Numerical modelling of the potential inside the cylindrical shaped nanocrystallite metal oxide semiconductors and its effect on gas sensor response

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Keywords: gas sensor, chemisorption, cylindrical grain, metal oxide

Abstract

The surface of metal oxide semiconductors exhibits great gas sensing response when the size of the grains becomes much smaller, i.e. in the range of the Debye length. In the presented work, the gas sensing properties of nanocrystalline cylindrical shaped metal oxide semiconductors have been studied. The effect of crystal size and surface states on gas sensor response has been investigated. The electric potential inside the grains has been calculated by solving the Poisson’s equation coupled with electroneutrality condition. The relationship between the electric potential and the size of the nanograins has been established as a function of available surface states, surface temperature and occupied surface states. It has been found that the critical value of available surface state density increases with an increase in the size of nanograins. Total carrier concentration inside the grain volume has been simulated as a function of available surface state density and grain size. Eventually, the sensitivity of the gas sensor has been simulated and compared for different sizes of nanocrystals. From the simulated studies, it is clear that the smaller cylindrical-shaped nanostructured grains could result in better gas sensing performances. Presented model has universal application for all metal oxides (both n-type and p-type) based semiconductors and can be extended for both oxidising and reducing gases with essential modifications.

1. Introduction

Metal oxide semiconductors (MOX) based chemo resistive gas sensors were among the first materials, which were studied vastly and have been used commercially for gas sensing applications [1–3]. These materials are quite famous and extensively used because of the easy fabrication processes, and very well explained gas-sensing mechanisms [3, 4]. Also, the possibility to change the conductivity by doping, capabilities to sense a large group of gases and chemical compounds and of course the cheaper implementation cost are the add-ons in the popularity of MOX materials [3].

The gas sensing mechanism of metal oxide semiconductors can be understood with the help of two steps. The first step is the adsorption of the ambient oxygen gas molecules on the sensor surface, and the second step is the reaction of the adsorbed oxygen gas molecules with the target gas. Wolkenstein’s has explained very well the adsorption mechanism of the oxygen gas molecules [5]. The Wolkenstein’s method to study the adsorption of gas species on the gas sensor surface considers the physical as well as chemical adsorption. Physical adsorption is considered as weak adsorption as the binding forces between the sensor surface and the target gas molecules are generally weak Van Der Wall’s forces, which result in shallow binding energy. Whereas, in the case of chemical adsorption, there exists a charge transfer between the adsorbed gas species and the sensor surface. The binding energy associated with the chemisorption of oxygen molecules is quite high due to charge sharing with the sensor surface [5–7]. The chemical adsorption of oxygen gas molecules/atoms results into the extraction of electrons from the conduction band of the n-type SnO2 semiconductors because of the higher electron
negativity of oxygen. Thus, chemisorption of oxygen on sensor surface results in increased resistance of sensor thin film as the formation of the depletion region at the sensor surface takes place. When these pre-adsorbed negatively charged oxygen molecules/atoms interact with the target gas, there is a change in the surface potential due to change in the density of occupied surface states. Eventually, the sensor film resistance decreases or increases depending upon the fact of whether the target gas is reducing or oxidising. The phenomenon of the chemical adsorption of environmental oxygen alters the charges in the trapped surface states. This change in charge distribution at the surface of the metal oxide semiconductor material as a function of the partial pressure of the gas has been studied in detail [8, 9]. The theoretical explanation of the change in the charge distribution inside MOX has been explained with the help of numerical solution of Poisson’s equation along with the Fermi–Dirac distribution function [10–12]. Both partial depletion and full depletion approximations have been employed for the modelling of nanoscale crystallite size of MOX based gas sensors [13, 14]. These simple models based upon the partial and full-depleted approximation use the estimated solution of Poisson’s equation, assuming that the whole grain is covered by the space charge region [15]. However, these devices as mentioned above models provide a simple and practical explanation for the gas sensing mechanism; there are various limitations of the grain size, shape, carrier concentration and the density of available surface states. More accuracy in the existing device models can be achieved by calculating the specific solution of the Poisson’s equation simultaneously with the chemisorption studies of the target gases at the sensor surface. So far, the various numerical models for the spherical shaped nanosized grains have been presented and discussed in detail [8, 16]. Moreover, there are available studies, which describe the relationship of gas sensitivity on the size of the spherical grain carried out by Xu et al [17]. Although, this device model is more quantitative still, it clears the doubts about the significant rise in gas sensitivity after a critical reduction in the size of the spherical grain. Moreover, in recent times, much emphasis has been given to the nanostructured gas sensors such as nanowires and nanorods. These cylindrical-shaped nanostructures exhibit excellent gas sensing characteristics [18–21]. Although, the primary sensing mechanism of these nanostructures can be explained based on similar theoretical work carried out for spherical shaped nanograins. Moreover, for the better understanding and more accurate modelling of the gas sensing response of cylindrical nanostructures like nanorods and nanowires, much more study is required in this area. In the presented work, an attempt has been made for the formulation of a useful model for predicting the behaviour of gas sensing mechanism of the cylindrical shaped nanostructures. This model consists of the numerical solution of Poisson’s equation in the cylindrical coordinates to get the electrostatic potential profile, distribution of carrier concentration and the gas sensor response as the function of grain size and the available surface state density.

