

Microstructure and Mineral Phase Evolution of Vanadium Slag by Modulating the CaO/V₂O₅ Ratio

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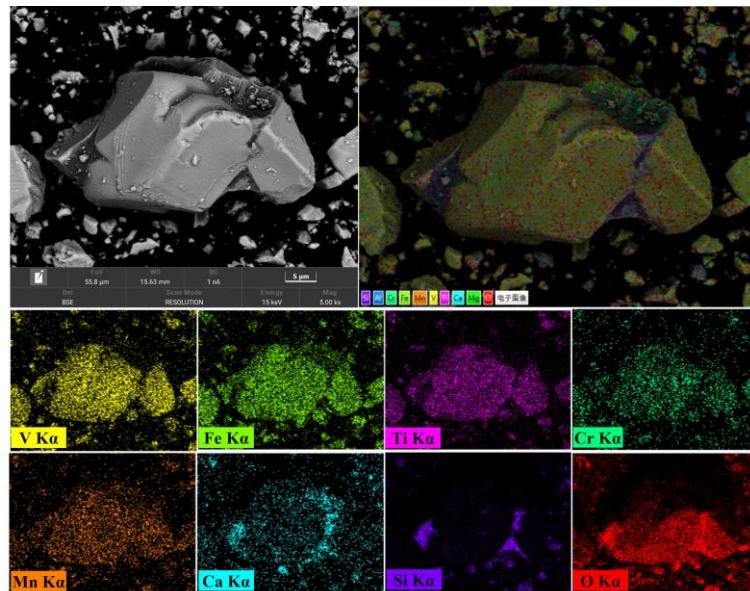


Figure S1. Microphotograph of raw slag and distribution of main elements.

Table S1. Buckingham potential and short-range corrected oxygen-cation pair interaction parameters.

Pair	A _{ij} (eV)	q _{ij} (Å)	C _{ij} (eV·Å ⁶)	r _s (Å)	B _{ij} (eV·Å ⁿ)	D _{ij} (eV/Å ²)	n _{ij}
O ^{1.2-} -O ^{1.2-}	2029.22	0.3436	192.58	1.906	46.251	3.424	-0.328
O ^{1.2-} -Si ^{2.4+}	13702.91	0.1938	54.681	1.172	28.905	3.932	-3.057
O ^{1.2-} -Ca ^{1.2+}	7747.183	0.2526	93.109	1.319	74.6787	3.168	-3.987
O ^{1.2-} -Fe ^{1.2+}	11777.07	0.207132	21.642	0.934185	103.903	2.67	-32.11
O ^{1.2-} -V ^{1.8+}	20506.78	0.1785	7.03	0.674	198.4726	2.3	-212.85
O ^{1.2-} -V ^{2.4+}	6199.731	0.2152	25.516	1.093	39.879	3.065	-5.599
O ^{1.2-} -V ³⁺	23300	0.1799	8.649	0.684	225.295	2.314	-229.279

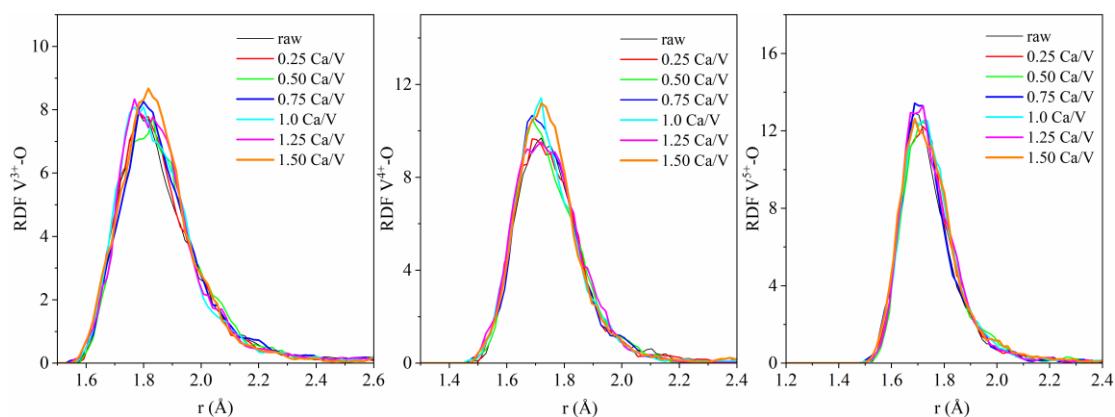


Figure S2. RDF distribution of V-O.

