

## Supplementary data

**Table S1** Common solid-state kinetic models and expressions of  $f(X)$  and  $g(X)$

	No.	symbol	kinetic model	differential form $f(x)= 1/k \cdot dx/dt$	integral form $g(x)= kt$
nucleation	1	P2	$n = 2$	$2X^{1/2}$	$X^{1/2}$
models	2	P3	power law $n = 3$	$3X^{2/3}$	$X^{1/3}$
	3	P4	$n = 4$	$4X^{3/4}$	$X^{1/4}$
	4	A2	$n = 2$	$2(1 - X)(-\ln(1 - X))^{1/2}$	$(-\ln(1 - X))^{1/2}$
Avrami–Erofeyev	5	A3	$n = 3$	$3(1 - X)(-\ln(1 - X))^{2/3}$	$(-\ln(1 - X))^{1/3}$
	6	A4	$n = 4$	$4(1 - X)(-\ln(1 - X))^{3/4}$	$(-\ln(1 - X))^{1/4}$
	7	R2	2-D (contracting area)	$2(1 - X)^{1/2}$	$1 - (1 - X)^{1/2}$
contraction	8	R3	3-D (contracting volume)	$3(1 - X)^{2/3}$	$1 - (1 - X)^{1/3}$
diffusion	9	D1	1-D	$1/(2X)$	$X^2$
	10	D2	2-D	$1/(-\ln(1 - X))$	$(1 - X)\ln(1 - X) + X$
models	11	D3	3-D (Jander)	$(3/2)(1 - X)^{2/3}(1 - (1 - X)^{1/3})$	$(1 - (1 - X)^{1/3})^2$
	12	D4	3-D (Ginstling–Brounshtein)	$(3/2)((1 - X)^{-1/3} - 1)$	$1 - (2/3)X - (1 - X)^{2/3}$
reaction-order	13	F0(R1) <sup>a)</sup>	zero-order	1	$X$
models	14	F1(A1) <sup>a)</sup>	first-order	$(1 - X)$	$-\ln(1 - X)$
	15	F2	second-order	$(1 - X)^2$	$(1 - X)^{-1} - 1$
	16	F3	third-order	$(1 - X)^3$	$(1/2)((1 - X)^{-2} - 1)$

Note: a) Same form

**Table S2** Linear fitting results of pure Fe<sub>2</sub>O<sub>3</sub> at all temperature ranges.  $R^2$  is the linear regression coefficient obtained with MS Excel<sup>®</sup>

No.	model	$R^2$				
		973 K	1023 K	1073 K	1123 K	1173 K
1	P2	0.811	0.844	0.865	0.875	0.877
2	P3	0.714	0.755	0.778	0.787	0.788
3	P4	0.643	0.684	0.705	0.708	0.706
4	A2	0.957	0.969	0.971	0.978	0.988
5	A3	0.922	0.941	0.951	0.957	0.958
6	A4	0.869	0.892	0.904	0.908	0.903
7	R2	0.994	0.996	0.996	0.996	0.997

8	R3	0.978	0.978	0.975	0.978	0.985
9	D1	0.997	0.992	0.987	0.985	0.984
10	D2	0.971	0.962	0.956	0.956	0.958
11	D3	0.811	0.806	0.794	0.807	0.839
12	D4	0.936	0.927	0.920	0.922	0.930
13	F0	0.949	0.962	0.969	0.971	0.970
14	F1	0.845	0.851	0.838	0.857	0.903
15	F2	0.140	0.178	0.172	0.217	0.358
16	F3	0.059	0.079	0.088	0.104	0.155

