\text{Sr}_{0.9}\text{Er}_{0.1}\text{CoO}_{2.689}$)	O	K_a	22.053	22.031	57.73
	Co	K_a	28.725	28.698	20.414
	Sr	L_a	41.768	41.728	19.965
$x = 0.2$ ($\text{Sr}_{0.8}\text{Er}_{0.2}\text{CoO}_{2.635}$)	Er	L_b	7.55	7.543	1.891
	O	K_a	20.606	20.614	56.598
	Co	K_a	28.984	28.996	21.612
$x = 0$ (Point, Co_3O_4)	Sr	L_a	35.831	35.845	17.97
	Er	L_b	14.538	14.544	3.82
	O	K_a	32.328	31.625	63.135
$x = 0$ (Point, Co_3O_4)	Co	K_a	68.787	67.292	36.47
	Sr	L_a	1.107	1.083	0.395

Table 4 ICP results of $\text{Sr}_{1-x}\text{Er}_x\text{CoO}_{3-\delta}$ ($x = 0, 0.1, 0.2$) polycrystals.

Sample	Sr	Er	Co	Sr	Er	Co
	(mg/L)	(mg/L)	(mg/L)	(mol/L)	(mol/L)	(mol/L)
$\text{SrCoO}_{2.626}$ (H)	1208	0	834	0.01415	0	0.01379
$\text{Sr}_{0.9}\text{Er}_{0.1}\text{CoO}_{2.689}$ (CP)	985	217	782	0.01124	0.00130	0.01327
$\text{Sr}_{0.8}\text{Er}_{0.2}\text{CoO}_{2.635}$ (OT)	852	413	747	0.00972	0.00250	0.01268

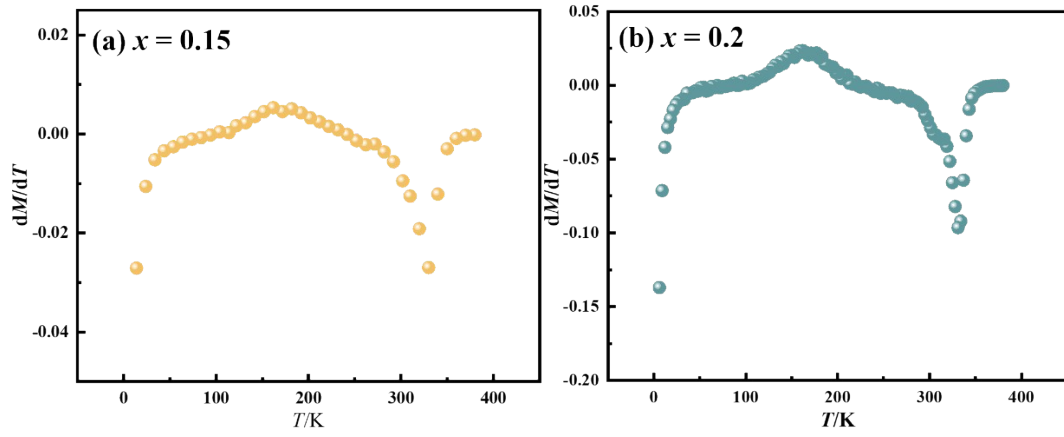


Figure 4. dM/dT curves of $Sr_{1-x}Er_xCoO_{3-\delta}$ ($x = 0.15, 0.2$) polycrystals.

Table 5. Effective and saturation magnetic moments of HS, IS, and LS in Co^{3+} and Co^{4+} ions.

Magnetic moments	Co^{3+}			Co^{4+}		
	LS	IS	HS	LS	IS	HS
μ_{eff} (μ_B)	0	2.83	4.90	1.73	3.87	5.92
μ_s (μ_B)	0	2	4	1	3	5