Supplementary Information

Kinetics and Mechanism of BaLaCuS3 Oxidation

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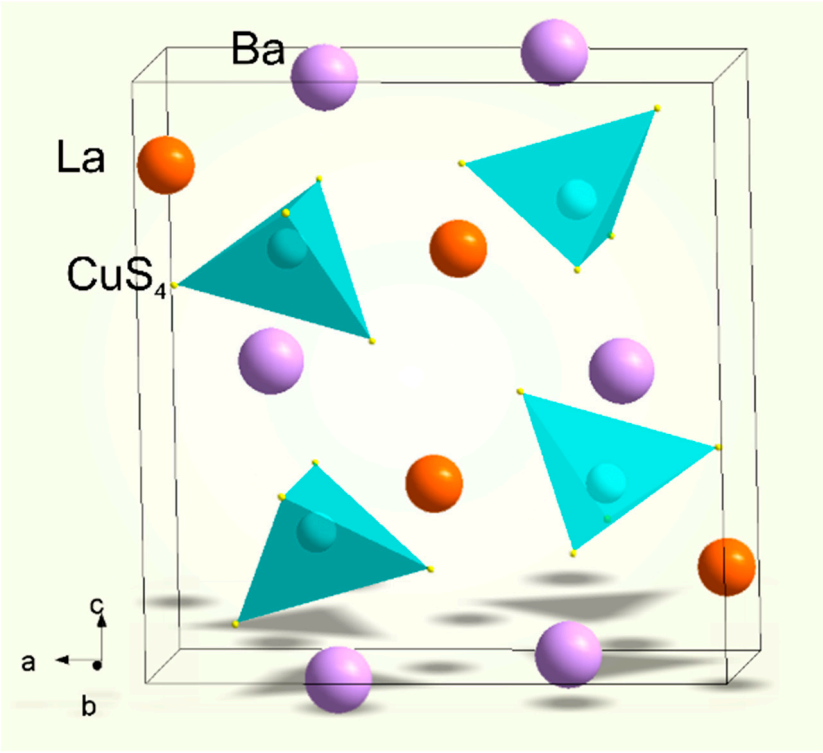
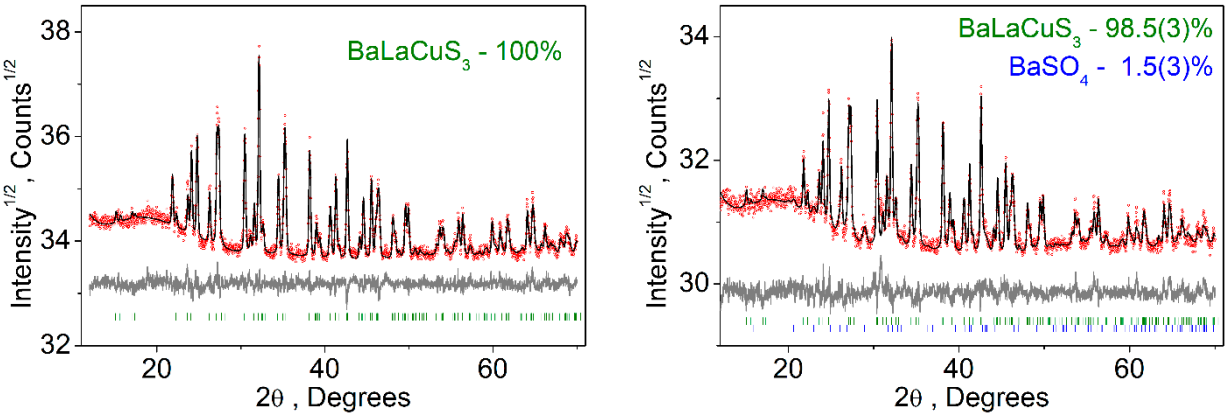
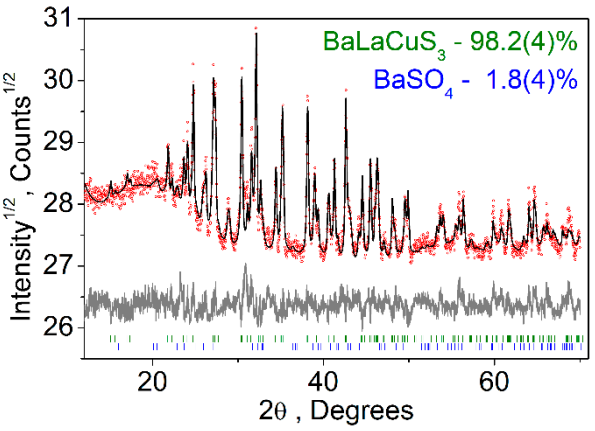


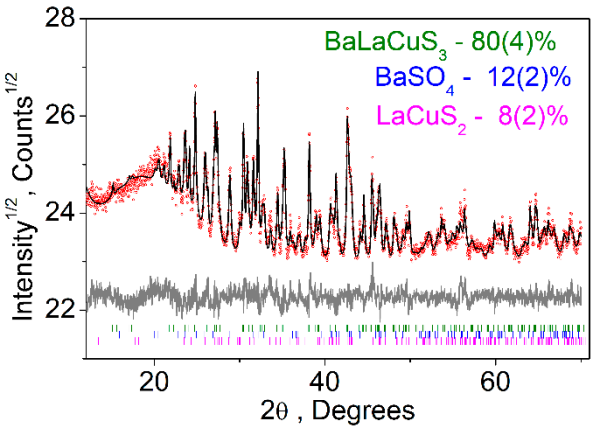
Figure S1. Crystal structure of $BaLaCuS_3$



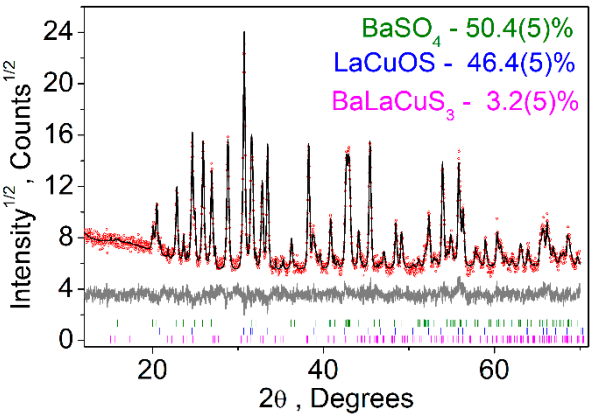
a) b)


