New insight of the structural evolution of the TiO_2-Ti_3O_5-Ti_2O_3-TiO-$Ti_xO_yC_z$-TiC Systems at Nanoscale During Reduction Process

Yuanyou Xiao[1,2], Pengliang Jin[1], Guocheng Wang[1,2,*] and Lifeng Zhang[3]

[1] School of Materials and Metallurgy, University of Science and Technology Liaoning, Anshan, Liaoning, 114051, PR China

[2] Key Laboratory of Metallurgy Engineering Liaoning Province, University of Science and Technology Liaoning, Anshan, Liaoning, 114051, PR China

[3] College of Materials Science and Engineering, Yanshan University, Qinhuangdao, Hebei, 066004 P. R China.

[*] Correspondence: wang_guocheng@163.com

Table S1 Normalized clustering energies ΔE_N, Ti−O bond distances r , and coordination number CN for the lowest energy structures of $(Ti_xO_y)_n$ (n=1-5) clusters

Clusters	Size	r (Å)		CN	ΔE_N (kJ/mol)
		Average	Range		
$(TiO_2)_n$	n=1	1.666	1.666	2	0
	n=2	1.792	1.647 to 1.864	3	237.084
	n=3	1.873	1.646 to 2.100	3.67	314.938
	n=4	1.891	1.637 to 2.122	4	352.553
	n=5	1.929	1.639 to 2.208	4.2	380.796
$(Ti_3O_5)_n$	n=1	1.840	1.645 to 1.900	3	0
	n=2	1.894	1.824 to 2.080	3.67	272.211
	n=3	1.843	1.827 to 1.853	3.33	356.579
	n=4	1.889	1.795 to 2.181	3.67	441.381
	n=5	1.912	1.790 to 2.215	3.8	458.125
$(Ti_2O_3)_n$	n=1	1.887	1.887	3	0
	n=2	1.862	1.862	3	316.134
	n=3	1.851	1.790 to 1.895	3	388.078
	n=4	1.935	1.840 to 2.050	3.75	439.345
	n=5	1.879	1.827 to 2.073	3.30	432.952
$(TiO)_n$	n=1	1.625	1.625	1	0
	n=2	1.869	1.869	2	215.892
	n=3	1.854	1.854	2	296.347
	n=4	1.895	1.838 to 1.978	2.25	363.870
	n=5	1.897	1.817 to 2.006	2.2	372.144

Table S2 Normalized clustering energies ΔE_N, Ti−C bond distances r , and coordination number CN for $(TiC)_n$ (n=1-10) clusters

Size	r (Å)		CN	ΔE(kJ/mol)
	Average	Range		
n=1	1.672	1.672	1	0
n=2	1.851	1.851	2	369.246
n=3	1.981	1.910 to 2.072	2.67	445.829
n=4	1.961	1.961	3	602.246
n=5	1.976	1.769 to 2.187	3	597.534
n=6	2.015	1.932 to 2.082	3.33	652.878
n=7	2.004	1.767 to 2.186	3.29	634.359
n=8	2.014	1.939 to 2.090	3.50	678.491
n=9	2.026	1.890 to 2.086	3.67	697.855
n=10	2.027	1.941 to 2.102	3.60	693.572