Supporting Information

Multi-element collaboration in $Cr_2TiAl_{1-x}Si_xC_2$ MAX for the oxide barrier formation in 550 °C LBE environment

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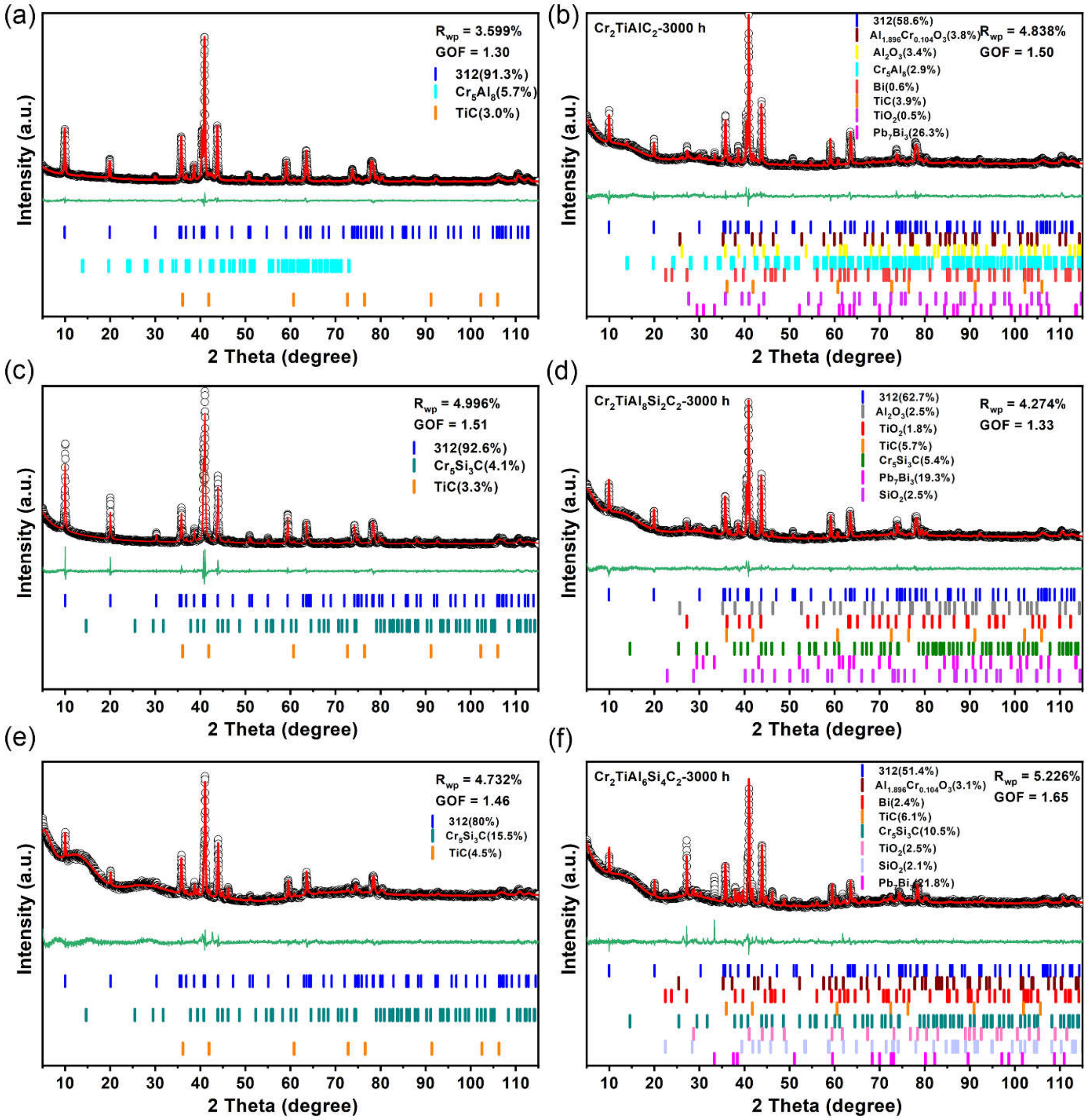

Fig. S1 (a) and (b) are the XRD Rietveld refinement patterns of Cr_2TiAlC_2 before corrosion and after corrosion in LBE for 3000 h; (c) and (d) are the XRD Rietveld refinement patterns of $Cr_2TiAl_{0.8}Si_{0.2}C_2$ before corrosion and after corrosion in LBE for 3000 h. (e) and (f) are the XRD Rietveld refinement pattern of $Cr_2TiAl_{0.6}Si_{0.4}C_2$ before corrosion and after 3000 h corrosion in LBE.

