Sensing performance of $CuO/Cu_2O/ZnO:Fe$ heterostructure coated with thermally stable ultrathin hydrophobic PV3D3 polymer layer for battery application

https://doi.org/10.1016/j.mtchem.2021.100642

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Abstract
Gas sensors are demanded in many different application fields. Especially the ever-growing field of batteries creates a great need for early hazard detection by gas sensors. Metal oxides are well known for gas sensing; however, moisture continues to be a major problem for the sensors, especially for the application in battery systems. This study reports on a new type of moisture protected gas sensor, which is capable to solve this problem. Sensitive nano-materials of CuO/Cu2O/ZnO:Fe heterostructures are grown and subsequently coated with an ultrathin hydrophobic cyclosiloxane-polymer film via initiated chemical vapor deposition to protect the sensor from moisture. The monomer 1,3,5-trimethyl-1,3,5-trivinylcyclotrisiloxane is combined with the initiator perfluorobutanesulfonyl fluoride to obtain hydrophobic properties. Surface chemistry, film formation and preservation of functional groups are confirmed by X-ray photoelectron spectroscopy and Fourier-transform infrared spectroscopy. It turns out that the hydrophobicity is retained even after annealing at 400 °C, which is ideal for gas sensing. Molecular distances in the polymer nanolayer are estimated by geometry optimization via MMFF94 followed by density functional theory. Compared with unprotected CuO/Cu2O/ZnO:Fe, the coated CuO/Cu2O/ZnO:Fe exhibit a much better sensing performance at a higher relative humidity, as well as tunability of the gas selectivity. This is highly beneficial for hazard detection in case of thermal runaway in batteries because the sensors can be used under high concentrations of relative humidity, which is ideal for Li–S battery applications.