

Investigation of Au doped SnO₂ gas sensors using transient IR spectroscopy

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For the rational design of sensor materials, a deep understanding of the underlying mechanism of gas sensing and the influence of surface doping is of great importance. For the investigation of gas sensors, powerful *in situ* spectroscopic techniques are available, as shown previously^[1-3]. For detailed analysis of the structural dynamics, leading to new mechanistic insight, these approaches can be supplemented with transient spectroscopic methods such as modulation-excitation (ME) DRIFT spectroscopy. Here, we present a detailed ME-DRIFTS study of the mechanism of gold-loaded tin oxide (Au/SnO₂) during ethanol gas sensing, in combination with resistance measurements and further characterization by XRD, UV-Vis and XPS^[4].

Resistance measurements show that the loading of Au on tin oxide leads to an increase in sensor response. In contrast to unloaded tin oxide, a maximum in sensor response is observed that shifts to lower operating temperature with increasing gold loading. Interestingly, the course of the resistance can be correlated with the integrated intensity of a broad mid-IR absorption, which occurs upon temperature changes and under reductive conditions. This mid-IR absorption is attributed to the absorption of electrons in the conduction band on the one hand and optical transitions of shallow trapped electrons into the conduction band on the other^[5]. In addition to time-resolved DRIFTS measurements and the analysis of the temporal progression of selected bands, modulation excitation spectroscopy (MES) was used to investigate ethanol gas sensing over SnO₂ and Au/SnO₂. This enabled the observation of a new surface species at 2030-2060 cm⁻¹, which is an intermediate not present for unloaded SnO₂ and which is tentatively assigned to CO adsorbed on negatively loaded gold particles (CO-Au^{δ-}). These findings were combined with results from XP and UV-VIS spectroscopy, confirming that there is no dominant electronic influence of gold on the sensor material, since gold is only present in its metallic state. No change in the absorption maxima and absorption edge is observed when SnO₂ is loaded with gold. Thus, we conclude that the increase in sensor response is caused by an oxygen spillover from gold to the SnO₂ surface.

Summarizing, we demonstrate the potential of transient IR spectroscopy to unravel new insight into the mode of operation of metal-oxide gas sensors as illustrated by gold loaded tin oxide used for ethanol gas sensing^[4].

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