Data in brief 24 (2019) 104010

Contents lists available at ScienceDirect

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Data Article

Data on TGA of precursors and SEM of reduced Cu/ZnO catalysts co-modified with aluminium and gallium for methanol synthesis

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A R T I C L E I N F O

Article history:
Received 19 March 2019
Received in revised form 6 May 2019
Accepted 9 May 2019
Available online 16 May 2019

Keywords:
Methanol synthesis
Copper
Zinc
Gallium
Catalysts

A B S T R A C T

The modification of Cu−Zn catalysts with low amount of Al and Ga (Al+Ga = 3%) was investigated and data corresponding to its influence on the decomposition of the calcined precursors and on the nanomorphology and surface concentration of reduced catalysts were presented in this contribution. The data presented here are supplementary material of the catalysts presented in the *research article "Structure and activity of Cu/ZnO catalysts co-modified with aluminium and gallium for methanol synthesis" published in Catalysis Today* [1].

DOI of original article: https://doi.org/10.1016/j.cattod.2019.03.034.
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https://doi.org/10.1016/j.dib.2019.104010

Specifications Table

Subject area	*Chemical Engineering*
More specific subject area	*Catalysis*
Type of data	*Images and figures*
How data was acquired	*Scanning Electron Microscope with energy-dispersive X-ray spectroscopy (Hitachi TM-1000)* *Thermo balance with* heat flow (DSC) and weight changes (TGA) *(Mettler Toledo 85e3)*
Data format	*Analysed*
Experimental factors	*Calcined precursors of catalysts were obtained* by thermal treatment in air of hydroxycarbonate precipitates. The reduced catalysts were obtained from reduction of calcined precursors under a mixture of H_2/Ar
Experimental features	Thermal decomposition of calcined precursors was studied by thermogravimetry analysing the gas produced by mass spectrometry. The nanomorphology and surface composition of the reduced catalysts were obtained by Scanning Electron Microscopy with energy-dispersive X-ray spectroscopy.
Data source location	*Sustainable energy and chemistry Group, Institute of Catalysis and Petrochemistry (CSIC) Madrid, Spain*
Data accessibility	*Data are provided in this article*
Related research article	*Associated to the research article "Structure and activity of Cu/ZnO catalysts co-modified with aluminium and gallium for methanol synthesis" in Catalysis Today* [1]

Value of the data

- The data corresponding to the thermal decomposition of calcined CuO/ZnO precursors indicated that the co-modification with low amount of Al and Ga (Al+Ga = 3%) influences on their carbonate retentionSEM data show that there are not significant differences in the structuration and agglomeration of Cu/ZnO reduced catalyst particles with the modification with Al and Ga.
- The energy-dispersive X-ray spectroscopy on reduced Cu/ZnO catalysts revealed the homogeneous composition of the catalyst particles modified with Al and Ga.

1. Data

Morphological changes of reduced Cu/ZnO catalysts modified with Al and Ga were analysed by SEM (Fig. 1). Reduced catalysts show similar irregular particles irrespective of the Al and Ga modification. Surface analysis by EDX of reduced Cu/ZnO catalysts modified with Al and Ga (Fig. 1) revealed the homogeneous composition in all analysed particles of catalysts.

The carbonate retention on calcined precursors was analysed by TGA-MS (Fig. 2). The precursors co-modified with Al and Ga show higher concentration of carbonates which decompose at temperatures higher than 500 °C. These carbonates improve the activity and stability of the catalysts obtained after reduction of the calcined precursors.

2. Experimental design, materials, and methods

The calcined precursors were prepared by coprecipitation of metal nitrates solutions with sodium or ammonium carbonate to generate mixed hydroxycarbonates [2] followed by calcination in air at 340 °C. Reduced catalysts were obtained by reduction of calcined precursors under diluted hydrogen flow (2.21 vol % H2) at 200 °C (see Table 1).

The morphology of the particles in the reduced catalysts was studied by Scanning Electron Microscopy (Hitachi TM-1000). Surface analysis was performed by energy-dispersive X-ray spectroscopy.

