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Electronic Supplementary Information (ESI)

Unraveling the role of substrate materials in governing the carbon/carbide growth of molten carbonate electrolysis of CO_2

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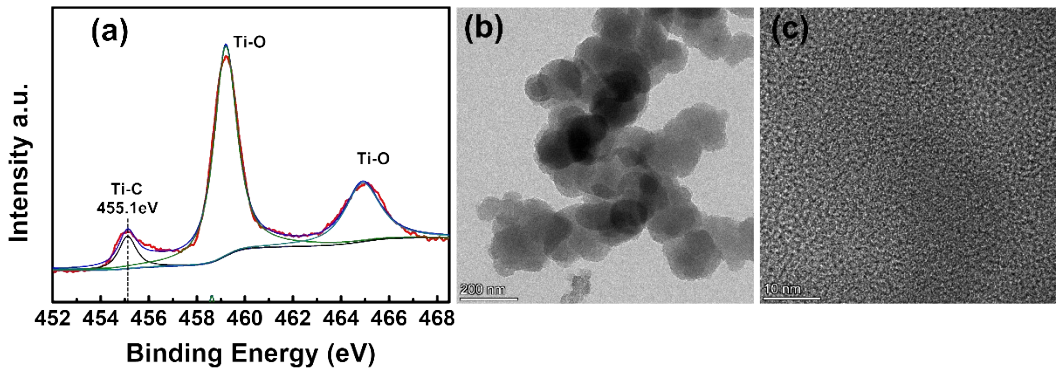

Fig. S1 (a) XPS spectra of Ti cathode after carbon deposition at 5 mA cm^{-2} for 120 min at 650 °C. (b-c) TEM image of carbon particles obtained on Ti cathode after 120 min electrolysis.

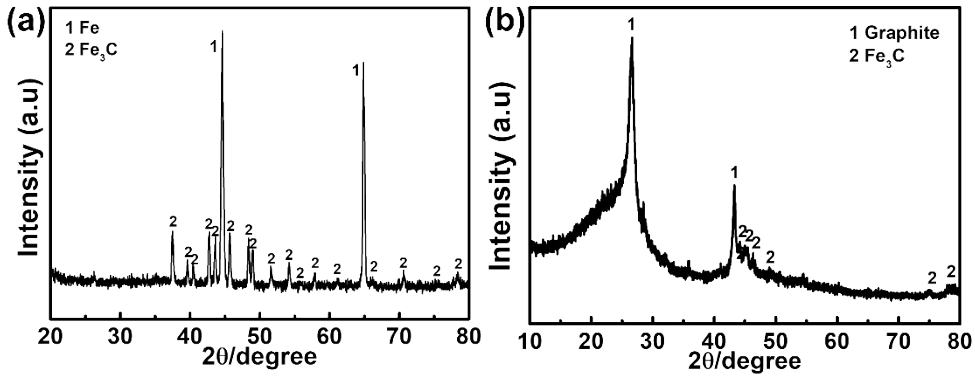

Fig. S2 (a) XRD pattern of Fe substrate after peeling off the powder on the surface after electrolysis at 5 mA cm^{-2} for 120 min at 650 °C. (b) XRD pattern of the peeled powder.