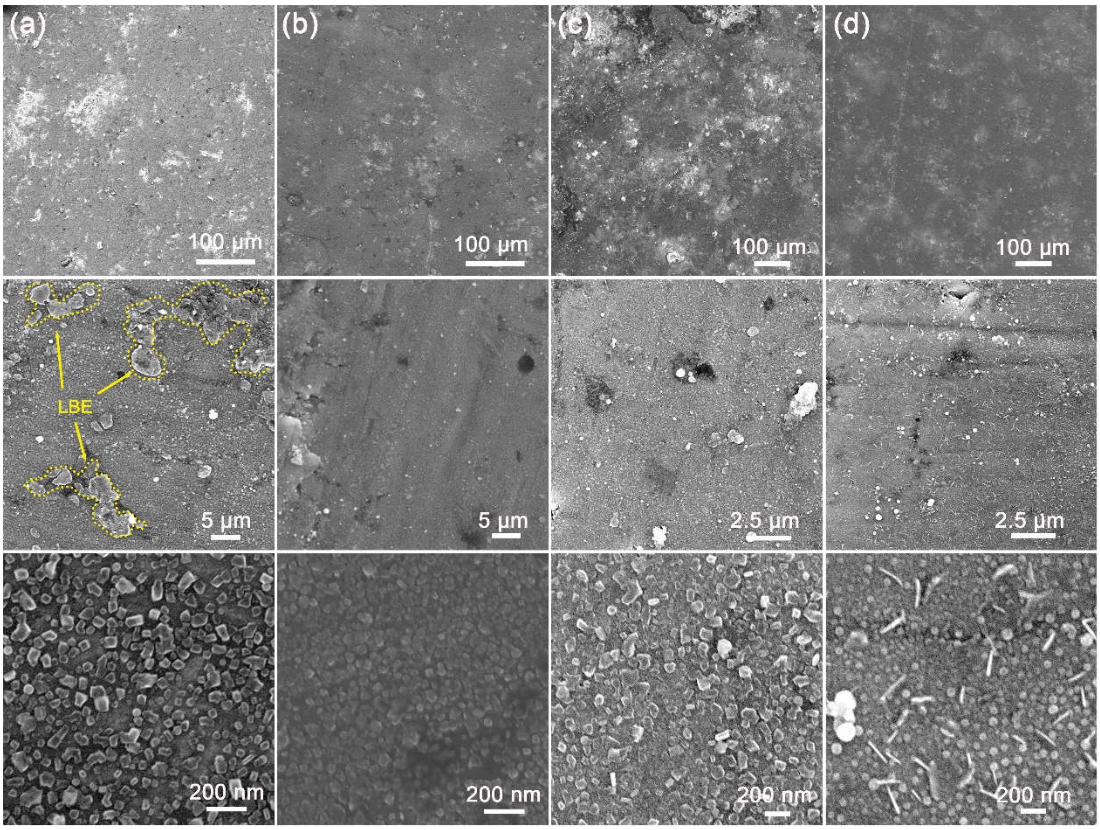

Fig. S2 Surface morphology of Cr_2TiAlC_2 after (a) 500 h, (b) 1000 h, (c) 2000 h, and (d) 3000 h corrosion in LBE.

