

Investigation of Carbothermic Reduction of Ilmenite Concentrate with Calcium Carbonate Addition Using the Rietveld Method

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Table S1. The Rietveld results of roasted products at different temperatures (lattice parameters).

	Temperature / °C				
	1000	1200	1300	1400	1500
R_{wp} / %	11.90	11.16	10.98	11.47	10.53
R_p / %	8.69	7.78	7.72	8.02	8.85
R_{exp} / %	6.93	6.89	6.52	7.06	6.60
χ^2 / %	1.72	1.59	1.68	1.62	1.60
Lattice parameters / nm					
Calcium titanate					
a	0.5440 (2)*	0.5439 (2)	0.5435 (1)	0.5439 (1)	0.5426 (1)
b	0.7640 (3)	0.7642 (3)	0.7633 (1)	0.7640 (2)	0.7618 (1)
c	0.5380 (2)	0.5382 (2)	0.5374 (1)	0.5377 (1)	0.5362 (1)
Iron					
a	0.2867 (1)	0.2866 (1)	0.2864 (1)	0.2867 (1)	0.2859 (1)
b	-	-	-	-	-
c	-	-	-	-	-
Ferropseudobrookite					
a	0.9765 (3)	0.9727 (4)	0.9802 (3)	0.9786 (1)	0.9761 (2)
b	1.0039 (2)	1.0001 (3)	0.9958 (3)	0.9979 (3)	0.9948 (1)
c	0.3767 (2)	0.3749 (2)	0.3773 (1)	0.3779 (1)	0.3772 (1)

*: the standard deviation.

Table S2. The Rietveld results of roasted products with different amounts of calcium carbonate (lattice parameters).

	CaCO₃ / %						
	0	20	30	40	50	60	70
$R_{wp} / \%$	11.43	10.77	10.33	12.81	12.53	11.92	11.93
$R_p / \%$	9.75	8.74	8.07	10.02	9.15	8.95	9.23
$R_{exp} / \%$	6.18	6.06	6.23	6.86	7.36	7.28	7.44
$\chi^2 / \%$	1.85	1.78	1.66	1.87	1.70	1.64	1.60
Lattice parameters / nm							
Calcium titanate							
<i>a</i>	-	0.5427 (3)	0.5419 (1)	0.5419 (1)	0.5426 (1)	0.5435 (1)	0.5439 (1)
<i>b</i>	-	0.7618 (2)	0.7608 (1)	0.7608 (1)	0.7618 (1)	0.7632 (2)	0.7638 (2)
<i>c</i>	-	0.5364 (3)	0.5356 (3)	0.5356 (1)	0.5362 (1)	0.5372 (1)	0.5377 (1)
Iron							
<i>a</i>	0.2866 (1)*	0.2859 (1)	0.2855 (1)	0.2856 (1)	0.2859 (1)	0.2864 (1)	0.2866 (1)
<i>b</i>	-	-	-	-	-	-	-
<i>c</i>	-	-	-	-	-	-	-
Ferropseudobrookite							
<i>a</i>	0.9778 (3)	0.9792 (3)	0.9769 (1)	0.9767 (1)	0.9761 (2)	0.9807 (1)	0.9667 (1)
<i>b</i>	1.0061 (3)	1.0026 (3)	1.0017 (2)	0.993 (2)	0.9948 (1)	1.0000 (1)	1.0119 (2)
<i>c</i>	0.3758 (2)	0.3773 (1)	0.3767 (1)	0.3779 (1)	0.3772 (1)	0.3712 (1)	0.3744 (1)

*: the standard deviation.

```

PHASE= Calcium titanate //
SpacegroupNo=62 HermannMauguin=P2_1/n2_1/m2_1/a //
PARAM=A=0.5442_0.5170^0.5714          PARAM=B=0.7640_0.7258^0.8022
PARAM=C=0.5380_0.5111^0.5649 //
RP=4 PARAM=B1=0_0^0.007 PARAM=k2=0_0^0.001 GEWICHT=SPHAR8 //
E=CA+2 Wyckoff=c PARAM=x=0.5360 PARAM=z=0.5068 TDS=0.0061
E=TI+4 Wyckoff=b TDS=0.0039
E=O-2 Wyckoff=c x=0.9838 z=0.4286 TDS=0.0053
E=O-2 Wyckoff=d x=0.2888y=0.0371 z=0.7108 TDS=0.0050

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Figure S1. Structure model of calcium titanate (including atomic coordinates) during the Rietveld refinement.

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PHASE=Iron_alpha //
SpacegroupNo=229 //
PARAM=A=0.28665_0.2838^0.2895 //
PARAM=B1=0_0^0.01 PARAM=k1=0_0^1 PARAM=k2=0_0^0.0001 GEWICHT=SPHAR5//
GEWICHT=SPHAR6 GOAL:ironalpha=GEWICHT*ifthenelse(ifdef(d),exp(my*d*3/4),1)
E=FE Wyckoff=a

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Figure S2. Structure model of iron (including atomic coordinates) during the Rietveld refinement.

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PHASE= Ferropseudobrookite //
SpacegroupNo=63 HermannMauguin=C2/c2/m2_1m Setting=2 Lattice=Orthorhombic //
PARAM=A=0.978980_0.969190^0.988770          PARAM=B=0.372610_0.368884^0.376336
PARAM=C=0.998160_0.988178^1.008142 //
RP=4 k1=0 k2=0 PARAM=B1=0_0^0.01 GEWICHT=SPHAR4 //
GOAL:pseudobrookite=GEWICHT*ifthenelse(ifdef(d),exp(my*d*3/4),1) //
E=FE Wyckoff=c x=0.187000 y=0.000000 z=0.750000 TDS=-0.000010
E=FE Wyckoff=f x=0.136000 y=0.000000 z=0.064000 TDS=-0.000010
E=O Wyckoff=c x=0.758000 y=0.000000 z=0.750000 TDS=0.000010
E=O Wyckoff=f x=0.048000 y=0.000000 z=0.883000 TDS=-0.000020
E=O Wyckoff=f x=0.310000 y=0.000000 z=0.929000 TDS=-0.000020

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Figure S3. Structure model of Ferropseudobrookite (including atomic coordinates) during the Rietveld refinement.