2. Numerical model

The presented model assumes that before oxygen gas adsorption, the surface is clean, and there is no charge exists at the sensor surface. In this condition, the energy bands of SnO2 are flat as shown in figure 2(A). When the environmental oxygen molecules/atoms are adsorbed on the surface of SnO2 as shown in figure 1, the oxygen atoms being higher electronegative takes the electron from the conduction band of the semiconductor and adsorbed as negatively charged adions. At this point, the energy bands of the semiconductor start banding and the formation of space charge region inside the material grain start as shown in figure 2(B). $E_C$ and $E_V$ are the energy levels of conduction band edges at the surface and in bulk respectively.

Similarly, $E_C^s$ and $E_V^s$ are the energy level of valence band edge at the surface and in bulk respectively. $E_{3s}$ is the energy level created during chemisorption of oxygen atoms. In the presented model, few more assumptions are considered for n-type SnO2 material:

1. The energy level ($E_{3s}$) created below the Fermi level is because of the chemisorption mechanism of oxygen atoms/ molecules at the surface of n-type SnO2 material. The effect of surface defects and other surface irregularities/impurities have been neglected in this model.
2. The semiconductor is homogeneously doped.
3. Environmental oxygen is chemisorbed in the dissociated form at the sensor surface at the available trap centres

The width of the space charge region after the adsorption of oxygen atoms, as shown in figure 3 is one of the most critical parameters, which is responsible for affecting the gas sensitivity in MOX based gas sensors [22]. Net effective carrier concentration inside the grain is a function of the potential ($\phi$) and the width of the depletion region ($X_0$) formed at sensor surface due to removal of electrons from the conduction band of the semiconductor by adsorbed oxygen [23] (figure 3). It has been reported in the literature that gas sensitivity
increases significantly when the crystallite size becomes smaller than the X0 [24]. A theoretical model has been suggested to demonstrate the effect of grain size on gas sensitivity [17]. Although this model is quantitative, still it clears the doubts about the significant rise in gas sensitivity after a critical reduction in size. This model describes three possible cases of grain size relative to the width of the depletion region X0, as shown in figure 3(a). When the size (Lateral diameter; D) of the cylindrical nanostructured grain is quite larger than X0, i.e. D \gg 2 \times 0. In this case, there exist a layer of negative charge at the sensor surface due to the removal of free electrons from the conduction band of the material. If the grain size is decreased further until the grain size becomes comparable to depletion region width, i.e. D \approx 2 \times 0 (figure 3(b)), in this situation, the depletion region width increases towards the centre of the crystallite. In these two events, the case of partial depletion of nanograins has been considered as shown in figure 4. Beyond the depletion region until the centre of the grain, the bulk is still neutral, and R0 represents its radius. The total potential in the grain exists at the surface only. This potential is denoted by the surface potential Vs. So, a barrier develops between the sensor surface and the oxygen gas adsorbates.