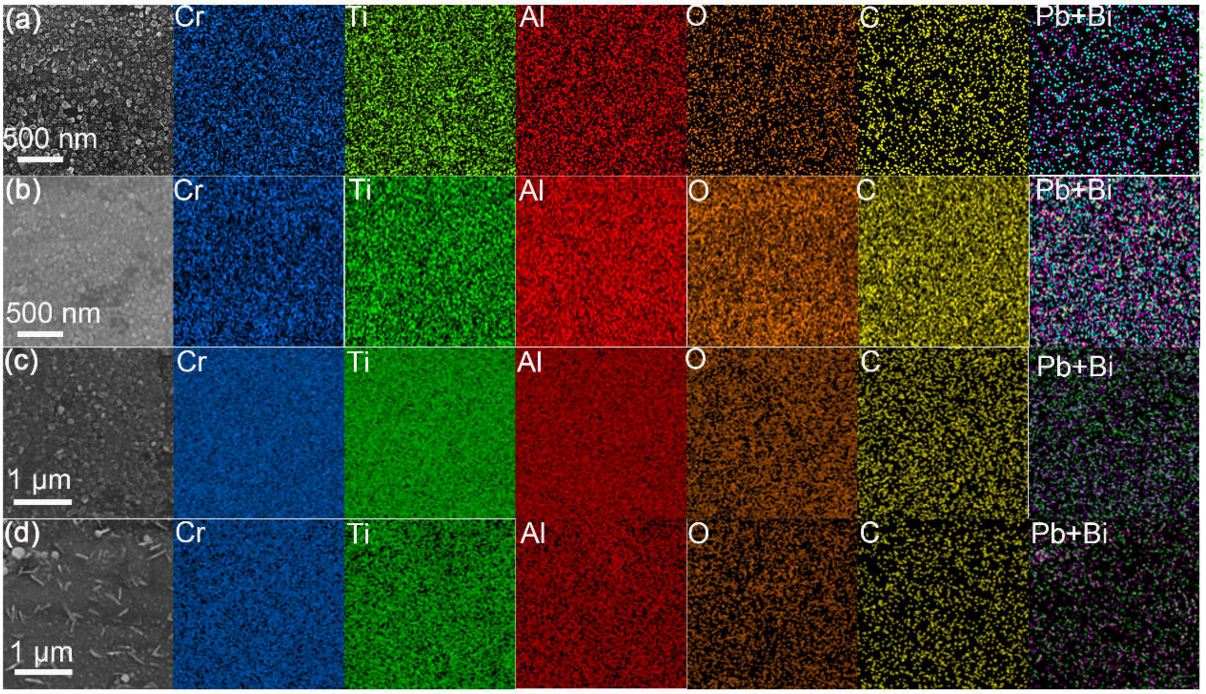

Fig. S3 EDS mapping of enlarged corroded surface of Cr_2TiAlC_2 after (a) 500 h, (b) 1000 h, (c) 2000 h, and (d) 3000 h corrosion in LBE.

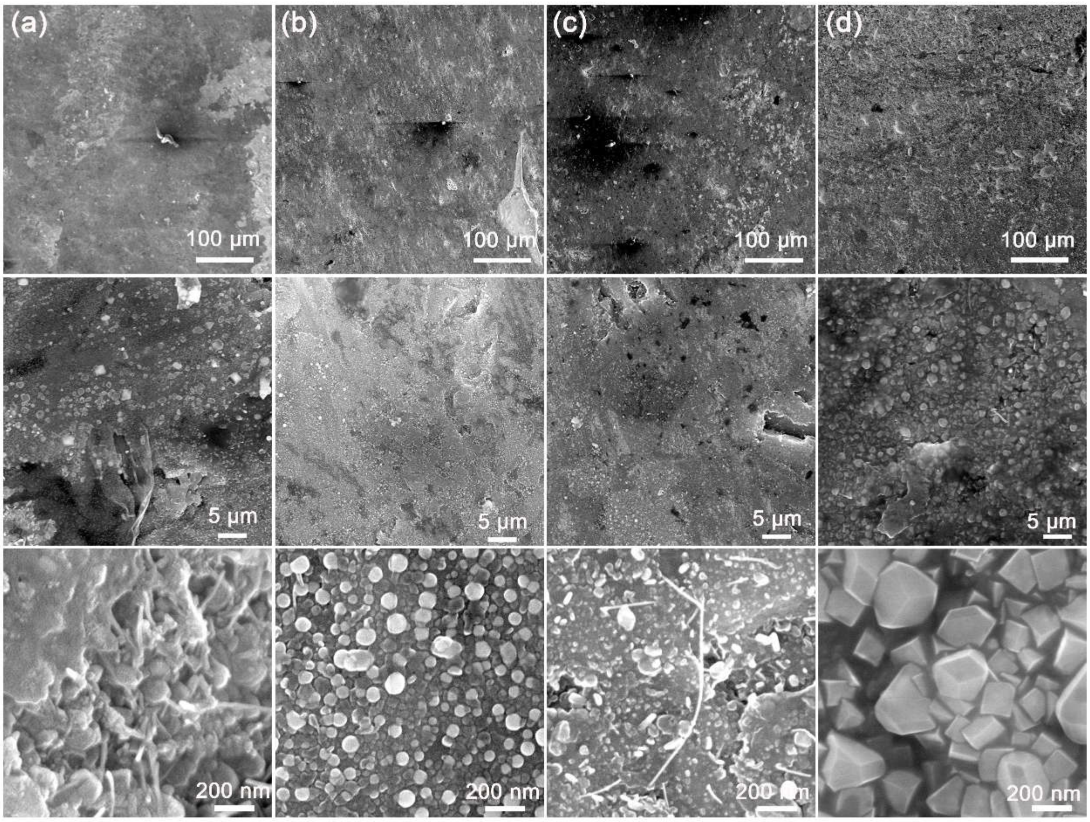

Fig. S4 Surface morphology of $Cr_2TiAl_{0.8}Si_{0.2}C_2$ after (a) 500 h, (b) 1000 h, (c) 2000 h, and (d) 3000 h corrosion in LBE.

