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Advanced hydrogen-gas sensing materials with a tailored architecture

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1 Motivation

The popularity of hydrogen in the energy market has heightened in the past few years since it is light, storable and energy dense while also producing no direct emissions of pollutants or greenhouse gases. Monitoring of hydrogen concentration through all technological steps (production, storage, transport and reconversion) is therefore of profound importance. The rapidly developing hydrogen based technologies demand new materials with enhanced response characteristics to hydrogen for precise monitoring of the gas concentration. Thanks to the significantly high specific surface area, nanostructured materials have shown promise as prompt and efficient hydrogen sensors.

In this work, we focus on nanomaterials composed of nanoparticles in the form of thin film prepared using a custom built magnetron-based gas aggregation source (MGA). Advantage of synthesis using MGA is that it can be used to produce nanoparticles in a relatively wide range of particle size and to an extend allow control of the size of nanoparticles by regulating operation parameters. Production is clean and the range of synthesizable materials is virtually unlimited since no precursors are used. The main goal of this project is to study the relationship between composition, structure, architecture and properties of the prepared films resulting in the development of functional thin-film materials with unique properties and thus having high application potential as conductometric hydrogen sensors – low cost, high sensitivity sensors. The experimental work will be supported by computer simulations

2 Principle

Very often, metal-oxide semiconductors (MOS) are employed as conductometric hydrogen sensors where the semiconductor works as a chemiresistor directly converting chemical response to electronic signal. The basic sensory mechanism of a conductometric sensor for a reducing gas such as hydrogen is explained below.

Oxygen in the atmosphere adsorbs onto the surface of the semiconductor (particularly n-type) and takes away electrons from the semiconductor. This leads to formation of depletion zone near the surface and consequently reduced electrical conductivity. When hydrogen is introduced, the hydrogen molecule is dissociated on the surface (due to elevated temperature or a noble-metal catalyst) and react with pre-adsorbed oxygen species. The reaction gives back

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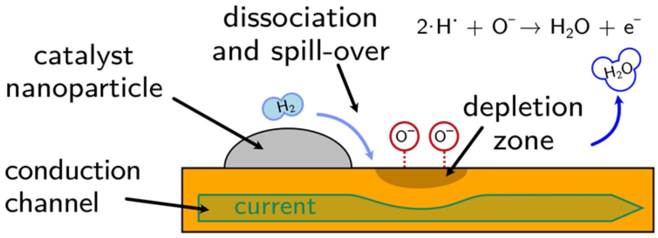

Figure 1: Illustration of explanation of sensing principle

electrons to the surface reducing the depletion zone and increasing conductivity.

Nanostructuring increases the effective active surface area for adsorption of gases. The changes induced by exposure to gas and the following reactions influence the overall transport of charge carriers through the material. The inter-grain necks formed on grain boundaries are highly sensitive to target gas. Hence the grain size, the inter-grain necks and the geometry of these inter-grain junctions affects the overall change of conductivity in the material when exposed to target gas.

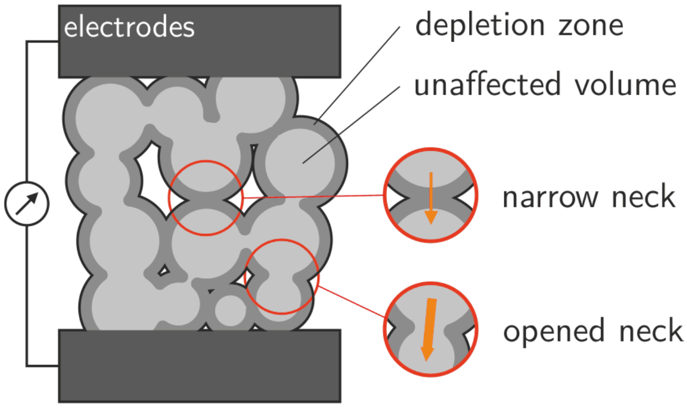

Figure 2: Illustration showing the effect of geometry of inter-grain junctions on conductivity - narrow necks with space charge region restricting charge carrier flow and open necks providing free path to flow of charge carriers

Tailoring the architecture of the percolated network of individual nanoparticles therefore has profound impact on the junctions formed between the individual blocks and the formed depletion zones. This in turn significantly affects the conduction channels in the material. Consequently, nanostructuring produces highly efficient conductometric sensors.

References

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