Thermal decomposition of calcined precursors was studied by thermogravimetry (Mettler Toledo TGA/SDTA 851e). Decomposition was performed under 25 mL/min of a mixture of O_2 (20 vol %)/Ar from 40 °C to 600 °C (heating ramp = 10 °C/min). The gas products during decomposition (H_2O, CO, CO_2) were analysed by mass spectrometry (Baltzer Prisma QMS 200 TM) quadrupole mass spectrometer.

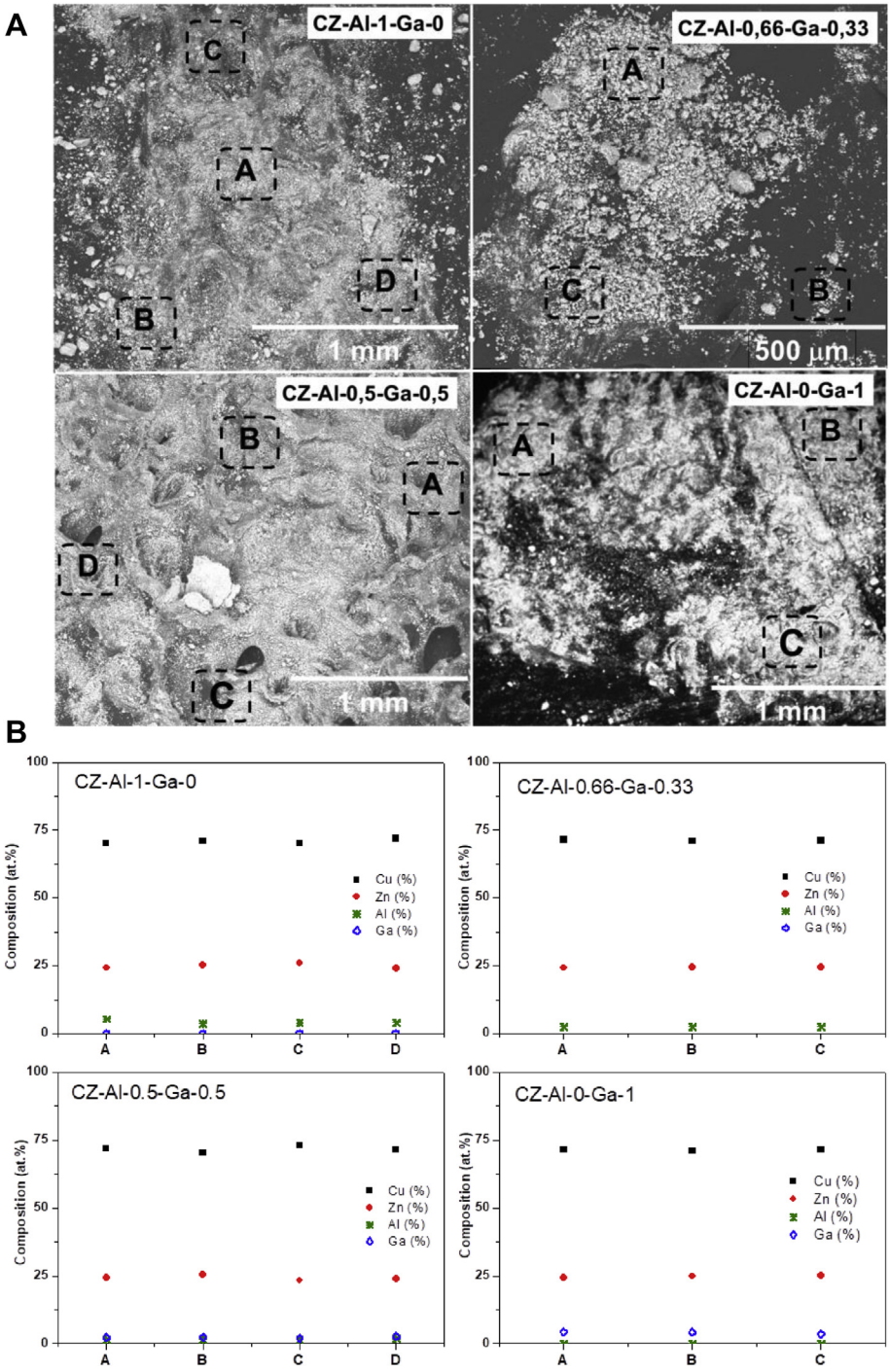

Fig. 1. SEM (a) and EDX composition (atomic %) (b) on different areas of CZ-Al-xGa catalysts: CZ-Al-1-Ga-0, CZ-Al-0.66-Ga-0.33 CZ-Al-0.5-Ga-0.5 and CZ-Al-0-Ga-1.