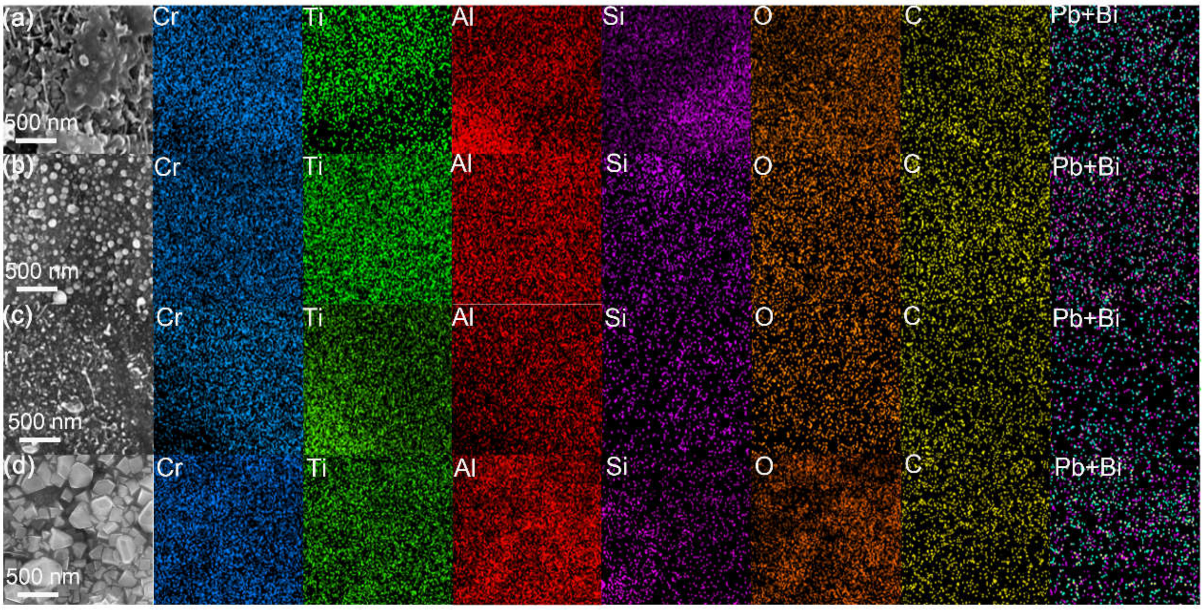

Fig. S5 EDS mapping of enlarged corroded surface of $Cr_2TiAl_{0.8}Si_{0.2}C_2$ after (a) 500 h, (b) 1000 h, (c) 2000 h, and (d) 3000 h corrosion in LBE.

