

Sensing Mechanisms for Carbon Nanotube Based NH₃ Gas Detection

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ABSTRACT

There has been an argument on carbon nanotube (CNT) based gas detectors with a field-effect transistor (FET) geometry: do the response signals result from charge transfer between adsorbed gas molecules and the CNT channel and/or from the gas species induced Schottky barrier modulation at the CNT/metal contacts? To differentiate the sensing mechanisms, we employed three CNTFET structures, i.e., (1) the entire CNT channel and CNT/electrode contacts are accessible to NH₃ gas; (2) the CNT/electrode contacts are passivated with a Si₃N₄ thin film, leaving the CNT channel open to the gas and, in contrast, (3) the CNT channel is covered with the film, while the contacts are open to the gas. We suggest that the Schottky barrier modulation at the contacts is the dominant mechanism from room temperature to 150 °C. At higher temperatures, the charge transfer process contributes to the response signals. There is a clear evidence that the adsorption of NH₃ on the CNT channel is facilitated by environmental oxygen.

The carbon nanotube (CNT)¹ has a great potential in miniaturized chemical/biological sensing applications. The small size, large surface to volume ratio, and highly sensitive electrical properties make CNTs arguably the ultimate candidate for nanosensors. Kong et al. demonstrated the first CNT gas sensors in 2000.² Since then, many techniques have been developed to improve the performance of CNT gas sensors, including polymer functionalization, metal nanoparticle decoration, etc.^{3–10} Although tremendous progress has been achieved, the underlying sensing mechanism still remains unclear. Previously proposed mechanisms include the indirect interaction through the hydroxyl group on SiO₂ substrate² or preadsorbed water layer,¹¹ adsorption of gas molecules at the interstitial sites in the CNT bundle,¹² direct charge transfer from the adsorbed gas molecules to CNT,¹³ and modulation of the Schottky barrier (SB) at CNT/metal contacts,¹⁴ etc. Until now, there is no unifying work able to identify the mechanisms. Furthermore, in order to optimize the CNT sensor for practical applications, it is important to understand whether the sensing signals result from the CNT channel and/or the CNT/metal contacts. Using a short-channel device with passivated CNT/metal contacts by thermally evaporated SiO, Bradley et al. found good sensitivity to NH₃ and suggested that NH₃ mainly interacts with the CNT channel.¹⁵ Zhang et al. argued that when the passivation length was comparable to the depletion length

in the CNT, the contacts could be indirectly affected. In their work, poly(methyl methacrylate) (PMMA) was applied to protect the CNT/metal contacts from NO₂ exposure and their devices became insensitive after contact passivation.¹⁶ Interestingly, Liu et al. also employed PMMA as a passivation layer. They observed changes in the transfer characteristics upon exposure to NH₃ and NO₂ for both contact-passivated and channel-passivated devices, suggesting that both the CNT channel and the CNT/metal contacts play a role in the detection process.¹⁷ The obvious ambiguity in those reports could arise from the permeable passivation materials used. Moreover, as the experiments were carried out at room temperature and air ambient only, exclusive identification of the sensing mechanisms is not possible.

In this paper, we differentiate the sensing mechanisms using a selective Si₃N₄ passivation technique. The sensing signals from the CNT channel and CNT/metal contacts are truly distinguished. Strikingly distinct sensing performance at various testing conditions is observed. From our results, a clear understanding of gaseous interactions in a CNT sensor with field-effect transistor (FET) geometry is obtained.

Single-walled CNTs (SWNTs) were aligned between Ti/Au source and drain electrodes predefined on a p-type silicon wafer using an ac dielectrophoresis (DEP) technique,^{18,19} which is simple and cost-effective, suitable for CNT sensor fabrications. Note that the CNTs in this work are on top of Au electrodes and the contact regions are fully accessible to the ambient. A heavily doped Si with a 200 nm thick

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