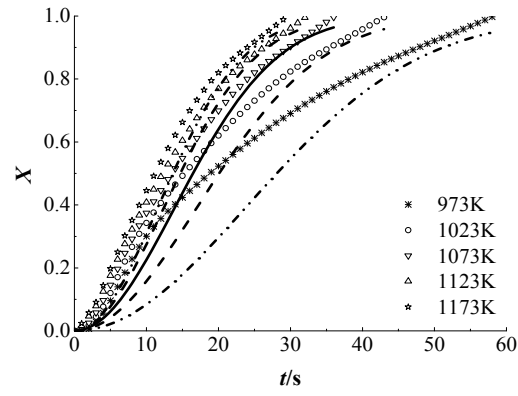
**Table S3** Linear fitting results of Fe<sub>5</sub>Al<sub>5</sub> at all temperature ranges.  $R^2$  is the linear regression coefficient obtained with MS Excel<sup>®</sup>

No.	model	$R^2$				
		973 K	1023 K	1073 K	1123 K	1173 K
1	P2	0.772	0.766	0.784	0.784	0.793
2	P3	0.647	0.639	0.658	0.658	0.667
3	P4	0.545	0.539	0.559	0.559	0.569
4	A2	0.927	0.919	0.906	0.954	0.964
5	A3	0.890	0.883	0.887	0.896	0.898
6	A4	0.822	0.813	0.822	0.814	0.812
7	R2	0.981	0.981	0.985	0.989	0.993
8	R3	0.963	0.961	0.957	0.980	0.987
9	D1	0.997	0.997	0.996	0.995	0.995
10	D2	0.979	0.980	0.979	0.981	0.980
11	D3	0.803	0.788	0.759	0.838	0.857
12	D4	0.942	0.941	0.937	0.950	0.953
13	F0	0.925	0.922	0.931	0.932	0.939
14	F1	0.812	0.780	0.717	0.878	0.909
15	F2	0.131	0.120	0.111	0.286	0.386
16	F3	0.064	0.078	0.094	0.140	0.188

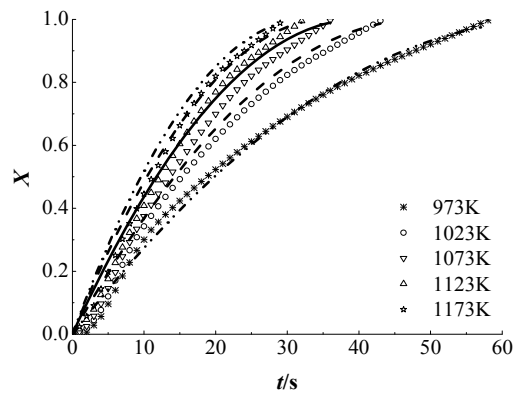
**Table S4** F-test on the best approximate models

oxygen carrier	model	973 K		1023 K		1073 K		1123 K		1173 K	
		$F$	$F_c^{a)}$	$F$	$F_c$	$F$	$F_c$	$F$	$F_c$	$F$	$F_c$
pure Fe <sub>2</sub> O <sub>3</sub>	R2	0.00 <sup>b)</sup>	3.92	0.22	3.95	0.44	3.97	0.41	3.99	0.33	4.01
Fe <sub>5</sub> Al <sub>5</sub>	D1	0.00 <sup>c)</sup>	3.94	0.02	3.97	0.19	4.00	0.21	4.03	0.29	4.07

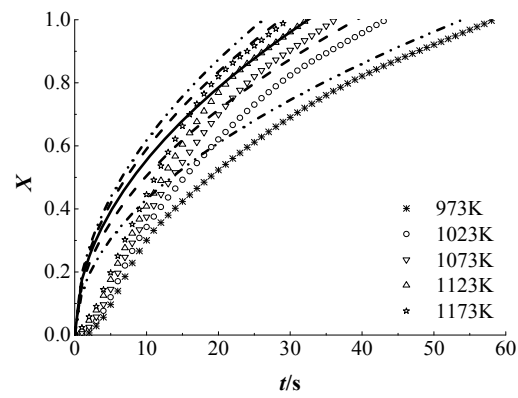
Notes: a)  $F_c$  is the critical value at 95% CL, i.e., the significant level  $\alpha = 0.05$ ; b)  $F = 0.0003$ ; c)  $F = 0.0004$