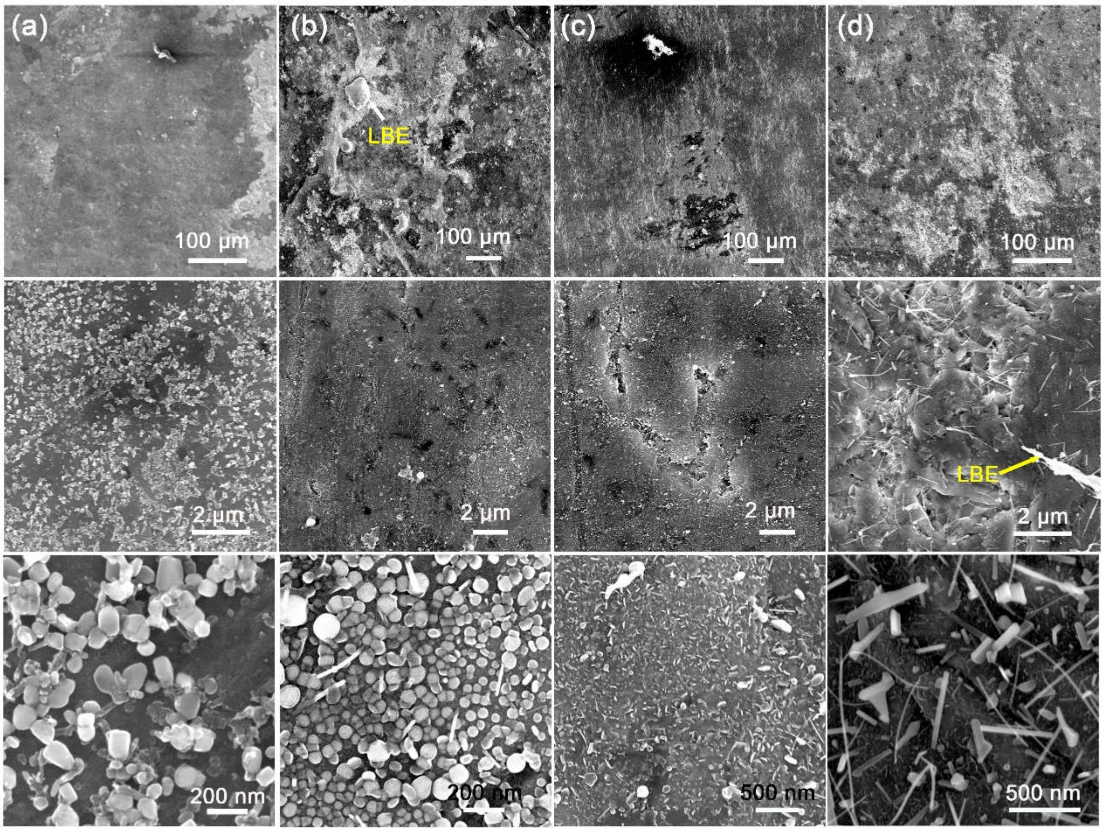

Fig. S6 Surface morphology of $Cr_2TiAl_{0.6}Si_{0.4}C_2$ after (a) 500 h, (b) 1000 h, (c) 2000 h, and (d) 3000 h corrosion in LBE.

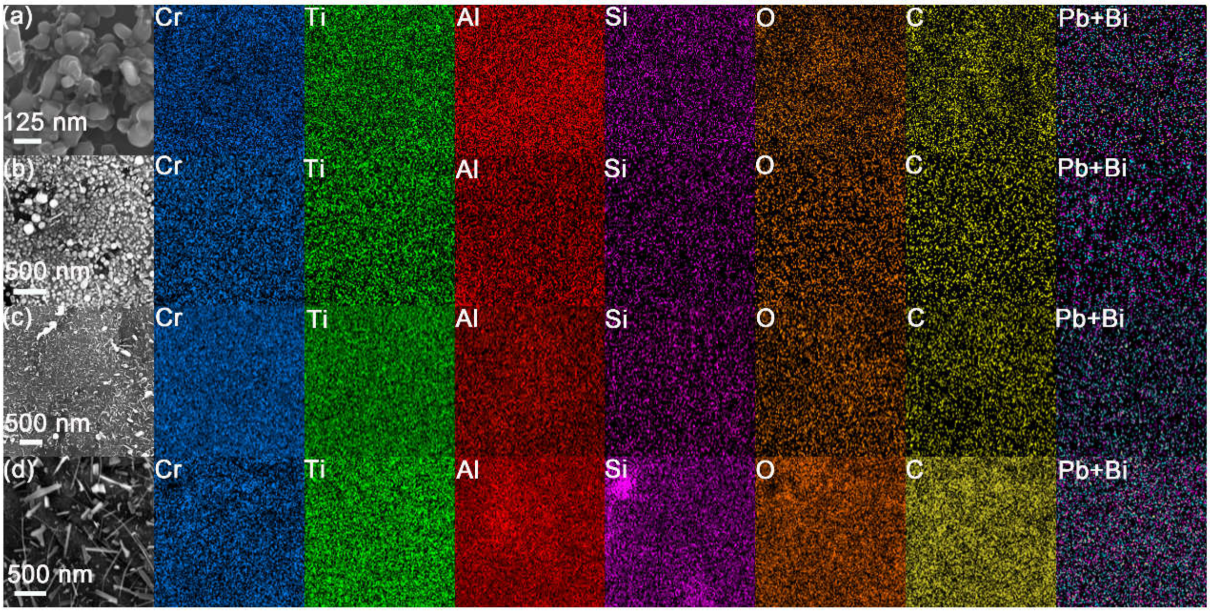

Fig. S7 EDS mapping of enlarged corroded surface of $Cr_2TiAl_{0.6}Si_{0.4}C_2$ after (a) 500 h, (b) 1000 h, (c) 2000 h, and (d) 3000 h corrosion in LBE.

