chemengineering

MDPI

Supplementary Materials

CNT and H_2 Production During CH_4 Decomposition over $Ni/CeZrO_2$. I. A Mechanistic Study

Agata Łamacz

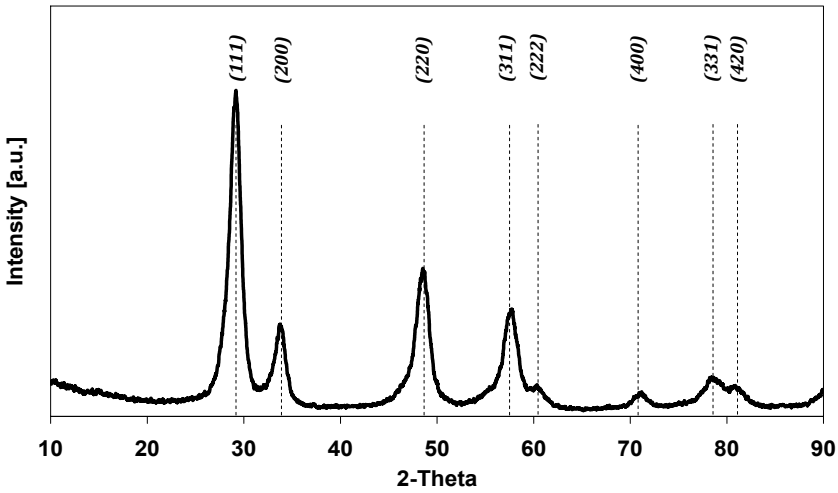

Figure S1. XRD of $CeZrO_2$ support.

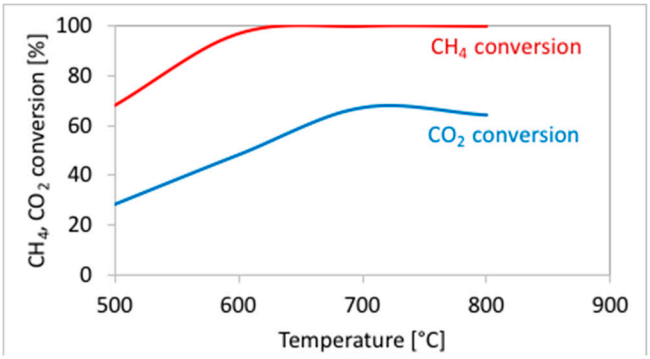

Figure S2. CH_4 and CO_2 conversion during dry reforming of methane over $Ni/CeZrO_2$@CNT hybrid catalyst.

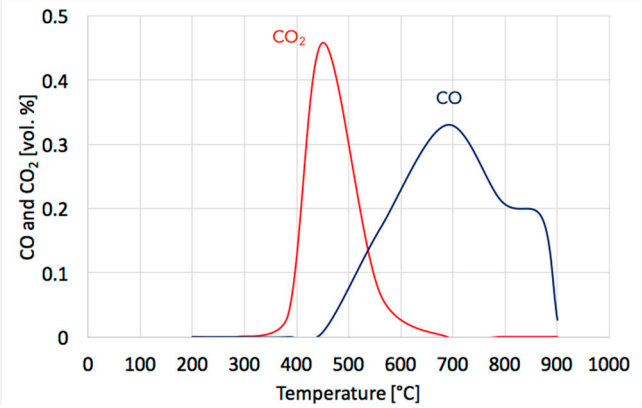

Figure S3. Temperature profile for spent $Ni/CeZrO_2$ in flowing Ar.

Table 1. Weight increase for powder Ni/$CeZrO_2$ after decomposition of 10 vol.% CH_4/Ar at 500, 600 and 700 °C for 3 h.

T (°C)	9.1 wt.% Ni/$CeZrO_2$		23.1 wt.% Ni/$CeZrO_2$	
	Mass Increase (%)	**C/Ni (mol/mol)**	**Mass Increase (%)**	**C/Ni (mol/mol)**
500	6.6	3.5	10.2	2.2
600	13.1	7.0	14.8	3.1
700	15.9	8.5	18.5	3.9
800	10.6	5.7	11.3	2.4

The powder Ni/$CeZrO_2$ after CO treatment at 500 °C (11 wt.% of carbon in the sample) was heated to 900 °C in flowing Ar (Figure S1). The oxidation of the most reactive carbon deposits to CO_2 with lattice oxygen from $CeZrO_2$ (Equation (S1)) occurred from ca. 350 °C. From 400 °C CO_2 and decreased with the simultaneous formation of CO, which indicates that CO_2 is consumed in the oxidation of carbon deposits (Equations (S2) and (S3)).

$$C^* + O^* = CO + 2^* \quad \text{(S1)}$$

$$CO_2 + * = CO + {}^*O(\text{ex. } CO_2) \quad \text{(S2)}$$

$$C^* + O^*(\text{ex. } CO_2) = CO + 2^* \quad \text{(S3)}$$