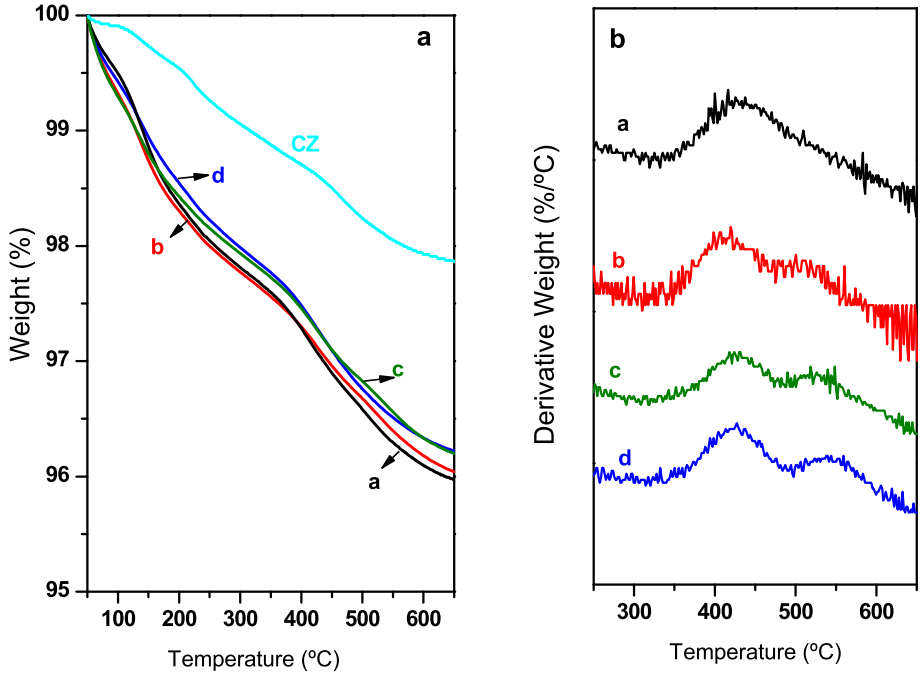

Fig. 2. TGA (a) and DTA (b) corresponding to the thermal decomposition of calcined precursors: (a) CZ-Al-1-Ga-0, (b) CZ-Al-0.66-Ga-0.33 (c) CZ-Al-0.5-Ga-0.5 and (d) CZ-Al-0-Ga-1.

Table 1
Composition of calcined precursors.

Nomenclature	wt %			
	CuO	ZnO	Ga_2O_3	Al_2O_3
CZ-Al-1-Ga-0	68.2	29.9	0.0	1.9
CZ-Al-0.66-Ga-0.33	67.8	29.7	1.3	1.2
CZ-Al-0.5-Ga-0.5	67.6	29.6	1.0	1.8
CZ-Al-0-Ga-1	67.1	29.4	3.5	0.0

Acknowledgments

The present investigation was performed within the research program CTQ2016-76505-C3-1 supported by the Spanish Ministry of Science, Innovation and Universities. Elena Millán would like to acknowledge the FPI programme from Spanish Ministry of Science, Innovation and Universities for the research grant.

Transparency document

Supplementary data to this article can be found online at https://doi.org/10.1016/j.dib.2019.104010.

References

[1] Structure and activity of Cu/ZnO catalysts co-modified with aluminium and gallium for methanol synthesis, Catalysis Today (2019). https://doi.org/10.1016/j.cattod.2019.03.034.
[2] J. Schumann, T. Lunkebein, A. Tarasov, N. Thomas, R. Schlögl, M. Behrens, ChemCatChem 6 (2014) 2889–2897.