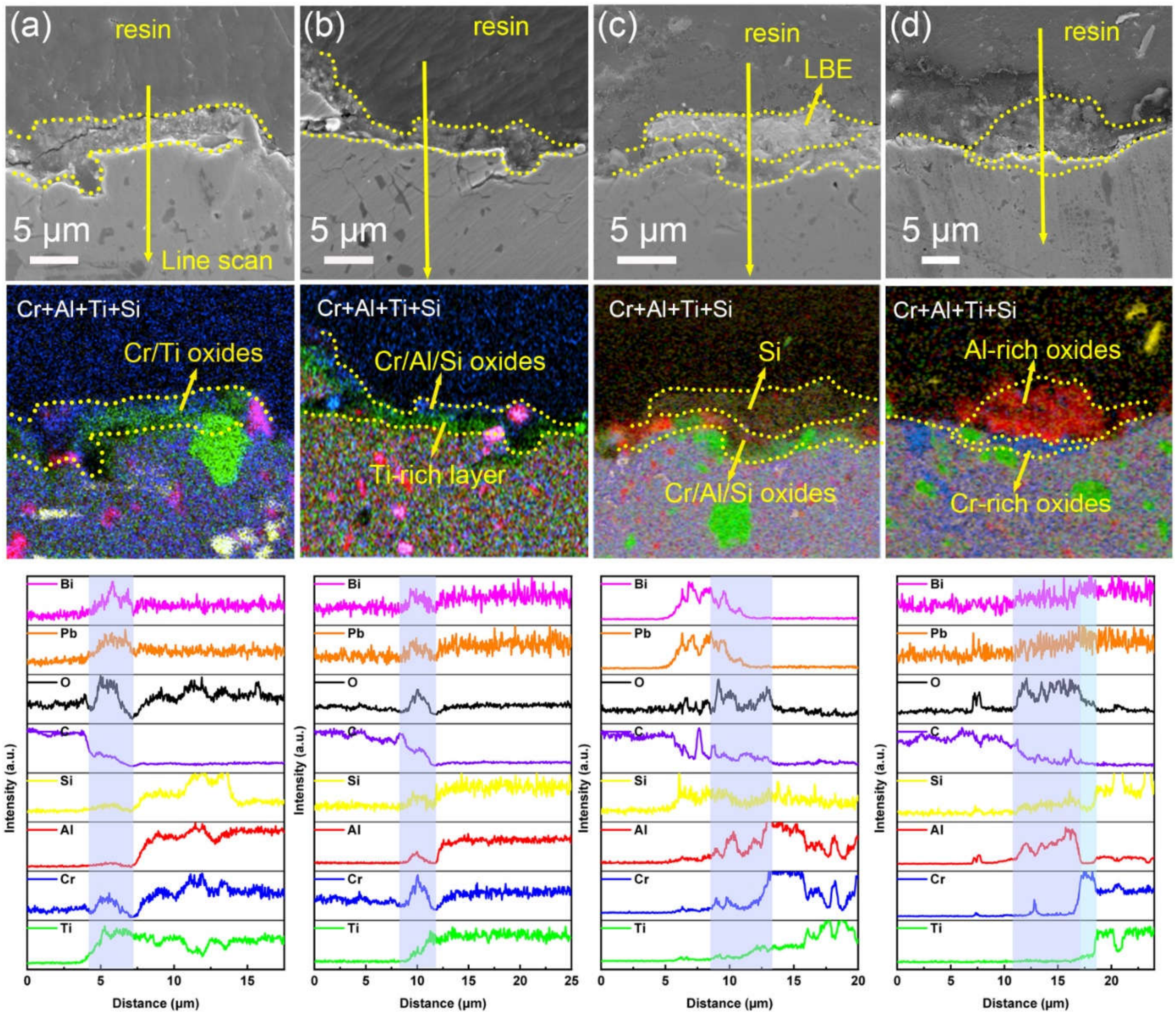

Fig. S8 Cross-section and corresponding EDS diagram of $Cr_2TiAl_{0.8}Si_{0.2}C_2$ corroded in LBE for (a) 500, (b) 1000, (c) 2000, and (d) 3000 h at 550 °C. Si, Al, Ti, and Cr element in the EDS mapping are colored in yellow, red, green, and blue, respectively.