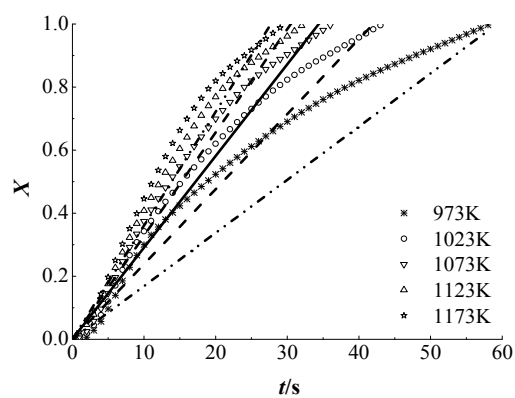
(a)



(b)

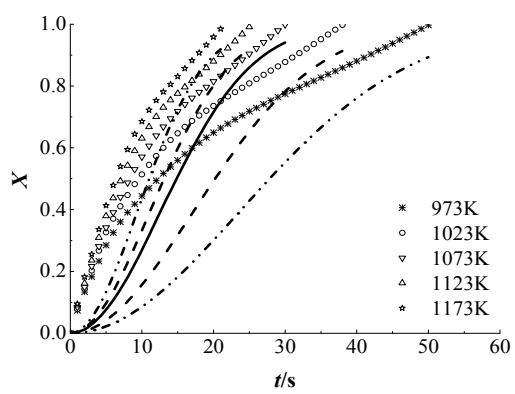


(c)

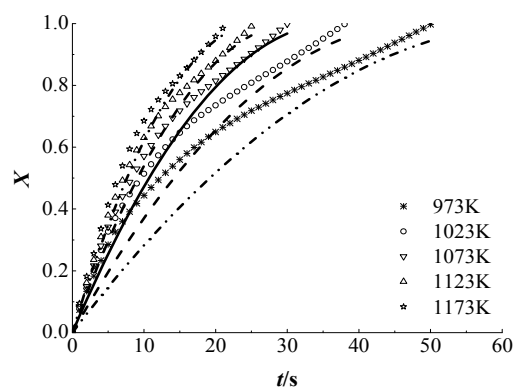


(d)

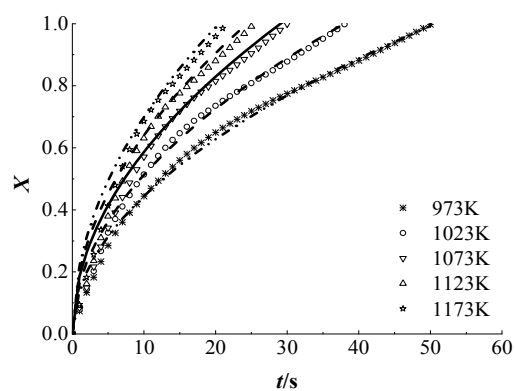
**Fig. S1** Comparison of the calculated conversion curves with the experimental data for pure  $\text{Fe}_2\text{O}_3$ : (a) A2, (b) R2, (c) D1, and (d) F0. Symbols denote the experimental data. Lines represent the calculated conversion curves



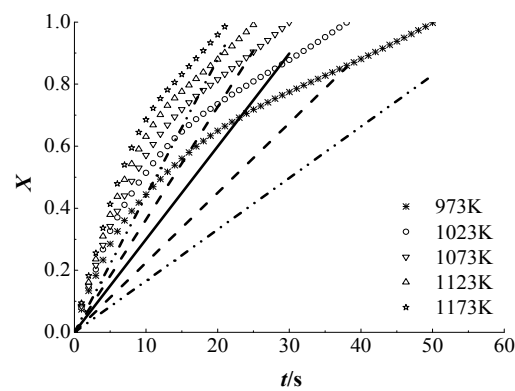
(a)



(b)



(c)



(d)

**Fig. S2** Comparison of the calculated conversion curves with the experimental data for  $\text{Fe}_5\text{Al}_5$ : (a) A2, (b) R2, (c) D1, and (d) F0. Symbols denote the experimental data. Lines represent the calculated conversion curves