In the third case, for a further decrease in the grain size so that D < 2 \times 0, depletion region will expand rigorously towards the centre of the grain as a large number of electrons are captured by the oxygen gas atoms at the surface. Eventually, the whole volume of the grain will be fully depleted of the free electrons as shown by figure 3(c). Despite the lesser conductivity in full depletion case, the sensitivity is remarkably high [24]. In this
paper, the gas sensor response of the nanosized cylindrical nanostructures has been simulated using numerical solution of Poisson’s equation superimposed with the Boltzmann approximation. The Bulk and surface parameters of n-type SnO$_2$ considered for the numerical solutions is listed in table 1.

**Case I.** Partial depletion (Cylindrical Shape).

If deposited sensing film consists of the nanostructured grain of cylindrical shape (i.e. nanorods, nanowires) and grain size is, such that the whole volume of the grain is not depleted, i.e. the case of partial depletion. This condition can be understood analytically as $qN_T[O^-] < qRN_0$, where $N_T[O^-]$ is the density of surface states occupied by negatively charged oxygen atoms and is a function of available surface state density ($N_T$) and the surface coverage by adsorbed oxygen atoms. The potential developed inside the grain can be demonstrated by the Poisson’s equation in cylindrical coordinates in the following form [4]:

$$\nabla^2 \phi(r) = \frac{d^2 \phi(r)}{dr^2} + \frac{1}{r} \frac{d \phi(r)}{dr} = -\frac{\rho(r)}{\varepsilon}$$

(1)
Where $\varphi$ is the potential inside the grain, $r$ is the distance from the centre of grain at any given point, $\rho$ is total charge density, and $\varepsilon$ is the permittivity of the semiconductor.

Total charge inside the depletion region can be expressed as:

$$\rho = \frac{2qN_D}{\varepsilon}$$

$q$ is the electronic charge, and $N_D$ is the doping concentration.

Equation (1) can be presented in the form of local potential to relate with the barrier height $|qV_S|$ as:

$$\frac{d^2V(r)}{dr^2} + \frac{1}{r} \frac{dV}{dr} = \frac{2qN_D}{\varepsilon}$$

The Solution of barrier voltage $V_S$ is obtained when $r = R$, i.e. at the sensor surface after integrating equation (3). In case of partial depletion approximation, one of the boundary conditions for this solution is that potential vanishes beyond the space charge region towards the centre of grain; i.e. $V = 0$ at $r \leq R_0$, as shown in figure 4.

Another boundary condition is that $\frac{dV}{dr} = 0$ at $r \leq R_0$. Applying these boundary conditions to equation (3), we get the following solution:

$$V(r) = \frac{qN_D}{\varepsilon} \left[ \frac{1}{2} (r^2 - R_0^2) - R_0^2 \log \left( \frac{r}{R_0} \right) \right]$$

The barrier height between grains is directly dependent upon the amount of oxygen adsorbed ($N_T$ $[O^-]$) with the available surface state density $N_T$ at the surface. So, to establish a relationship between barrier height and occupied surface states; equation (4) must be written as a function of $N_T$ $[O^-]$). From the electroneutrality condition of space charge region, it is known that electrons removed from conduction band must be equal to the electrons trapped by adsorbed oxygen atoms. Thus, implying this relation, the following equation emerges:

$$2qN_TA_1 = qN_TA_2$$

Where $A_1$ is the volume of cylindrical grain and $A_2$ is the surface area of the cylinder. Equation (5) becomes as:

$$2qN_0 \pi (R^2 - R_0^2) h = qN_T [O^-] 2\pi R \left( \frac{R}{2} + h \right)$$

$R$ - $R_0$ = radius of space charge region, as shown in figure 4.

$h$ = height of nanostructured cylindrical grain.