BaLaCuS3 - 98.2(4)%
BaSO4 - 1.8(4)%
Intensity1/2, Counts1/2
2θ , Degrees

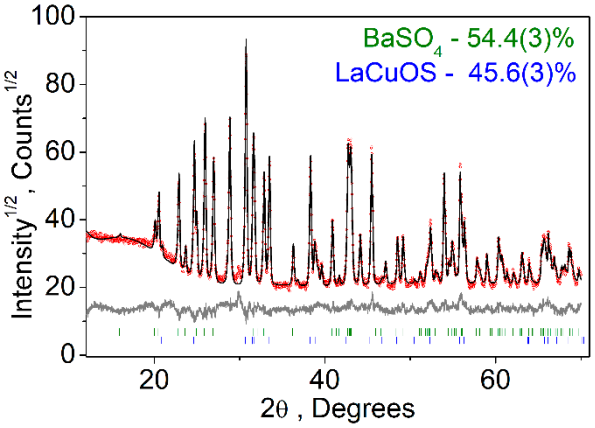
c)


BaLaCuS3 - 80(4)%
BaSO4 - 12(2)%
LaCuS2 - 8(2)%
Intensity1/2, Counts1/2
2θ , Degrees

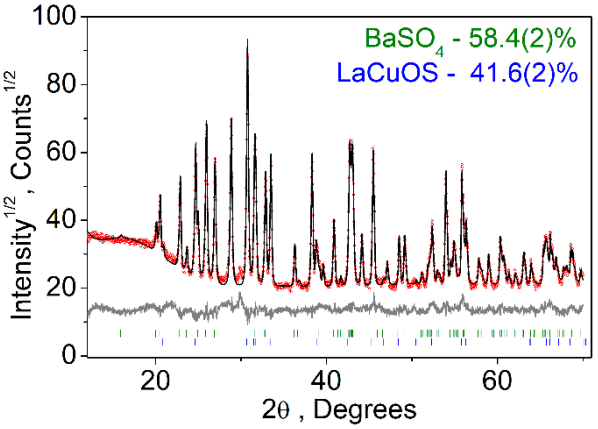
d)


BaSO4 - 50.4(5)%
LaCuOS - 46.4(5)%
BaLaCuS3 - 3.2(5)%
Intensity1/2, Counts1/2
2θ , Degrees

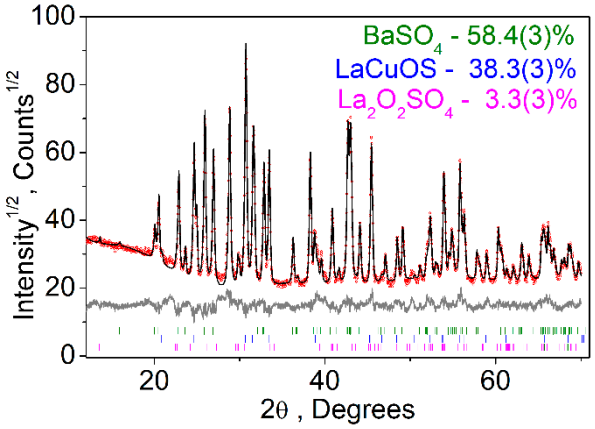
e)


BaSO4 - 54.4(3)%
LaCuOS - 45.6(3)%
Intensity1/2, Counts1/2
2θ , Degrees

f)


BaSO4 - 58.4(2)%
LaCuOS - 41.6(2)%
Intensity1/2, Counts1/2
2θ , Degrees

g)


BaSO4 - 58.4(3)%
LaCuOS - 38.3(3)%
La2O2SO4 - 3.3(3)%
Intensity1/2, Counts1/2
2θ , Degrees

h)

