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Correction: Enhanced room temperature NO₂ response of NiO–SnO₂ nanocomposites induced by interface bonds at the p–n heterojunction

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Correction for 'Enhanced room temperature NO₂ response of NiO–SnO₂ nanocomposites induced by interface bonds at the p–n heterojunction' by Jian Zhang *et al.*, *Phys. Chem. Chem. Phys.*, 2016, 18, 5386–5396.

The authors wish to revise several paragraphs of their article, beginning on page 5393, left column, line 31 in order to correct an error with an equation used and the subsequent discussion in the text. The amended section is provided below:

To further elaborate the sensing mechanism of the heterojunction, the surface band bending diagrams, involving the interface potential, are employed, as shown in Fig. 10. Commonly, the conductance of materials is dependent on carrier density and mobility, therefore, the conductance of NiO can be expressed as:⁴⁸

$$\sigma = qp\mu \quad (2)$$

where μ is the hole mobility, and q is the elementary electron charge, and p is the hole density. For the bare NiO, there is no contact potential because the Fermi level is kept always constant before or after the NiO nanosheets exposure to NO₂ gas, so that the NO₂ adsorption has little influence on the contact potential and the hole mobility. Therefore, the change in the conductance of the bare NiO is mainly dependent on the change in the surface accumulated hole density induced by NO₂ adsorption. According to eqn (1), the sensitivity of the bare NiO can be expressed as:

$$S_{\text{NiO}} = \frac{G_{\text{NO}_2} - G_{\text{air}}}{G_{\text{air}}} = \frac{p_{\text{NO}_2}}{p_{\text{air}}} - 1 \quad (3)$$

For a p-type semiconductor, the conduction process is mainly dominated by the surface hole accumulation layer component. And the hole density in the surface accumulation layer can be expressed as:⁵⁰

$$p_s = p_b \exp\left(\frac{qV_s}{2kT}\right) \quad (4)$$

where qV_s is the surface band bending, p_b is the hole concentration in bulk and p_s is the hole density in the surface accumulation layer. Coming back to the relationship between the sensor signal and the surface band bending, as defined by eqn (3) and (4), one can obtain that:

$$S_{\text{NiO}} = \frac{p_{\text{NiO}} \exp\left(\frac{qV_{\text{NO}_2}}{2kT}\right)}{p_{\text{NiO}} \exp\left(\frac{qV_{\text{air}}}{2kT}\right)} - 1 = \exp\left(\frac{q\Delta V}{2kT}\right) - 1 \quad (5)$$

For the NiO–SnO₂ nanocomposites, the situation is different. The interface potential is formed as a result of the differences in the Fermi level of the p-type NiO and the n-type SnO₂, and the electron transfer from the SnO₂ to NiO should overcome the interface

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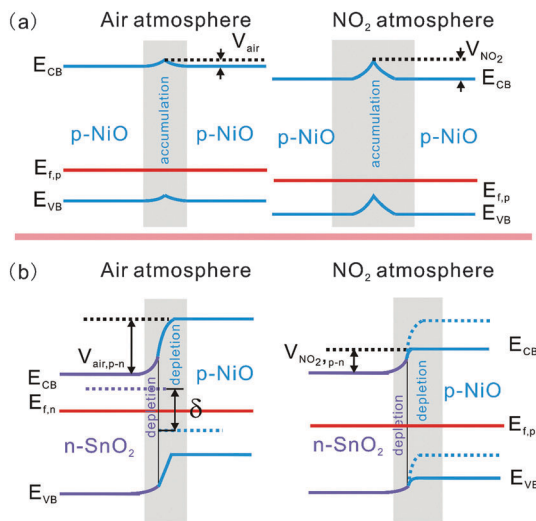


Fig. 10 The schematics and band diagrams of the bare NiO (a) and the NiO-SnO₂ heterojunction (b).

potential. Therefore, the sensitivity of the NiO-SnO₂ depends not only on the carrier density but also on the carrier mobility, and it can be expressed as:

$$S_{\text{NiO-SnO}_2} = \frac{G_{\text{NO}_2} - G_{\text{air}}}{G_{\text{air}}} = \frac{n_{\text{NO}_2} \mu_{\text{NO}_2}}{n_{\text{air}} \mu_{\text{air}}} - 1 \quad (6)$$

As the carrier mobility is dependent on the interface potential, the carrier mobility can be expressed as:⁴⁹

$$\mu = \mu_0 \exp\left(-\frac{qV_{p-n}}{kT}\right) \quad (7)$$

where μ_0 is the mobility without interface potential. And V_{p-n} is the interface potential, which is equal to the contact potential δ without surface states. It should be noted that the interface potential attenuates drift mobility of carriers and thus increase the resistance of the heterojunction nanocomposites, which is consistent with the former results of the largely decreased initial conductance of the NiO-SnO₂. After exposure to NO₂, the interface band bending aroused by the NO₂ adsorption leads to the decrease of the interface potential. Therefore, from eqn (6) and (7), one obtains:

$$S_{\text{NiO-SnO}_2} = \frac{n_{\text{NO}_2}}{n_{\text{air}}} \exp\left[\frac{q(V_{\text{air},p-n} - V_{\text{NO}_2,p-n})}{kT}\right] - 1 \quad (8)$$

Additionally, the carrier concentration of heterojunction nanocomposites is determined by the interface potential, and the carrier concentration of the nanocomposites can be expressed as:

$$n_s = n_b \exp\left(-\frac{qV_{s,p-n}}{kT}\right) \quad (9)$$

where $V_{s,p-n}$ is the interface potential. Accordingly, the sensitivity of the NiO-SnO₂ nanocomposites, as defined by eqn (8), can be further expressed as:

$$\begin{aligned} S_{\text{NiO-SnO}_2} &= \frac{n_{\text{NiO-SnO}_2} \exp\left(-\frac{qV_{\text{NO}_2,p-n}}{kT}\right)}{n_{\text{NiO-SnO}_2} \exp\left(-\frac{qV_{\text{air},p-n}}{kT}\right)} \exp\left[\frac{q(V_{\text{air},p-n} - V_{\text{NO}_2,p-n})}{kT}\right] - 1 \\ &= \exp\left[\frac{q(V_{\text{air},p-n} - V_{\text{NO}_2,p-n})}{kT}\right] \exp\left[\frac{q(V_{\text{air},p-n} - V_{\text{NO}_2,p-n})}{kT}\right] - 1 \end{aligned} \quad (10)$$

Comparing eqn (5) with eqn (10), the sensitivity of the NiO-SnO₂ heterojunction is characterized by two factors, involving the changes both in the carrier density and in the carrier mobility induced by NO₂ adsorption, while the sensitivity of the bare NiO is only dependent on the changes in the surface band bending, as shown in Fig. 10. For the nanocomposites, the higher electron concentration in the SnO₂ could attract NO₂ gas more easily, and then more NO₂ molecules adsorbed on the NiO-SnO₂ nanocomposites, leading to the largely decreased interface potential of the heterojunction nanocomposites, as shown in Fig. 10.



Therefore, the variation of the interface potential of nanocomposites induced by NO_2 adsorption is larger than the changes in the surface band bending of bare NiO, leading to a more obvious decrease of the interface potential and a drastic effect on the transducer function for gas sensing. This means that NO_2 adsorption affects the heterojunction conductance doubly, first through the carrier density term and second through the mobility term, enhancing the transducer function up to the square of that of the bare NiO. Therefore, the response of heterostructured NiO– SnO_2 nanocomposites is largely enhanced at room temperature compared to the bare NiO.

The Royal Society of Chemistry apologises for these errors and any consequent inconvenience to authors and readers.

