DOI 10.5162/EUROSENSORS2025/MP5

(MgCoNiCuZn)O High-Entropy Oxide as Novel Gas Sensing Material

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Summary:
We report the performance of (MgCoNiCuZn)O material as chemoresistive gas sensor, both against reducing and oxidizing agents at different temperatures. The active material has been synthetized by mixing the different oxides in the form of nanopowers and applying a thermal treatment at 1000 ºC for several hours, quenching the resulting rock-salt compound by a rapid cooling. The structural characterization confirms the formation of a uniform elemental distribution and single-phase formation. The chemoresistive response of the material has been assessed against several gases, such as humidity, sulfur dioxide and methane. We determined the p-type semiconductor character of the material and get first insights of its temperature behavior and its sensing mechanisms.

Keywords: high entropy oxide, chemoresistor, gas sensing, humidity sensor, sulfur dioxide.

Headlines

We are exploring the gas sensing performance of (MgCoNiCuZn)O material, belonging to the so-called High Entropy Oxides category, a novel class of materials that owns a wide range of interesting properties and behaviors.

We demonstrate the semiconducting and chemoresistive nature of this material via its optical and electrical properties as well as characterizing its gas sensing behavior when working at different temperatures.

Background, Motivation and Objective

Since 2015 (MgCoNiCuZn)O has been synthesized as a rock salt belonging to the so-called High Entropy Oxides (HEO). This class of materials can present a stable single phase, despite the variety of crystalline structures of the individual binary oxides which are composing it [1]. Their complex composition gives rise to enhanced functional properties, such as outstanding thermal stability, low thermal conductivity and tunable electronic, magnetic, and catalytic properties [2].

We are interested in exploring the performance of this material as a gas sensor. Similarly to other HEOs with a different composition, the chosen multicomponent oxide is thought to behave as an improved gas sensor due to its peculiar properties. Among the features that would enhance its sensing ability, one would include the large variety of sites at the surface for absorption of gas molecules and the strong thermal endurance at high temperatures and under extreme conditions such as resilience to harsh gas species [3]. One can foresee a large flexibility in tailoring the composition of the material to adapt it to a specific sensing application.

We aim at fabricating dedicated test samples of this material to convert them into the active region of a gas sensor. A comprehensive structural analysis is mandatory in order to fully assess the actual composition and crystalline status of the fabricated compound. Finally, a set of dedicated experiments are able to provide the chemoresistive response towards reducing and oxidizing gases, enabling us to assess the quality of the material as gas sensor.

Methodology

Starting from a homogenous mixing of the single oxide components in the form of nanopowders, the resulting mixture was annealed at 1000 ºC for several hours and then rapidly cooled in order to stabilize the material to the desired structure.

X-ray diffraction confirmed the rock-salt crystalline structure, and at the same time allowed to discard the presence of secondary phases. Additionally, the lattice parameters are in agreement with the ones reported in literature within a range of 2%.

Elemental mapping by Energy Dispersive X-Ray Spectroscopy confirms the homogeneous distribution of all the metallic components in the resulting powder, with an average grain size of few micrometers, while from optical transmission measurements we estimated a direct optical bandgap of 1.4 eV.

In order to perform the gas measurements, the fabricated powder was dispersed onto an interdigitated metallic pattern engraved on a silica slab, mounted on a TO8 support together with a micro-heater and a temperature sensor. The resulting sensor is shown in Figure 1.

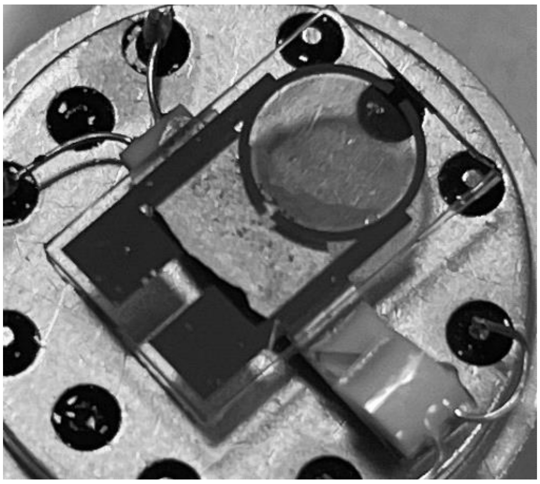

Fig. 1. Picture of one the fabricated gas sensors based on the synthetized (MgCoNiCuZn)O powder acting as active media.

Results

We will present and discuss the gas sensing behavior observed for the fabricated structures when exposed to humidity, CH_4, and SO_2, in a wide range of temperatures and gas concentrations. The temperature behavior of the device resistance and the rectifying characteristics of the electrical contacts point to the semiconducting character of the active synthetized material. A typical example of the recorded chemoresistive change under the flow of a train of gas pulses is depicted in Figure 2. The tracking of the relative response of the sensor as a function of temperature enables us to single out the optimal operation temperature. A value of 140 ºC was attained, which corresponds to a maximum response of 60% towards a humidity pulse of 80%. A complete analysis of the interaction and recovery time allows us to get insight on the detection mechanisms. The demonstration of the chemoresistive character of such novel material paves the way to further studies and applications in the field of the chemical resistive sensors.

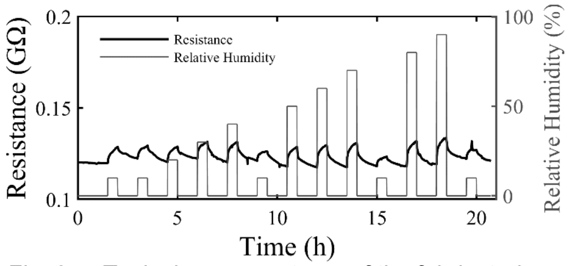

Fig. 2. Typical response trace of the fabricated sensor towards a train of relative humidity pulses.

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Acknowledgements

This work has been financially supported by the MICIU/AEI/10.13039/501100011033 and ERDF, EU under project PID2023-151565OB-C44 and by the Horizon Europe's Marie Skłodowska-Curie grant agreement No 101109501.