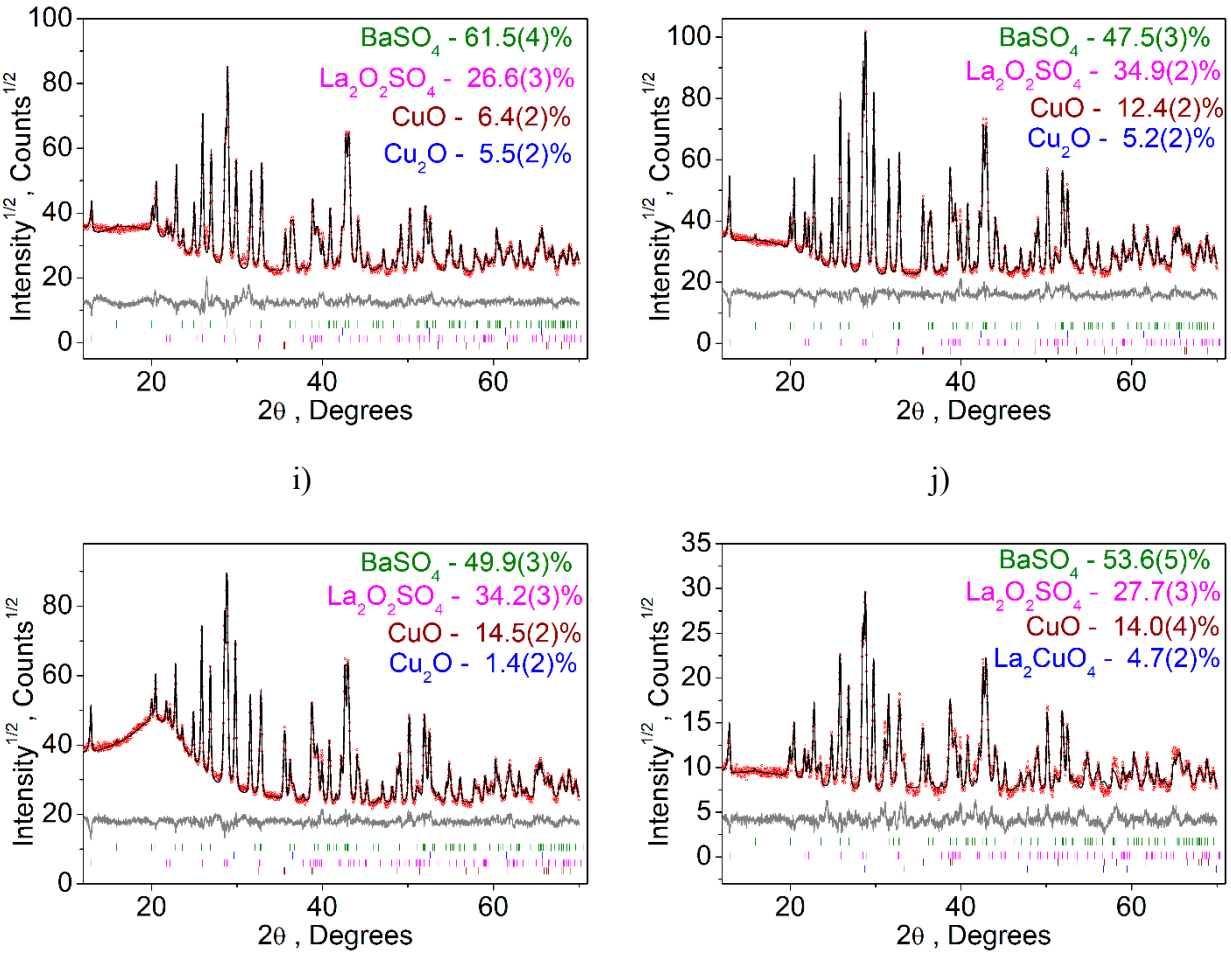
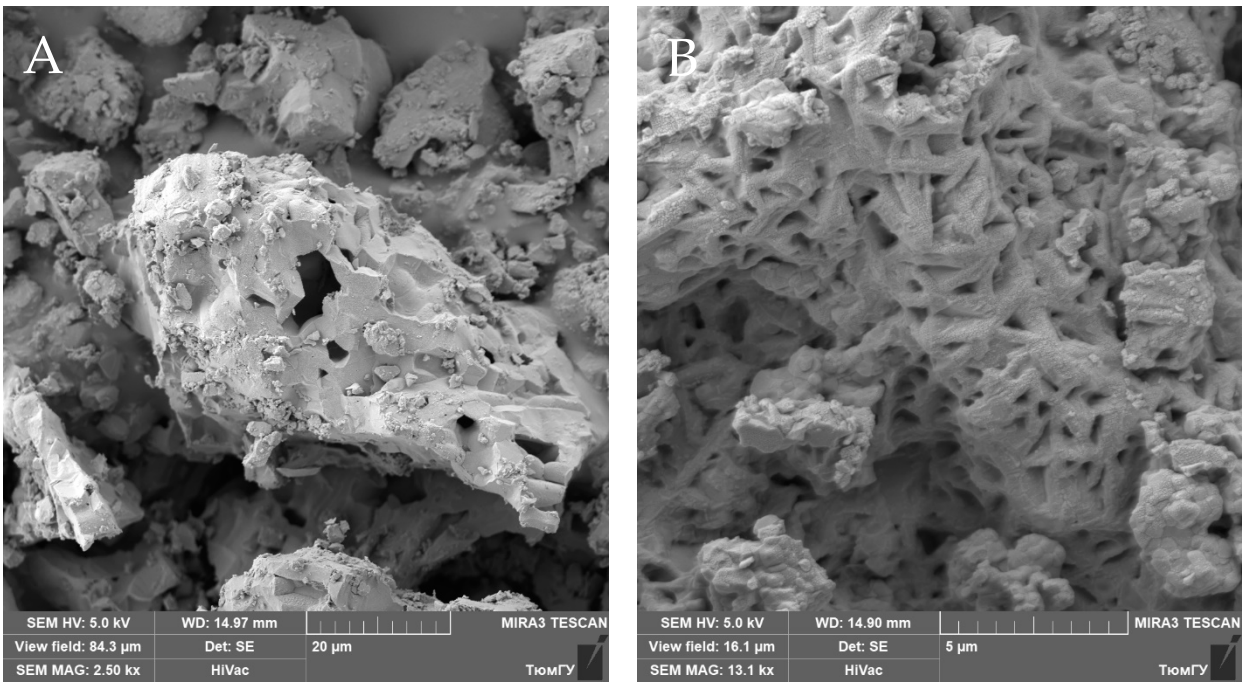


Figure S2. Difference Rietveld plot of $BaLaCuS_3$ at temperature: a) T = 380 ºC; b) T = 518 ºC; c) T = 560 ºC; d) T = 630 ºC; e) T = 760 ºC; f) T = 790 ºC; g) T = 872 ºC; h) T = 940 ºC; i) T = 1020 ºC; j) T = 1045 ºC; k) T = 1137 ºC; l) T = 1165 ºC.



