

Electronic supplementary information (ESI)

Depolymerization mechanism of MgO on silicate microstructure under different CaO content: A theoretical and experimental study

Maierhaba Abudourehman^a, Lanzhen He^a, Fangru Ma^a, Bo Wei^{a*}, Jianjiang Wang^a, Quan Zhu^b,
Hong Yao^c

^a *State Key Laboratory of Chemistry and Utilization of Carbon Based Energy Resources, Xinjiang Key Laboratory of Clean Conversion and Chemical Engineering Process, School of Chemical Engineering and Technology, Xinjiang University, Urumqi, 830017, China;*

^b *School of Chemical Engineering, Sichuan University, Chengdu 610065, China;*

^c *State Key Laboratory of Coal Combustion, Huazhong University of Science and Technology, Wuhan 430074, China;*

* Corresponding authors, E-mail: weiboxju@163.com (B. Wei)

1. Theoretical details

Table S1 Potential parameters between different particles and oxygen ions in MgO-CaO-SiO₂-Al₂O₃ system

Atom 1	Atom 2	$A_{ij}/(\text{eV})$	$B_{ij}/(\text{\AA}^{-1})$	$C_{ij}/(\text{eV}\cdot\text{\AA}^6)$
Si	O	62794.37	6.06	0
Al	O	86057.58	6.06	0
Ca	O	717827.00	6.06	8.67
Mg	O	154917.90	6.06	1.73
O	O	1497049.00	5.88	17.34

Table S2 Particle number and density of MgO-CaO-SiO₂-Al₂O₃ system in high calcium system

Mole fraction (%)			Atomic number			Density	Box
MgO	Ca	Si	Al	Mg	O	(g/cm ³)	length (Å)
1	653	576	771	16	2982	2.762	40.594
3	661	560	753	50	2971	2.765	40.595
5	669	543	736	84	2960	2.767	40.603
7	677	526	718	118	2949	2.768	40.61
9	685	509	699	154	2937	2.769	40.616
11	694	491	680	191	2925	2.77	40.633
13	703	474	661	228	2913	2.771	40.648

Table S3 Particle number and density of MgO-CaO-SiO₂-Al₂O₃ system in low calcium system

Mole fraction (%)			Atomic number			Density (g/cm ³)	Box length (Å)
MgO	Ca	Si	Al	Mg	O		
1	292	693	923	15	3077	2.699	40.205
3	295	682	910	44	3069	2.704	40.595
5	299	672	896	75	3060	2.708	40.603
7	302	661	881	106	3051	2.713	40.611
9	305	650	866	137	3041	2.717	40.616
11	308	638	851	170	3032	2.724	40.633
13	312	627	836	203	3022	2.721	40.648

2. FTIR experiment details

Table S4 Specific components of samples with MgO content of 1, 5, 9 mol% under high calcium

Group	Ash weight(wt%)				Ash composition(mol%)			
	CaO	SiO ₂	Al ₂ O ₃	MgO	CaO	SiO ₂	Al ₂ O ₃	MgO
I	32.9	31.2	35.3	0.6	40	35.4	23.6	1
II	33.6	29.7	33.6	3.0	40	33	22	5
III	34.4	28.2	31.9	5.6	40	30.6	20.4	9

Table S5 Specific components of samples with MgO content of 1, 5, 9 mol% under low calcium

Group	Ash weight(wt%)				Ash composition(mol%)			
	CaO	SiO ₂	Al ₂ O ₃	MgO	CaO	SiO ₂	Al ₂ O ₃	MgO
I	15.5	39.4	44.6	0.6	20	47.4	31.6	1
II	15.8	38.2	43.2	2.9	20	45	30	5
III	16.2	36.9	41.7	5.2	20	42.6	28.4	9