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Evolution of ZnO microstructures from hexagonal disk to prismoid, prism and pyramid and their crystal facet-dependent gas sensing properties

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Gas concentration calculation

To obtain the desired gas concentration, injection volume of the gas or liquid can be calculated as follow:

When the test target is gas:

$$V_x = V \times C \times 10^{-6} \times \frac{273 + T_r}{273 + T_c} \quad (1)$$

When the test target is liquid vapor:

$$V_x = \frac{V \times C \times M}{22.4 \times d \times p} \times 10^{-9} \times \frac{273 + T_r}{273 + T_c} \quad (2)$$

where V_x os the injection volume (ml), V is the test chamber volume (ml), C is the gas or liquid vapor concentration (ppm), M is the liquid mole mass (g/mol), d is the liquid specific gravity (g/cm^3), p is the liquid purity, Tr is the room temperature (℃) and Tc is the chamber temperature (℃).

Gas sensing properties of the sensors

O_2 (gas) ↔ O_2 (adsorbed) (3)

O_2 (ads) + e^- ↔ O_2^- (ads) (4)

O_2^- (ads) + e^- ↔ $2O^-$ (ads) (5)

O^- (ads) + e^- ↔ O^{2-} (ads) (6)

$V_O + O_2$ (g) ↔ O_2^- (ads) $+V_O^\bullet$ (7)

$V_O + O_2$ (g) ↔ O_2^- (ads) $+V_O$ ↔ $2O^- + 2V_O^\bullet$ (8)

wherein "g" and "ads" refer to gas and adsorbate, V_O oxygen vacancy, and $V_O^\bullet$ single electropositive oxygen vacancy.

In addition, C_2H_5OH gas can be either dehydrated at the surface of acidic oxide:

C_2H_5OH (g) → C_2H_4 (g) + H_2O (g) (9)

or dehydrogenated at the surface of basic oxide:

C_2H_5OH (g) → CH_3CHO (g) + H_2 (g) (10)

Since ZnO is a basic metal oxide, the catalytic oxidation of C_2H_5OH on the ZnO surface will happen according to Eq. 10. The sequent gas sensing reaction is shown in Eq. 11:

CH_3CHO (ads) + $5O^-$ (ads) → $2CO_2 + 2H_2O + 5e^-$ (11)

When the sensor is exposed to the other gases:

H_2 (ads) + O^- (ads) → $H_2O + e^-$ (12)

CH_3OH (ads) + $3O^-$ (ads) → $CO_2 + 2H_2O + 3e^-$ (13)

$HCHO$ (ads) + $2O^-$ (ads) → $CO_2 + H_2O + 2e^-$ (14)