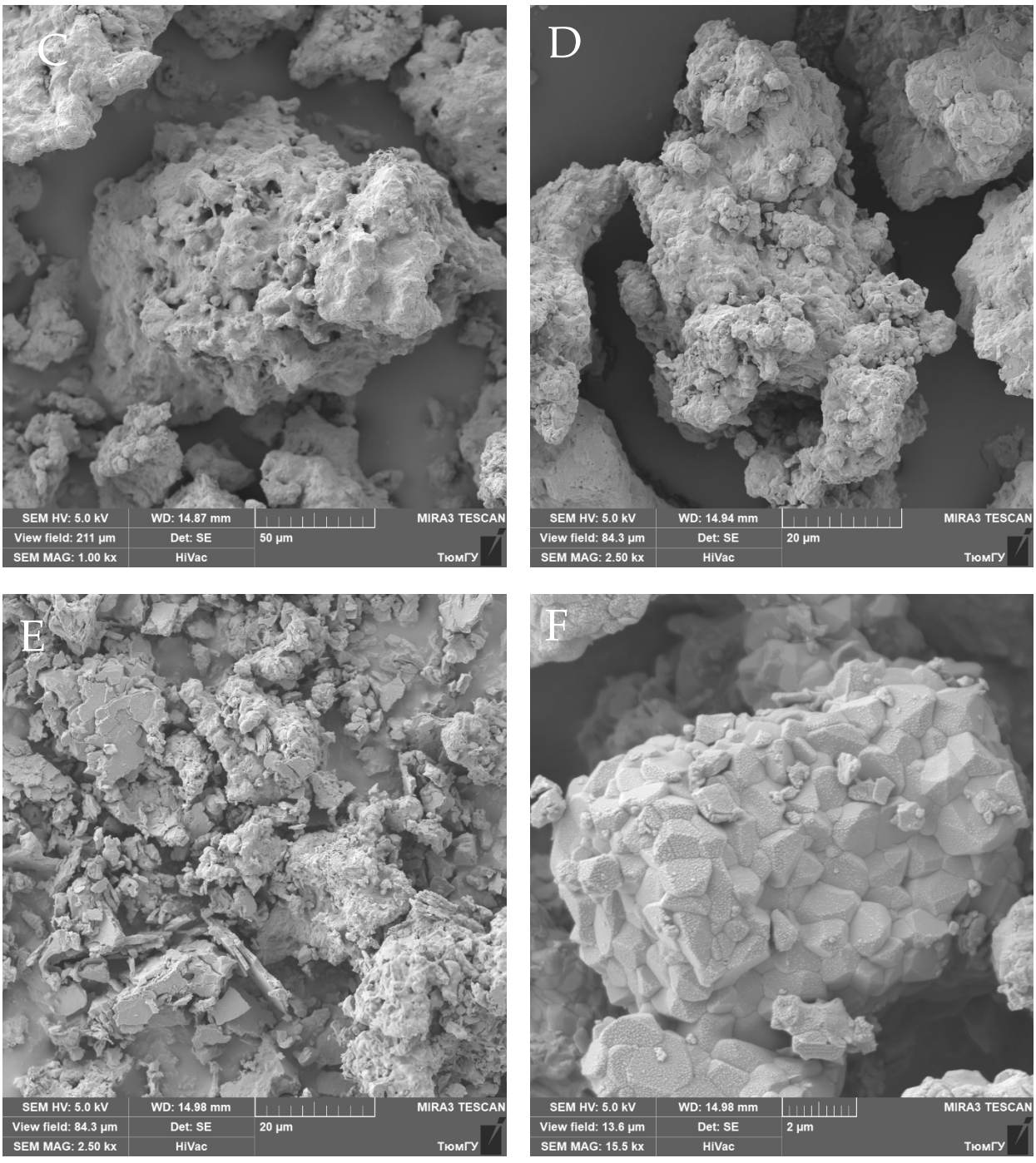


Figure S3. SEM patterns recorded for the intermediate products of the $BaLaCuS_3$ oxidation. A – first state at 380ºC, B – at 650 ºC, C – at 900 ºC, D – 1000 ºC, E – 1100 ºC, F – 1200 ºC.

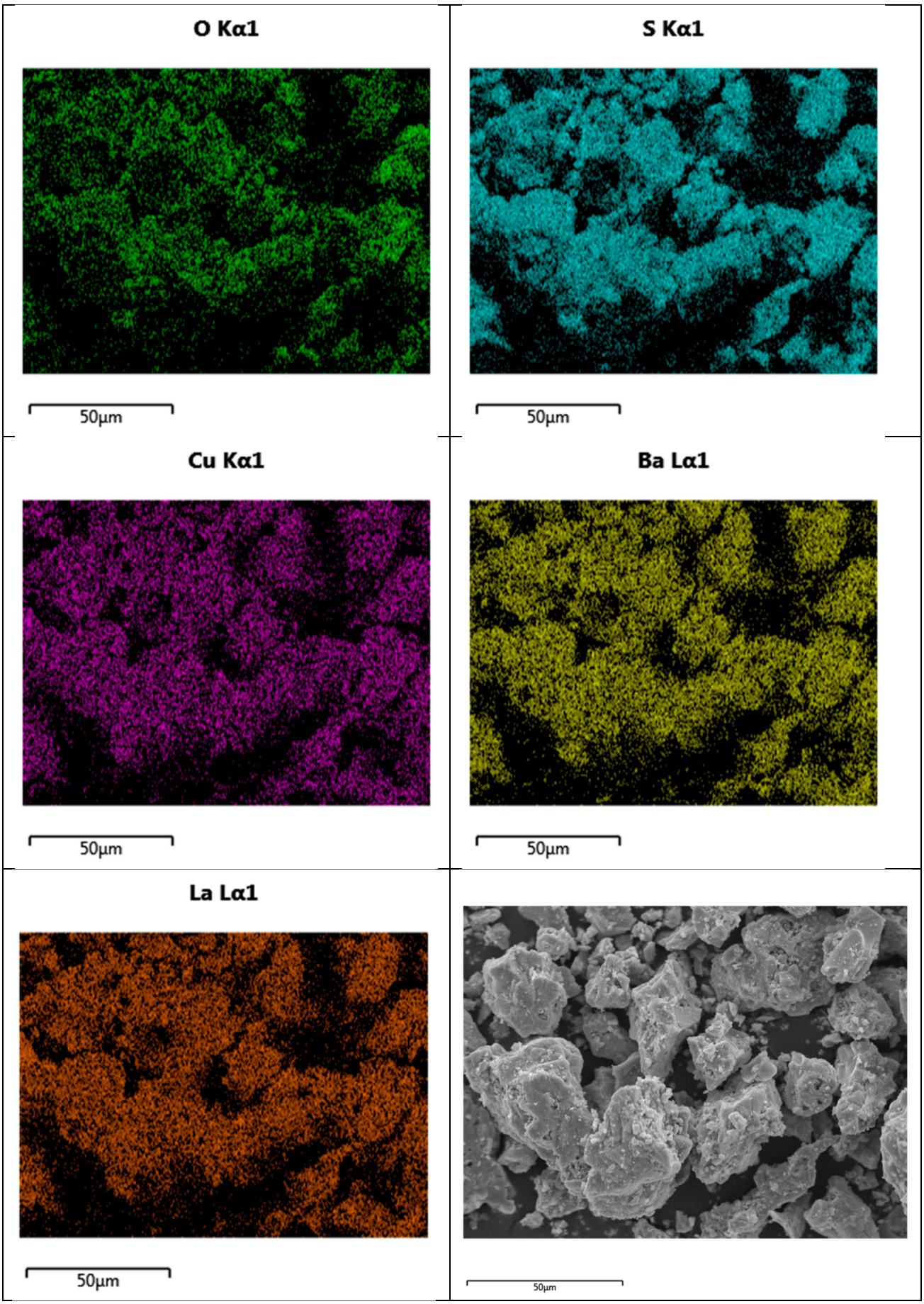


Figure S4. SEM and Energy dispersive X-ray (EDX) mapping analysis of $BaLaCuS_3$ oxidation at 380ºC

