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Supplementary Materials

Substitution preference of chromium ions in ordinary Portland cement clinker phases

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1. XRD patterns of raw materials.

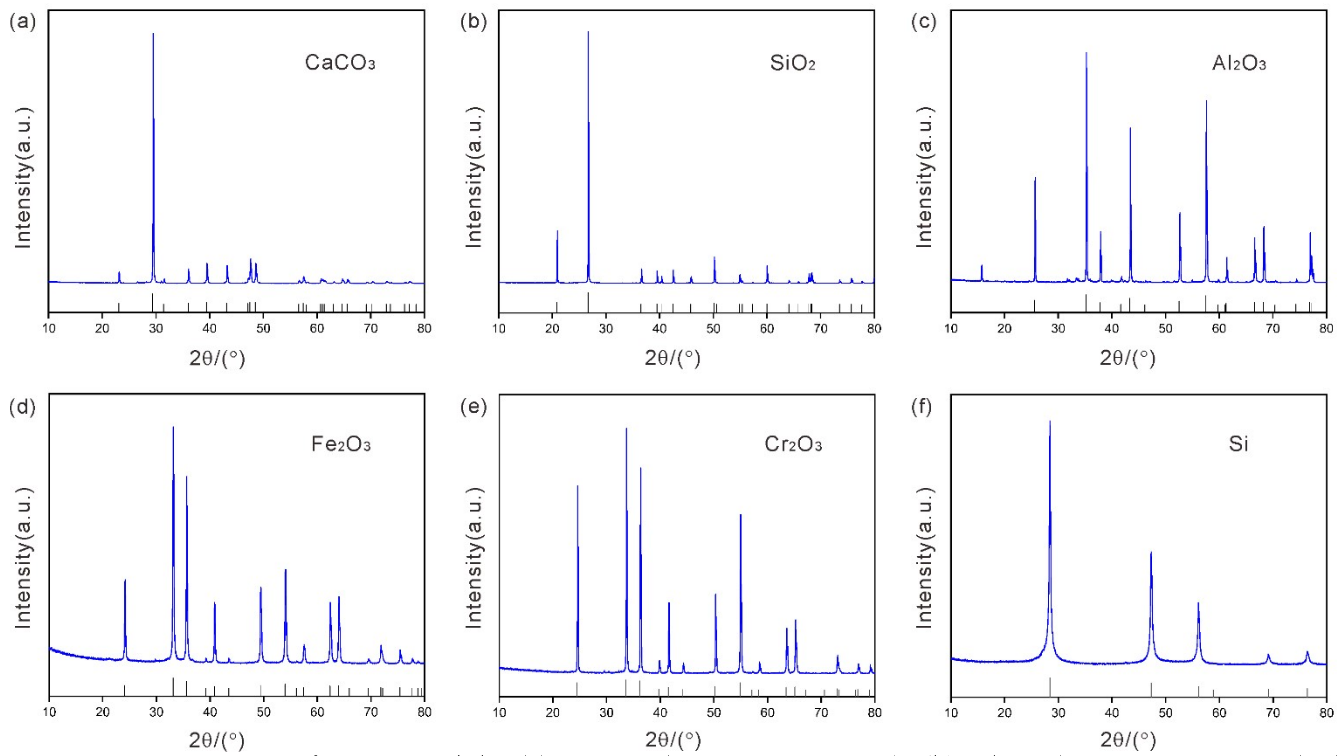

Fig. S1 XRD patterns of raw materials: (a) $CaCO_3$ (Space group, R-3), (b) Al_2O_3 (Space group, R-3c), (c) SiO_2 (Space group, $P3_221$), (d) Fe_2O_3 (Space group, R-3c), (e) Cr_2O_3 (Space group, R-3c), (f) Si (Space group, Fd-3m). The standard cards are also shown in each panel for comparison.

2. Detailed calculations, the potential contents of minerals in OPC clinker and masses of raw materials.

Bogue equations[1] were used to estimate the contents of OPC clinker minerals and quality of raw materials:

$$C_3S = 4.07C - 7.6S - 6.72A - 1.43F - 2.86\,\bar{S} \quad (1)$$

$$C_2S = 2.87S - 0.754C_3S \quad (2)$$

$$C_3A = 2.65A - 1.69\,F \quad (3)$$

$$C_4AF = 3.04\,F \quad (4)$$

Where C = CaO, S = SiO_2, A = Al_2O_3, F = Fe_2O_3, $\bar{S}$ = SO_3

KH = 0.899, SM = 2.07 and IM = 1.172 of Portland cement clinker were estimated by the following formula.

$$KH = \frac{C_3S + 0.8838C_2S}{C_3S + 1.3256C_2S} \quad (5)$$

$$SM = \frac{C_3S + 1.3256C_2S}{1.4341C_3A + 2.0464C_4AF} \quad (6)$$

$$IM = \frac{1.1501C_3A}{C_4AF} + 0.6383 \quad (7)$$

Table S1 The content of minerals in OPC clinker samples.

Minerals	C_3S	C_2S	C_3A	C_4AF
Content (wt%)	59	19	7	19

Table S2 The percentage of raw materials used to prepare OPC clinker samples.

Samples	$CaCO_3$ (%)	Al_2O_3 (%)	SiO_2 (%)	Fe_2O_3 (%)	Cr_2O_3* (%)
S_0	78.47	3.79	14.51	3.23	0
S_1	78.47	3.79	14.51	3.23	12.5
S_2	78.47	3.79	14.51	3.23	25.0
S_3	78.47	3.79	14.51	3.23	37.5
S_4	78.47	3.79	14.51	3.23	50.0

*Note: The quality of Cr_2O_3 is calculated according to that of Fe by supposing 0, 12.5, 25.0, 37.5 and 50 mol% was substituted.

3. Minerals, supercells, parameters and K-point meshes of Cr-doped configurations.

Table S3 Minerals, supercells, parameters and k-point meshes of Cr-doped configurations.

Minerals	Supercells	Parameter (Å)	K-points	
			Relax	PDOS
C_3S*	1 × 1 × 1	a = 12.24, b = 7.07, c = 9.30	2 × 2 × 2	4 × 4 × 4
C_2S*	2 × 2 × 1	a = 11.010, b = 13.510, c = 9.311	2 × 2 × 3	5 × 4 × 5
C_3A*	1 × 1 × 1	a = 5.57, b=14.52, c=5.35	2 × 2 × 2	3 × 3 × 3
C_4AF*	2 × 1 × 2	a = 11.168, b=14.600, c = 10.748	2 × 2 × 2	5 × 3 × 5

*Notes: C_3S [2-4], C_2S [5], C_3A [6], C_4AF [7].

4. Ions, coordination numbers and ionic radius.

Table S4 Ion types, coordination numbers and radius of Cr and atoms been substituted [8].

Ion types	Coordination numbers	Radius/pm
Mn^{4+}	6	53
Mn^{2+}	6	67
Ca^{2+}	6	100
Al^{3+}	4	39
S^{6+}	4	12
Si^{4+}	4	26
Fe^{3+}	6	55

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