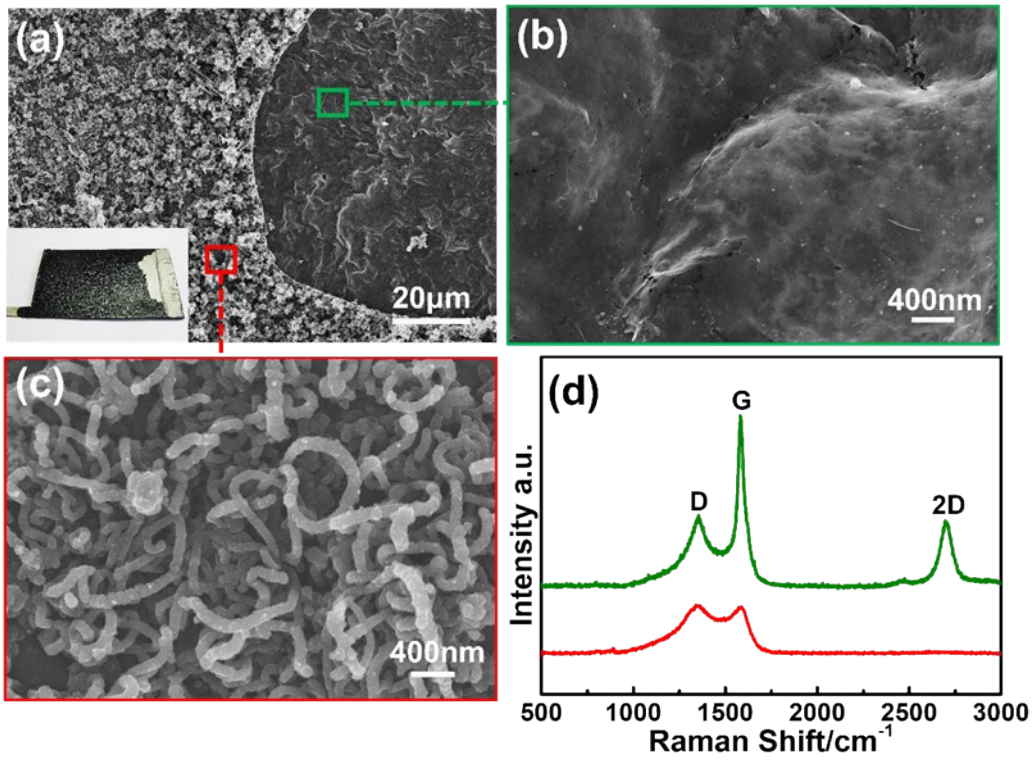

Fig. S3 (a) SEM image of carbon products obtained on Ni at 5 mA cm^{-2} for 120 min at 650 °C. Inset: optical image of the Ni cathode after electrolysis. SEM image of the grey area (b) and the black area (c) in the optical image. (d) Raman spectra of the corresponding areas.

Table S1 Gibbs free energies and equilibrium constants of the reactions between metals/carbides and carbon (carbon-binding ability of metals) at different temperatures (thermodynamic data was calculated by HSC Chemistry 6.0)

Reaction	450 °C		550 °C		650°C		750 °C		850 °C	
	ΔG kJ mol^{-1}	K	ΔG kJ mol^{-1}	K	ΔG kJ mol^{-1}	K	ΔG kJ mol^{-1}	K	ΔG kJ mol^{-1}	K
Ti + C = TiC	-176.2	12.7	-175.1	11.1	-174.1	9.85	-173	8.83	-172	8
2V + C = V_2C	-105.3	7.61	-103.7	6.59	-102.3	5.79	-100.8	5.15	-99.4	4.62
7/3Cr + C = 1/3Cr_7C_3	-59.9	12.9	-61.2	11.6	-62.6	10.6	-64.1	9.82	-65.7	9.16
3/5Cr_7C_3 + C = 7/5Cr_3C_2	-19.9	2.40	-20.1	2.12	-20.3	1.91	-20.5	1.75	-20.8	1.62
2Mo + C = Mo_2C	-52.6	3.80	-53.4	3.39	-54.2	3.06	-55.1	2.81	-55.9	2.6
W + C = WC	-36.6	2.64	-36.3	2.3	-36	2.04	-35.8	1.83	-35.5	1.65
W_2C + C = 2WC	-52.7	3.81	-51.5	3.26	-49.9	2.83	-48.2	2.46	-46.3	2.15
3Fe + C = Fe_3C	8.42	-0.608	5.49	-0.349	2.86	-0.162	0.71	-0.036	-0.87	-0.04
2Co + C = Co_2C	24.8	-1.79	30.7	-1.95	37.7	-2.13	45.7	-2.33	54.6	-2.54
3Ni + C = Ni_3C	57.3	-4.14	55.7	-3.53	54.1	-3.06	52.4	-2.67	50.7	-2.36