$R_0$ can be obtained from equation (6) as a function of $N_T$ $[O^-]$ as:

$$R_0 = \left[ R^2 \left( 1 - \frac{N_T [O^-]}{2N_0} \right) + R \left( \frac{hN_T [O^-]}{N_0} \right) \right]^{1/2}$$

Using the value of $R_0$ from equation (7) in equation (4), we obtain local potential at any distance ‘$r$’ as a function of $N_T$ $[O^-]$:

### Table 1. Semiconductor device parameters used for numerical simulations.

| Physical property | Symbol | Value |
|-------------------|--------|-------|
| Bandgap           | $E_g$  | 3.6 eV$^a$ |
| The energy level of the induced states with respect to Fermi level | $E_{SS} - E_F$ | $-1.21$ eV$^b$ |
| The energy level of the induced states caused by chemical adsorption | $E_{SS}^c - E_F$ | $1$ eV$^c$ |
| Doping concentration | $N_D$ | $10^{24}$ m$^{-2}$ |
| Depletion region width | $X_0$ | 21.8 nm |
| Effective mass for electrons in the conduction band | $m^*_e$ | $0.3 m_0$ |
| Effective mass for holes in the valence band | $m^*_h$ | $0.3 m_0$ |
| The relative permittivity of the metal oxide semiconductor | $\varepsilon$ | $12$ $^a$ |
| Temperature | $T$ | 600 K |
| Boltzmann Constant | $k$ | $1.38 \times 10^{-23}$ J/K |
| Available surface state density | $N_T$ | $10^{15}$ m$^{-2}$ $^a$ |
| Height of the cylindrical grain | $h$ | 1 $\mu$m |

$^a$ Reference [8].

$^b$ Reference [7, 25].
As shown in figure 5, the normalised surface potential \( V(s) \); at \( r = R \) increases with the increase in grain size. It is concluded from this observation that higher is the value of potential barrier on the sensor surface, lesser will be the concentration of electron trapping at the sensor surface. Eventually, the sensor response will decrease with an increase in grain size. It has also been observed from this figure that the surface potential in case of spherical grains is less for the same grain size. This can be attributed to the fact that the trapping of electrons from the conduction band at the surface is less in case of spherical grains. It has also been shown in figure 6 that the sensor response will be higher for smaller cylindrical-shaped grains. In figure 6, the response of a gas sensor can be given by the following relationship, as discussed in detail in section 3:

\[
V(r) = \frac{qN_0}{\varepsilon} \left[ \frac{1}{2} \left( r^2 - \left( R^2 \left( 1 - \frac{N_T [O^-]}{2N_D} \right) + R \left( \frac{hN_T [O^-]}{N_D} \right) \right) \right) - \left( R^2 \left( 1 - \frac{N_T [O^-]}{2N_D} \right) + R \left( \frac{hN_T [O^-]}{N_D} \right) \right) \right] \\
\times \log \left[ \left( \frac{r}{R^2 \left( 1 - \frac{N_T [O^-]}{2N_D} \right) + R \left( \frac{hN_T [O^-]}{N_D} \right)} \right) \right]^\frac{1}{2}
\]

(8)


\[
S = -\frac{\partial}{\partial \left( \frac{N_{T}[O^{-}]}{N_{D}} \right)} \left( \frac{N_{total}}{N_{totalڝ}} \right)
\]

**Case II.** full depletion (Cylindrical Shape).

As represented earlier in figure 3(c), the condition of full depletion can be achieved if the lateral diameter 'D' of the cylindrical grain is such that \( D < 2 \times R \); all the mobile electrons in the grain volume would be trapped at the sensor surface. This case can be expressed analytically as:

\[
qN_{T}[O^{-}] = qRN_{D}
\]

Equation (8) can be modified for full depletion as:

\[
V(r) = \frac{qN_{D}}{\varepsilon} \left[ \frac{1}{2}r^{2} - \left( \frac{R^{2}}{2} - \frac{R^{2}}{2} + R^{2} \right) + \left( \frac{R^{2}}{2} - \frac{R^{2}}{2} + R^{2} \right) \log \left( \frac{r}{ \left( \frac{R^{2}}{2} - \frac{R^{2}}{2} + R^{2} \right)^{\frac{1}{2}}} \right) \right]
\]

Where Value of R can be derived from equation (9) and can be written as:

\[
R = \frac{N_{T}[O^{-}]}{N_{D}}
\]