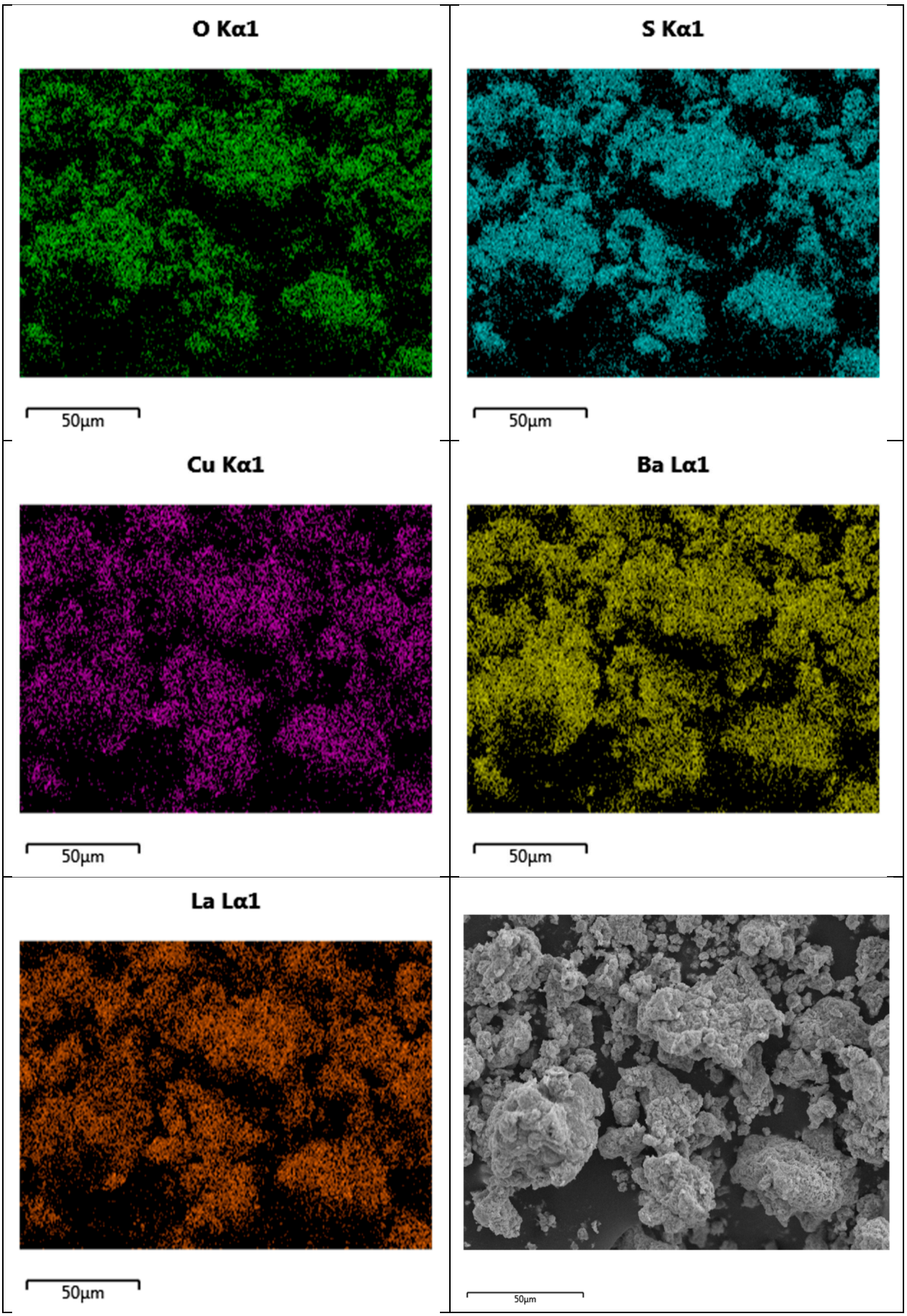


Figure S5. SEM and Energy dispersive X-ray (EDX) mapping analysis of $BaLaCuS_3$ oxidation at 650ºC

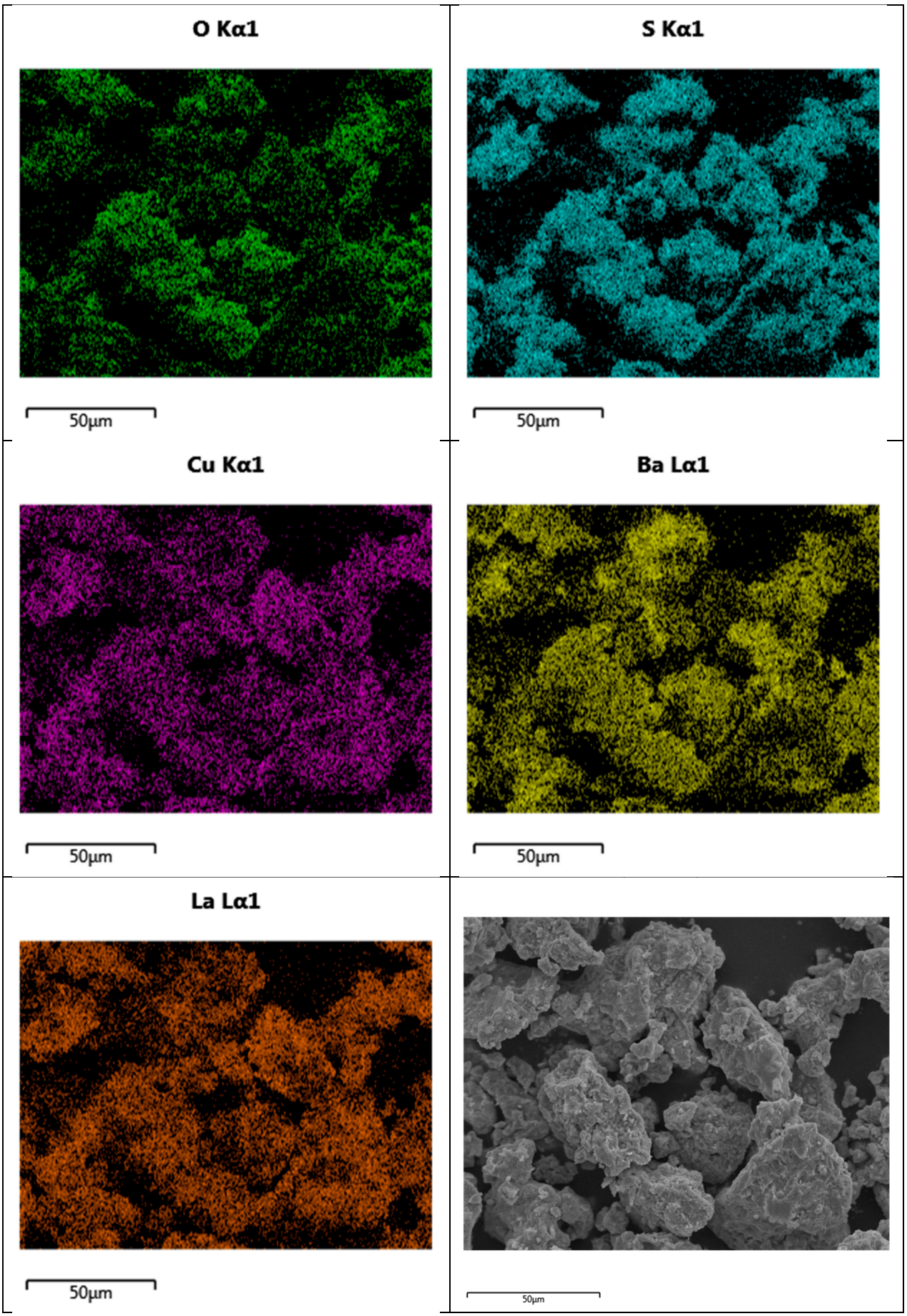


Figure S6. SEM and Energy dispersive X-ray (EDX) mapping analysis of $BaLaCuS_3$ oxidation at 900 °C