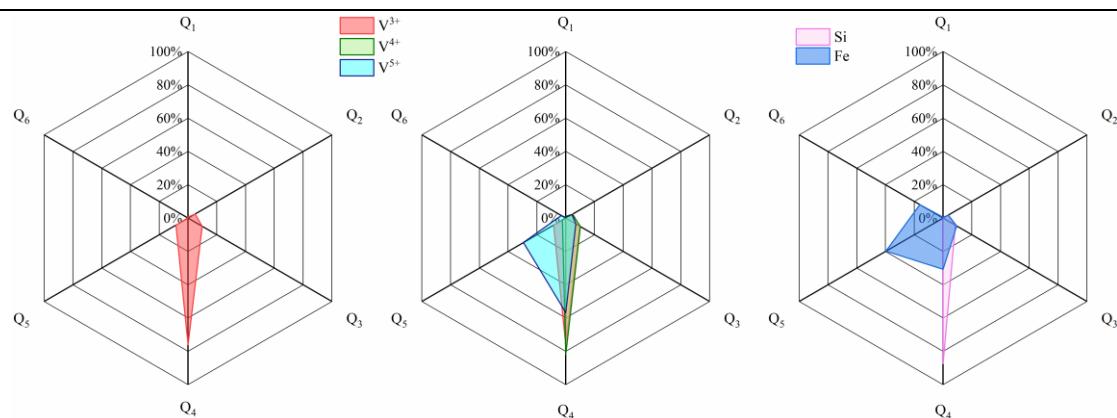


Figure S3. Coordination distribution of cations and oxygen.

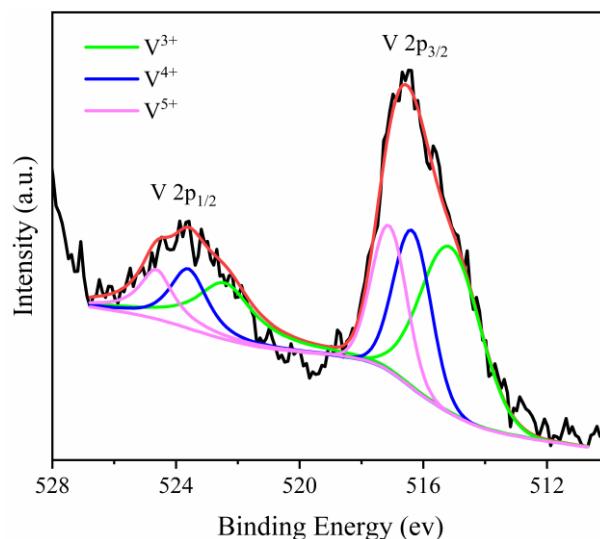


Figure S4. V2p XPS fitting curve of 1.5Ca/V.

Table S2. Proportions of different valence states of vanadium in modified vanadium slag.

Raw slag	0.25	0.5	0.75	1.0	1.25	1.50	
V ³⁺	37.66	38.27	38.27	36.08	43.73	43.72	41.44
V ⁴⁺	32.27	29.64	30.62	32.68	32.20	26.73	31.16
V ⁵⁺	30.08	32.09	31.11	29.24	24.07	29.54	27.39

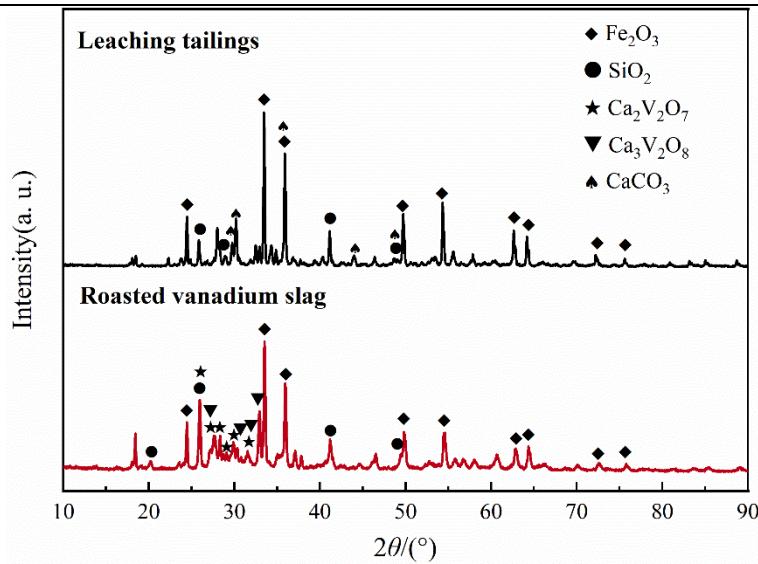


Figure S5. Roasted vanadium slag and leaching tailings XRD pattern for 1.0Ca/V (800 °C, 2 h).

Table S3. The chemical constituent of roasted clinker and leaching tailings under 1.0Ca/V (800 °C, 2 h) condition (%).

Constituent	MgO	Al ₂ O ₃	SiO ₂	P ₂ O ₅	CaO	TiO ₂	V ₂ O ₅	Cr ₂ O ₃	MnO	Fe ₂ O ₃	CO ₂
Roasted vanadium slag	1.79	4.63	9.78	0.0899	13	9.66	13.8	1.51	7.13	33.8	\
Leaching tailings	1.74	5.49	11.4	0.0679	13.3	9.33	2.27	1.53	6.01	34.8	13.1