Accordingly, equation (10) can be expressed in the form of relationship between the local potential and the occupied surface state density at the sensor surface as:

\[
V(r) = \frac{qN_{D}}{\varepsilon} \left[ \frac{1}{2}r^{2} - \left( \frac{N_{T}[O^{-}]}{N_{D}} \right)^{2} \left( 1 - \frac{N_{T}[O^{-}]}{N_{D}} \right) + \left( \frac{N_{T}[O^{-}]}{N_{D}} \right)^{2} \right] \log \left( \frac{r}{ \left( \frac{N_{T}[O^{-}]}{N_{D}} \right)^{2} \left( 1 - \frac{N_{T}[O^{-}]}{N_{D}} \right) + \left( \frac{N_{T}[O^{-}]}{N_{D}} \right)^{2} \right)^{\frac{1}{2}} \right)
\]

The normalised potential inside grain can be derived as a function of \( V(r) \) as:

\[
\phi(r) = -\frac{qV(r)}{kT}
\]

Where; \( k = \) Boltzmann constant, \( T = \) Temperature of the sensor surface.

The radial distribution of electric potential inside the nano crystallite has been shown in figure 7. It is evident from the figure that the potential at the centre of grain does not fall to zero but has some positive value in case of full depletion of the grain. As we move away from the centre of grain towards the sensor surface, the magnitude of the electric potential starts increasing and becomes maximum at the surface, i.e. when \( r = R \).

In full depletion case of grain volume, the electrical conduction will take place through the grain volume and will be a function of total conduction carrier concentration inside the grain. Considering this, \( n_{total}(r) \), the total Carrier concentration in a nanocrystalline grain can be written as a function of Normalised potential \( \phi(R) \) at surface i.e. for \( r = R \) is given as:

\[
n_{total}(R) = \frac{1}{\pi R^{2}h} \int_{0}^{\pi R^{2}h} N_{D} \exp(-\phi(R))dR
\]

To calculate the total carrier concentration as a function of doping density and the potential inside the grain volume, Electroneutrality condition was solved to get \( \phi_{0} \), as shown in figure 8. Left-hand side (LHS) term in this condition gives the total charge appeared after removal of the free electrons from the grain. The right-hand side
(RHS) represents the charge at the surface due to acceptance of electrons by chemisorbed oxygen. \( N_T \) is the available surface density for oxygen adsorption. After the interaction of oxygen gas with sensor surface, some of these surface states will be occupied. The surface state density, which has been occupied by a negatively charged oxygen atom, is denoted by \( N_T^-[O^-] \). \( N_T^-[O^-] \) is a function of \( N_T \) and \( E_{SS} \). Where \( E_{SS} \) is the corresponding energy level created by the chemisorption of oxygen gas at the surface.

3. Conduction mechanism and discussion of results

To explain the gas sensor response, two well-established mechanisms are there; receptor and transducer function of the gas sensing thin film. The receptor function is dependent upon the various parameters related to the interaction of the target gas with the sensor surface like morphology of surface, the density of occupied surface states, humidity variations, deposition method of the sensing thin film and concentration of the target gas etc as studied by Korotcenkov et al [26]. As discussed in section 2.1, after the exposure of a reducing gas like CO at the sensor surface, the interaction of CO and \( O_2 \) will result into a free electron shown in following equation [7]:

---

**Figure 7.** Radial distribution of the electric potential inside the fully depleted cylindrical grain as a function of the distance from the centre of grain towards the grain surface. The radius of the grain is \( R = 40 \) nm, \( N_D = 10^{24} \) m\(^{-2}\), \( N_T = 10^{15} \) m\(^{-2}\) and \( T = 600 \) K.

**Figure 8.** The solution of Electroneutrality condition given by equation (6) for cylindrical grains. The intersection of two shown curves represents the optimum solution for the grain potential \( \phi \), where \( \phi \) is related to surface barrier potential \( V_s \) as \( \phi(R) = V(R) / KT \). \( N_D = 10^{24} \) m\(^{-2}\) and \( T = 600 \) K.
After the interaction of the target gas, the occupied surface state density $N_T[O^-]$ decreases as the trapped oxygen atoms will be consumed by test gas, as shown in equation (14). The equation (14) describes the receptor case for CO target gas. This model has been discussed and studied widely by N Barsan et al [4].

