Developing Surface-Functionalized Gallium Nitride Nanostructured Devices for Resolving Cross-sensitivity of Chemical/Gas Sensors: Modeling and Experimental

ECE Doctoral Research Seminar Presentation

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There is a great need for the development of highly selective sensors for detecting various toxic gases and their mixtures in many industrial, medical, space exploration and environmental monitoring applications. Metal oxide-based sensors to detect these environmental pollutants have been the subject of intensive research for several decades. However, these metal oxide sensors lack precise selectivity towards any specific analyte. In this work, GaN nanowires have been formed on Si substrate using industry standard stepper lithography and top-down approach. Different functionalized devices were prepared by the deposition of metal oxides- TiO_2, ZnO, WO_3 and SnO_2 by optimized RF sputtering on nanowires followed by rapid thermal annealing. To examine the real-world applicability of the fabricated sensor devices, their gas sensing properties, including adsorption and desorption rate, cross-sensitivity to interfering gases, and long-term stability at various environmental conditions were investigated. Fundamental electronic interactions and thermodynamics between the gas molecular adsorption on ideal metal-oxide surfaces have been investigated with Density Functional Theory (DFT) molecular simulations. The functionalized GaN in contact with gas molecules was designed and geometrically optimized. Simulation results revealed the most energy favorable surface for chemical/gas adsorption. In addition, the electronic properties of these oxide functionalized GaN have been studied in terms of the total density of states (TDOS) and projected density of states (PDOS).

A sensor array has been designed and developed comprising of functionalized GaN nanowires. The receptor metal/metal-oxide combinations within the array have been determined from prior molecular simulation results. Each gas produced a unique response pattern across the sensors within the array by which cross-sensitive gases were precisely identified. Unsupervised principal component analysis (PCA) technique was applied on the array response. It is found that each analyte gas forms a separate cluster in the score plot for all the target gases and their mixtures, indicating a clear discrimination among them. Then, supervised machine learning algorithms such as- Decision Tree, Support Vector Machine (SVM), Naive Bayes (kernel), k-Nearest

Neighbor (k-NN), and artificial neural network (ANN) were trained and optimized using their significant parameters with our array dataset for the classification of gas type. Statistical and computational complexity results indicated that back-propagation neural network stands out as the optimal classifier among the considered ANN algorithms. Then, ppm concentrations of the identified gases have been estimated using the optimal model. In another study, TiO_2 functionalized GaN nanowire-based back-gate FET device has been designed and implemented to address the well-known cross-sensitive nature of metal oxides. Here, Si back-gate with C-AlGaN as the gate-dielectric has been demonstrated as a tunable parameter, which enhances discrimination of these cross-sensitive gases at room temperature (20 ^{o}C). Compared to no bias, back-gate bias resulted in a significant 60% increase in NO_2 response, whereas the increase is an insignificant 10% in SO_2 response. At last, sensor die/process and packaging reliabilities of metal-oxide/GaN nanowire-based gas sensors have been studied for the first time, using industry standard accelerated lifetime tests, such as- High Temperature Operating Life, High Temperature Storage Life, Temperature Cycling Test and Highly Accelerated Stress Test. The method for estimating failure rate and lifetime of GaN nanowire devices has been developed. Using statistical data from the performed accelerated stress tests, chi-square distribution has been implemented to predict the failure rate and lifetime of GaN nanostructured sensor devices.