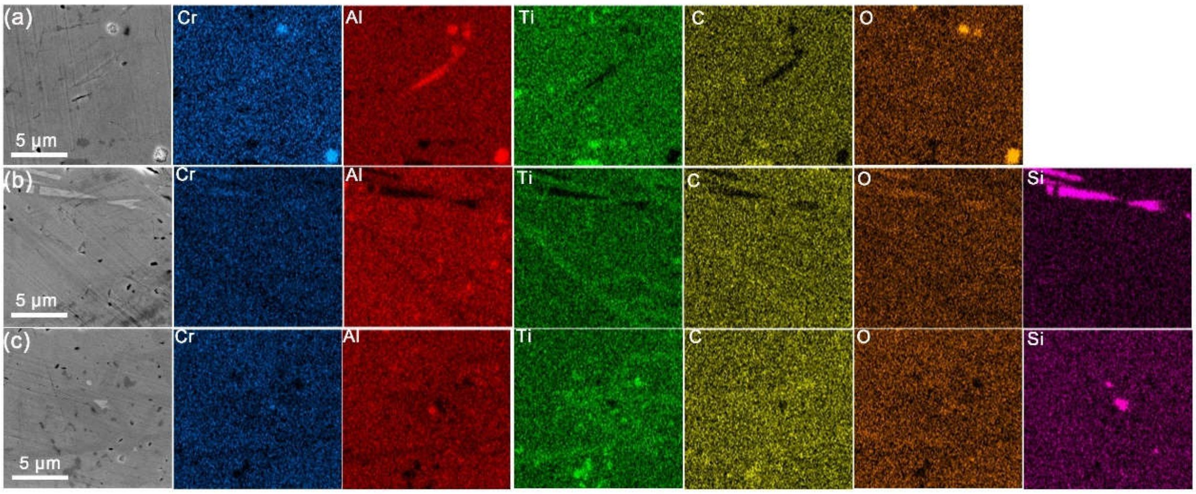

Fig. S9 EDS of the pristine surface of $Cr_2TiAl_{1-x}Si_xC_2$, (a) Cr_2TiAlC_2 (b) $Cr_2TiAl_{0.8}Si_{0.2}C_2$ (c) $Cr_2TiAl_{0.6}Si_{0.4}C_2$.

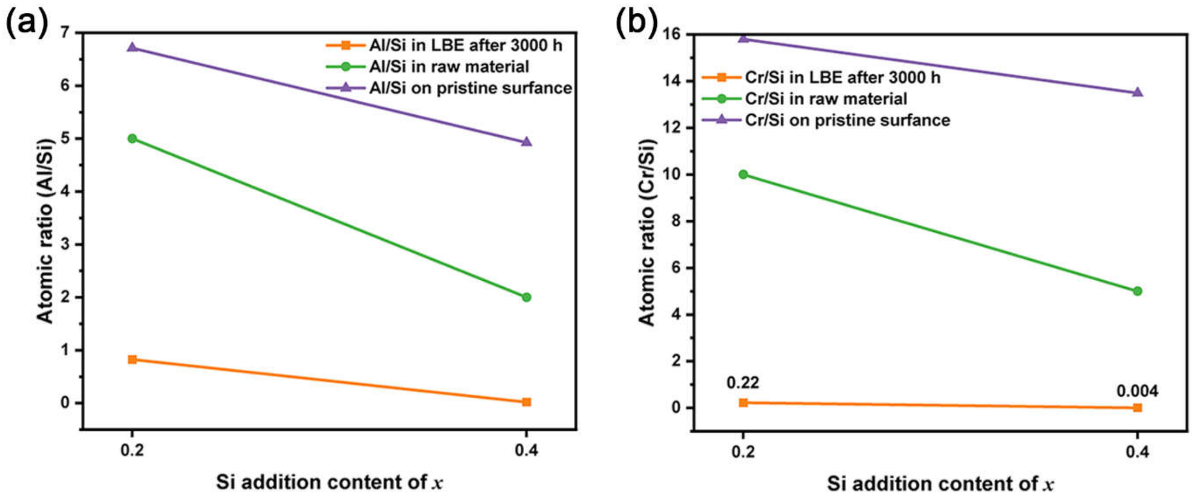

Fig. S10 (a) The atomic ratio of Al/Si in the raw materials, on the pristine surface, and in LBE residue after 3000 h corrosion. (b) The atomic ratio of Cr/Si in the raw materials, on the pristine surface, and in LBE residue after 3000 h corrosion.