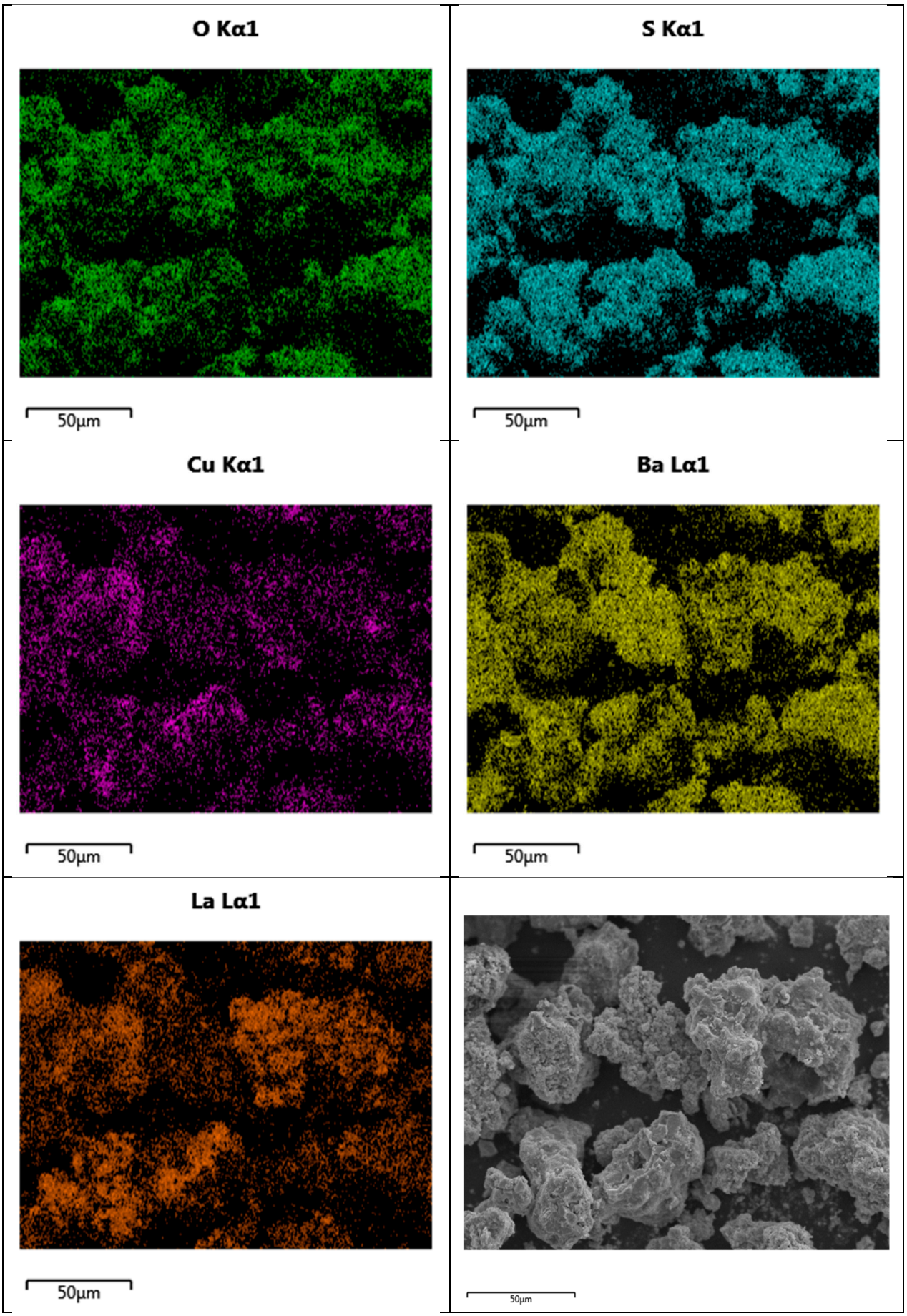


Figure S7. SEM and Energy dispersive X-ray (EDX) mapping analysis of $BaLaCuS_3$ oxidation at 1000 ºC

