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Heterostructure-based devices with enhanced humidity stability for H2 gas sensing applications in breath tests and portable batteries

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Abstract

Semiconducting metal oxide - based gas sensors exhibit outstanding sensitivity, although humidity in the analyte typically hampers precise measurements. In this work it was shown that a 5–6 nm thin Al2O3 nano-layer is particularly beneficial in reducing the interference due to humidity of p-type conductivity copper oxide-based gas sensors. An effective approach from chemical solutions at 75 °C and thermal annealing at 600 °C was used to grow copper oxide nano-crystallite layers. The Al2O3 nano-layers were subsequently deposited on top of copper oxide by atomic layer deposition in a high-aspect-ratio regime at 75 °C. The morphological, structural, chemical, vibrational, electronical and sensor characteristics of the heterostructured nano-crystallite layers have been studied. The final nano-Al2O3/CuO heterostructure showed an increase in the response to H2 gas by 140 %, while long-term stability at low and high relative humidity was observed. The initial sensing response varied by only 10 % for an Al2O3 layer of 5–6 nm on top of CuO with a post-thermal annealing at 600 °C acting as an effective barrier for water vapor and oxygen. A comparison with CuO nanocrystallite layers covered by ALD with 6 nm and 15 nm of Al2O3 ultra-thin films on top

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demonstrates an exceptional stability of the hydrogen gas response at high relative humidity (84 % RH). Density functional theory-based calculations showed that the H2 molecule spontaneously dissociates over the formed Al2O3/CuO heterostructure, interacting strongly with the surface Al atoms, showing different behavior compared to the pristine CuO (111) surface, where H2 gas molecules are known to form water over the surface. The present study demonstrates that a thorough optimization of technology and surface properties due to coverage and formation of heterostructured nano-materials improves the humidity stability during H2 gas sensing applications which is important for real-world applications, e.g. portable battery analysis, H2 breath tests, along with environmental, medicine, security, and food safety diagnostic tests.