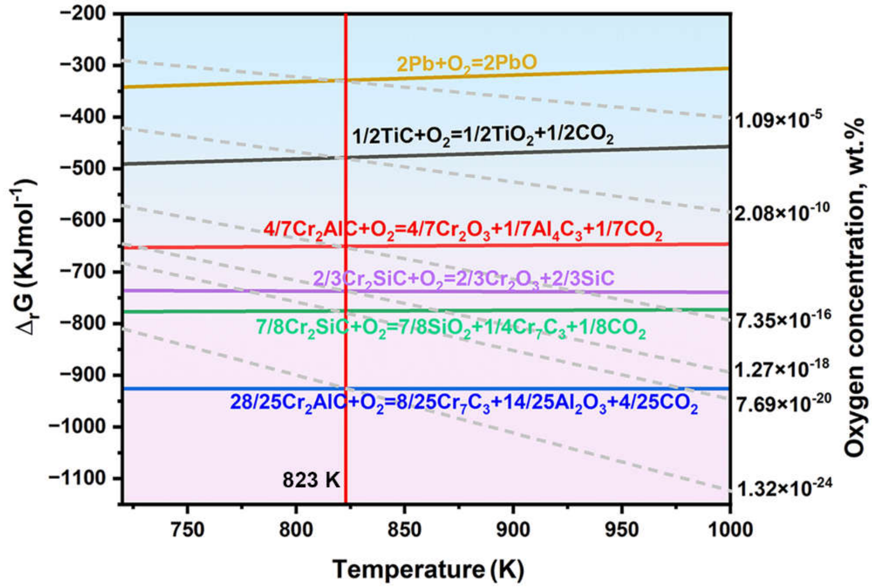

Fig. S11 The Ellingham diagram of oxides formed by oxidation of $Cr_2TiAl_{1-x}Si_xC_2$ at 550 ℃ liquid LBE.

Table S1 The phase composition of $Cr_2TiAl_{1-x}Si_xC_2$ obtained based on XRD refinement.

MAX	Phase & content (wt.%)		
Cr_2TiAlC_2	312 (91.3 wt.%)	TiC (3.0 wt.%)	Cr_5Al_8 (5.7 wt.%)
$Cr_2TiAl_{0.8}Si_{0.2}C_2$	312 (92.6 wt.%)	TiC (3.3 wt.%)	Cr_5Si_3C (4.1 wt.%)
$Cr_2TiAl_{0.6}Si_{0.4}C_2$	312 (80.0 wt.%)	TiC (4.5 wt.%)	Cr_5Si_3C (15.5 wt.%)

Table s2 Refined lattice parameters of $Cr_2TiAl_{1-x}Si_xC_2$ based on XRD patterns

Parameters	Cr_2TiAlC_2	$Cr_2TiAl_{0.8}Si_{0.2}C_2$	$Cr_2TiAl_{0.6}Si_{0.4}C_2$
Crystal system	hexagonal	hexagonal	hexagonal
Space group	$P6_3/mmc$	$P6_3/mmc$	$P6_3/mmc$
a (Å)	2.93003	2.92781	2.9265
c (Å)	17.88182	17.7481	17.6947
R_{wp}(%)	3.599	4.996	4.732
GOF	1.30	1.51	1.46

Table S3 The bond lengths of $Cr_2TiAl_{1-x}Si_xC_2$ in the pristine sample

MAX	Bond	Length (Å)
	Cr-A	2.702
Cr_2TiAlC_2	Cr-C	1.996
	Ti-C	2.136
	Cr-A	2.678
$Cr_2TiAl_{0.8}Si_{0.2}C_2$	Cr-C	1.987
	Ti-C	2.142
	Cr-A	2.673
$Cr_2TiAl_{0.6}Si_{0.4}C_2$	Cr-C	1.937
	Ti-C	2.197

Table S4 Refined lattice parameters of $Cr_2TiAl_{1-x}Si_xC_2$ after corroding in LBE for 3000 h

Parameters	$\mathbf{Cr_2TiAlC_2}$	$\mathbf{Cr_2TiAl_{0.8}Si_{0.2}C_2}$	$\mathbf{Cr_2TiAl_{0.6}Si_{0.4}C_2}$
Crystal system	hexagonal	hexagonal	hexagonal
Space group	$P6_3/mmc$	$P6_3/mmc$	$P6_3/mmc$
a **(Å)**	2.93099	2.93093	2.92685
c **(Å)**	17.88722	17.8314	17.69509
$\mathbf{R_{wp}}$**(%)**	4.838	4.157	5.54
GOF	1.50	1.31	1.75

Table S5 The bond lengths of $Cr_2TiAl_{1-x}Si_xC_2$ after 3000 h of corrosion

MAX	**Bond**	**Length (Å)**	**Length variation**
$\mathbf{Cr_2TiAlC_2}$	Cr-A	2.680	−0.814%
	Cr-C	1.984	−0.6%
	Ti-C	2.170	1.59%
$\mathbf{Cr_2TiAl_{0.8}Si_{0.2}C_2}$	Cr-A	2.668	−0.37%
	Cr-C	1.967	−1.0%
	Ti-C	2.190	2.24%
$\mathbf{Cr_2TiAl_{0.6}Si_{0.4}C_2}$	Cr-A	2.653	−0.7%
	Cr-C	1.920	−1.78%
	Ti-C	2.238	1.87%