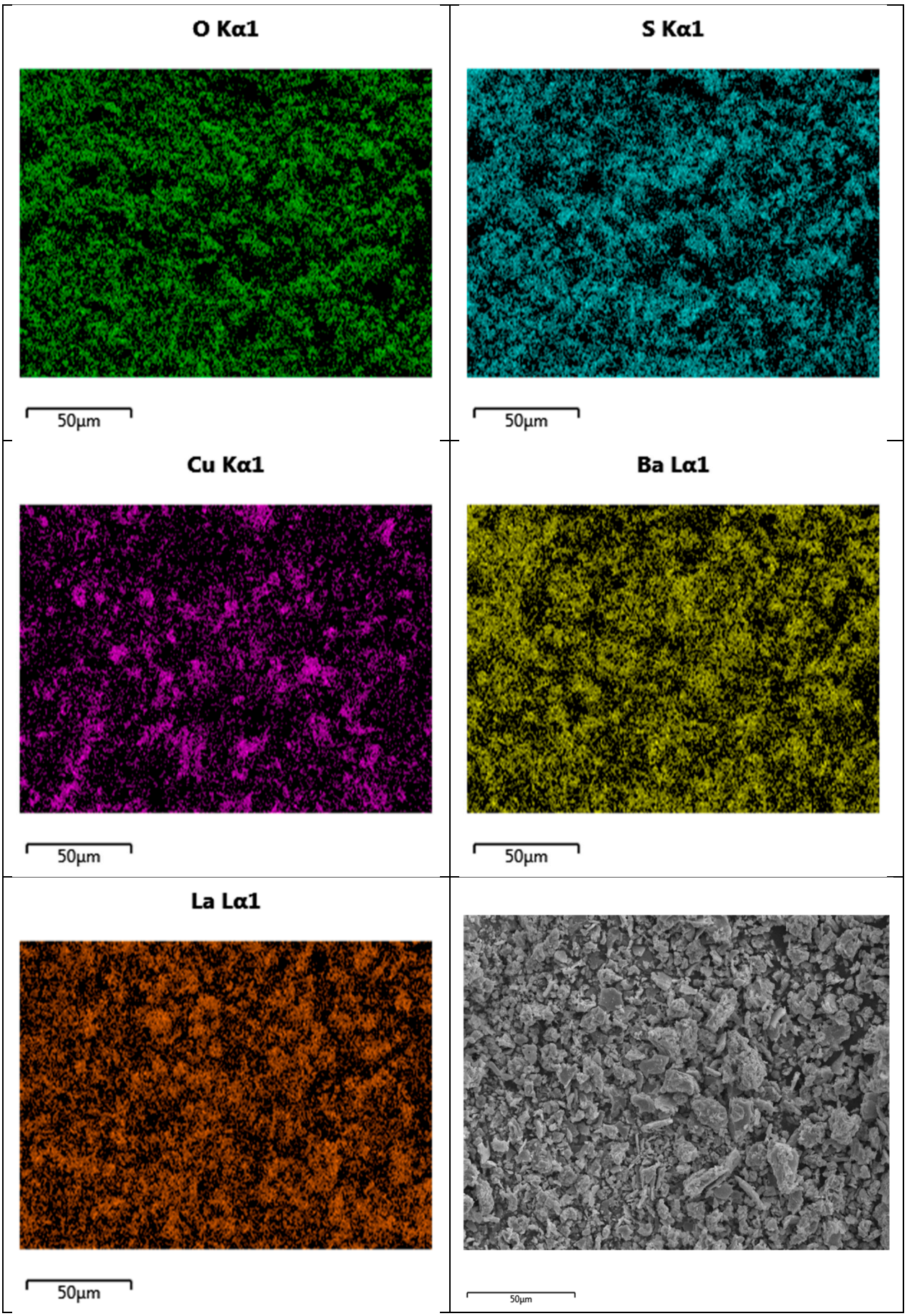


Figure S8. SEM and Energy dispersive X-ray (EDX) mapping analysis of $BaLaCuS_3$ oxidation at 1100 ºC

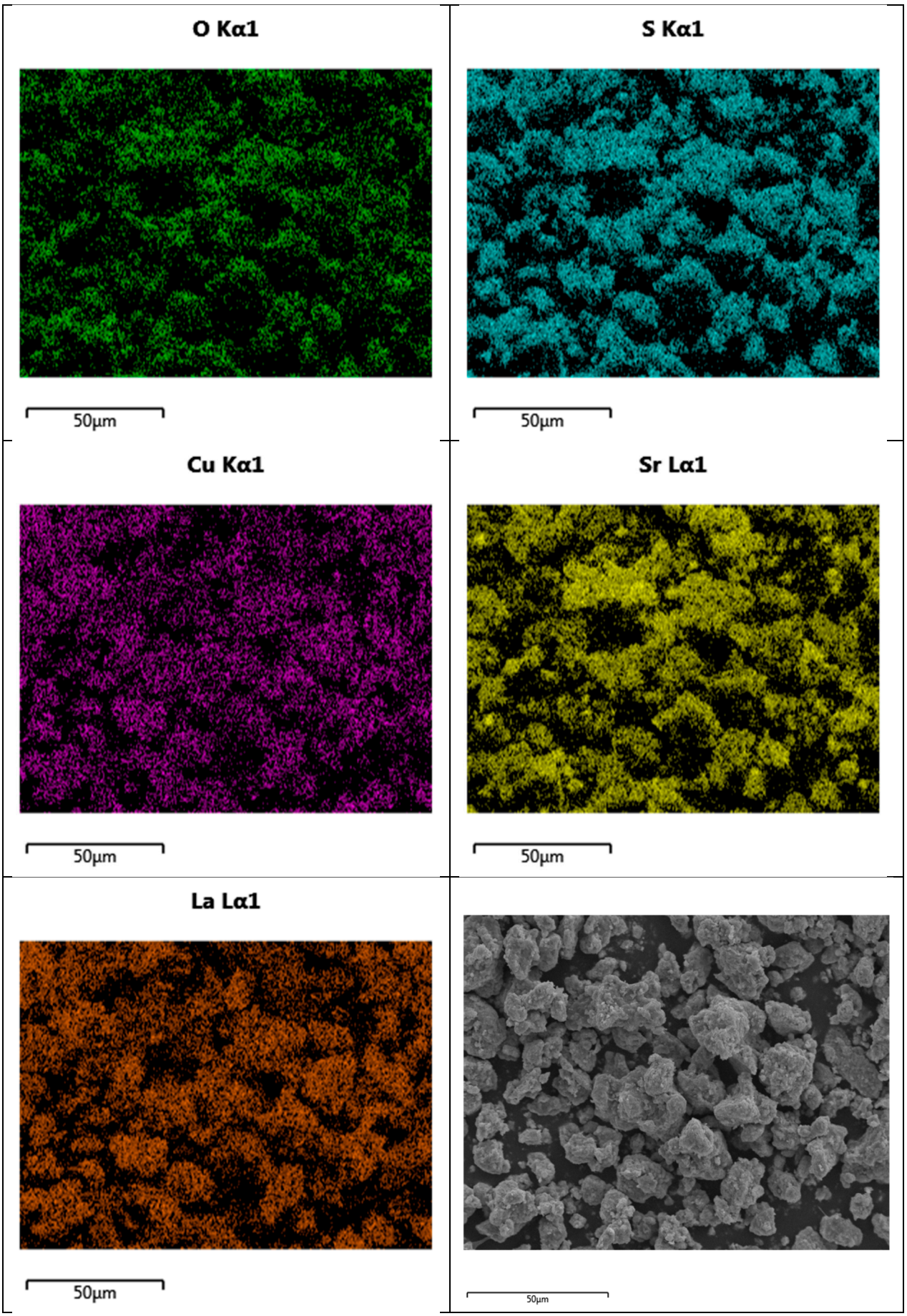


Figure S9. SEM and Energy dispersive X-ray (EDX) mapping analysis of $BaLaCuS_3$ oxidation at 1200 ºC