Moreover, the more generalised methodology, i.e. the transducer function [23, 27], to demonstrate the gas sensor response has been used in the presented study in this paper. With the help of this methodology, we can draw the generalised conclusions for the gas sensitivity without caring much about the different parameters involved during the interaction of the target gas species and that of sensing thin film. The Presented study has been carried out for the gas sensitivity discussing the dependence of grain size on potential profile inside the grain, chemisorbed surface states and the carrier concentration. The response of a gas sensor can be given by the following relationship:

$$CO_{(gas)} + O_{(s)}^{−} \xrightarrow{k_{CS}} CO_{2(gas)} + e^-$$ \hspace{1cm} (14)

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$$S = \frac{-\partial}{N_T[O^-]} \left( \frac{n_{total}}{n_{total,o}} \right)$$ \hspace{1cm} (15)

In equation (15), $n_{total}$ and $n_{total,o}$ are total carrier concentrations of conducting electrons after the gas exposure and in ambient conditions without gas interaction. Similarly, $N_T[O^-]$ and $N_T[O^-]_o$ are occupied surface state density with and without target gas exposure. The negative sign in the equation (15) indicates that $N_T[O^-]$ will decrease after interaction with target gas from its value in the ambient exposure of oxygen gas $N_T[O^-]_o$.

It is clear from the figure 9 that the electric potential at the centre of the grain increases with the increase in the density of available surface states, $N_T$. Furthermore, this increment is significant at a threshold value of surface state density ($N_{TC}$) below which the observed increment in the potential is very less. It clearly shows that the role of surface state density is very critical in deciding the barrier height and ultimately, the net carrier concentration responsible for the conduction and ultimately, the gas sensor response.

As discussed earlier, the density of surface states occupied by the negatively charged oxygen atoms; $N_T[O^-]$ also depends upon the lateral diameter of cylindrical grain, i.e. size of the grain. The increase in the value of $N_T[O^-]$ is significant up to a critical size and after that, it is saturated, as shown in figure 10. The critical size up to which the value of $N_T[O^-]$ increases has been observed as 26.38 nm for $N_T = 10^{15}$ m$^{-2}$. It implies that the grains having a larger size than the critical size will not affect the density of occupied surface states.

The relationship between the total carrier concentrations inside the grain volume with the available surface state density as a function of grain sizes has been depicted in figure 11. It is clear that at a critical value of surface state density, the carrier concentration decreases and then becomes saturated. The significance of this phenomenon lies in the fact that a specific value of surface states available for oxygen gas adsorption affects the sensing mechanism. It is also clear from figure 11 that the value of critical surface density increases as the grain...
Figure 10. Occupied surface state density as a function of grain size for the specific value of surface state density. \( N_D = 10^{24} \text{ m}^{-2} \), \( N_T = 10^{15} \text{ m}^{-2} \) and \( T = 600 \text{ K} \).

Figure 11. Relationship of total carrier concentration responsible for conduction with the available surface state density as a function of grain size. \( N_D = 10^{24} \text{ m}^{-2} \) and \( T = 600 \text{ K} \).

Figure 12. Sensor response of cylindrical shaped nanograins as a function of grain size.
size increases. The simulated sensor response for full depletion case for cylindrical nanograins has been shown in figure 12. The sensor response has been calculated as per the equation (15).

4. Conclusion

The effect of grain potential and surface states on the gas sensing response of nanostructured SnO₂ metal oxide semiconductor has been studied. The cylindrical shapes of the grains have been considered to simulate the sensor response. The effect of shapes (cylindrical) on barrier potential height at the surface ([ΣqVₛ]), normalised potential (σ) inside the grain has been studied. Full depletion approximation was considered to present an extensive numerical study. Role of the density of surface states and surface preparation is very crucial while selecting the gas sensing material. A mathematical model for the approximate analytical and numerical solution of Poisson’s equation along with the charge neutrality condition has been presented. It has shown that smaller cylindrical-shaped nanostructured grains comparable with the twice of depletion width, could result in better gas sensing alternate. The presented model is general in nature, which can be extended for both oxidising and reducing gases and p-type semiconductor model with necessary modifications.

Data availability

The raw/processed data required to reproduce these findings cannot be shared at this time as the data also forms part of an ongoing study.

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