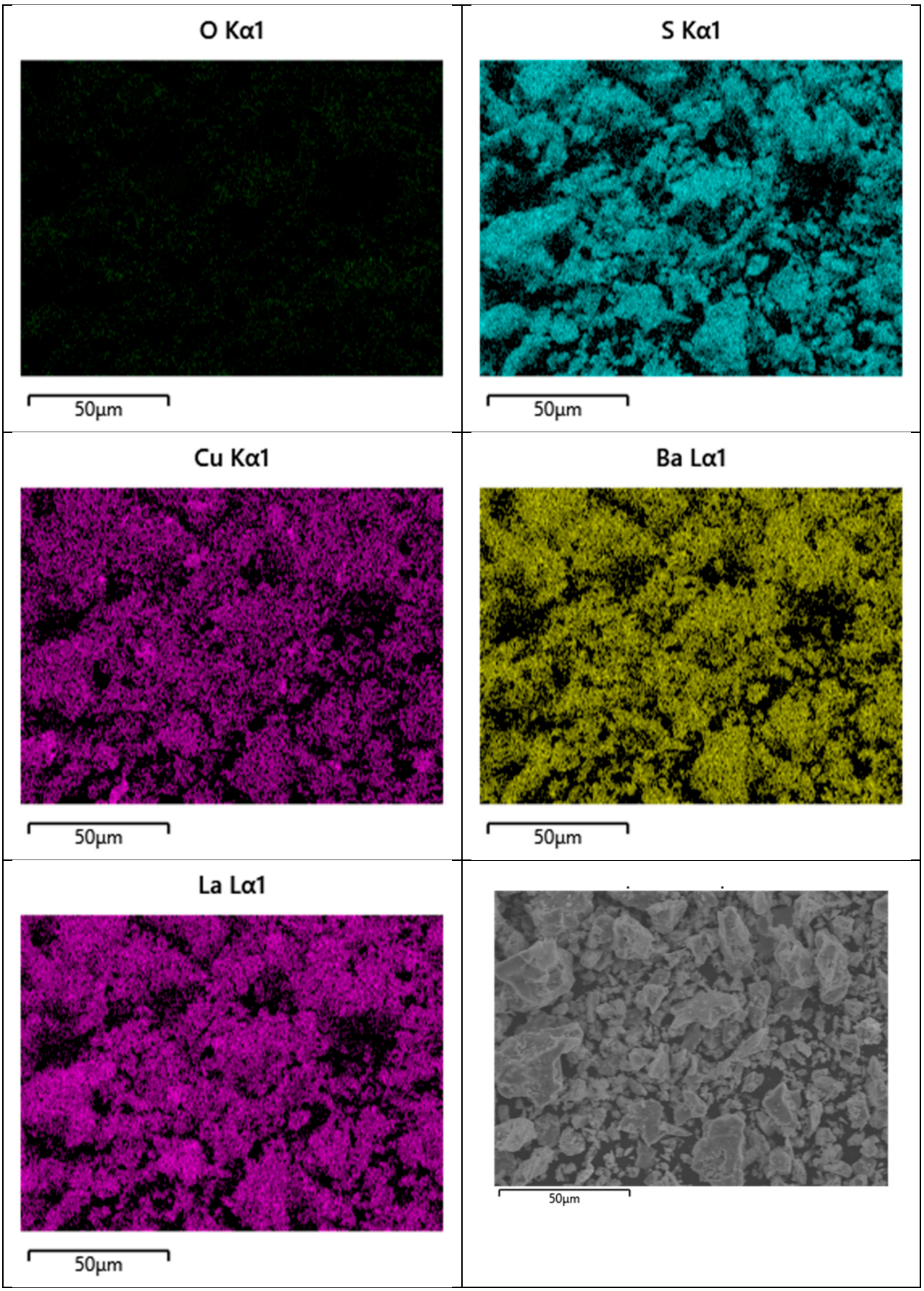


Figure S10. SEM and Energy dispersive X-ray (EDX) mapping analysis of $BaLaCuS_3$

Table S1. Fractional atomic coordinates and isotropic displacement parameters (Å^2) of $BaLaCuS_3$

Atom	*x*	*y*	*z*	B_{iso}	*Occ.*
La	-0.01065(4)	0.25	0.81895(4)	0.201(19)	1
Ba	0.31635(3)	0.25	0.00671(4)	0.201(19)	1
Cu	0.24522(9)	0.25	0.29110(8)	0.96(3)	1
S1	0.04955(14)	0.25	0.35169(14)	0.40(4)	1
S2	0.22578(14)	0.25	0.70312(14)	0.56(5)	1
S3	0.38852(15)	0.25	0.44404(14)	0.30(4)	1

Table S2. Main bond lengths (Å) of $BaLaCuS_3$

La—S1^{i}	2.9530(11)	La—S2	3.0076(16)
La—S2^{ii}	3.0019(16)	La—S3^{iii}	2.9310(11)
La—S3^{ii}	3.0078(17)	Ba—S1^{iv}	3.1844(12)
Ba—S1^{v}	3.1247(16)	Ba—S2^{iv}	3.1713(12)
Ba—S3^{iv}	3.2342(13)	Cu—S1	2.3314(18)
Cu—S2^{iv}	2.38524(85)	Cu—S3	2.4220(19)

Symmetry codes: (i) -x, y+1/2, -z+1; (ii) x+1/2, -y+1/2, -z+3/2; (iii) -x+1/2, -y, z+1/2; (iv) -x+1/2, -y, z+1/2; (v) x+1/2, -y+1/2, -z+1/2;

Table S3. Main parameters of processing and refinement of the $BaLaCuS_3$ samples after heating to specified temperature and cooling

T, C	Phase	Weight, %	R_{wp}, R_p (%)
380	$BaLaCuS_3$	100	0.52, 0.40
518	$BaLaCuS_3$	98.5(3)	0.65, 0.49
	$BaSO_4$	1.5(3)	
560	$BaLaCuS_3$	98.2(4)	0.98, 0.76
	$BaSO_4$	1.8(4)	
630	$BaLaCuS_3$	80(4)	1.18, 0.91

	$BaSO_4$	12(2)	
	$LaCuS_2$	8(2)	
	$BaLaCuS_3$	50.4(5)	
760	$BaSO_4$	46.4(5)	9.17, 7.24
	$BaLaCuS_3$	3.2(5)	
790	$BaSO_4$	54.4(3)	8.36, 6.60
	LaCuOS	45.6(3)	
872	$BaSO_4$	58.4(2)	7.06, 5.47
	LaCuOS	41.6(2)	
	$BaSO_4$	58.4(3)	
940	LaCuOS	38.3(3)	7.45, 5.77
	$La_2O_2SO_4$	3.3(3)	
	$BaSO_4$	61.5(4)	
1020	$La_2O_2SO_4$	26.6(3)	6.98, 5.16
	CuO	6.4(2)	
	Cu_2O	5.5(2)	
	$BaSO_4$	47.5(3)	
1045	$La_2O_2SO_4$	34.9(2)	6.80, 5.27
	CuO	12.4(2)	
	Cu_2O	5.2(2)	
	$BaSO_4$	49.9(3)	
1137	$La_2O_2SO_4$	34.2(3)	5.33, 4.05
	CuO	14.5(2)	
	Cu_2O	1.4(2)	
	$BaSO_4$	53.6(5)	
1165	$La_2O_2SO_4$	27.7(3)	10.48, 7.84
	CuO	14.0(4)	
	La_2CuO_4	4.7(2)	