Dimension Effect on Intrinsic Carrier Concentration of Semiconductor Calculated from Density of State

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ABSTRACT

Dimension effect is an important effect to understand nanoscience and nanotechnology. In this work, dimension effect on intrinsic carrier concentration of semiconductor has been studied. The study is based on the calculation from the density of state at 3, 2, 1 and 0 dimensions at temperature $k_BT<<E_g / 2$where E_g is energy gap. Since the density of state at different dimension has different function, intrinsic carrier concentration calculated from density of state is expected to vary as a function of dimension. For 2, 1 and 0 dimensions, the energy level are discrete outside the energy gap. Moreover, 1 and 0 dimensions also have degenerated state and the degeneracy has an effect on density of state. From the calculation, it has been found that the intrinsic carrier concentration of semiconductor depends on the dimension and is proportional to $T^{D/2} \exp(-E_g / 2k_BT)$ where D is a dimension.

Key words: Density of state, Dimension effect, Intrinsic carrier concentration

INTRODUCTION

Dimension effect is an important effect to understand nanoscience and nanotechnology. Due to dimension effect, the properties of nanostructures are different from the properties of microstructures or bulk. For example, density of state (DOS) at different dimension has a different function as shown in Figure 1. For 3 dimension, DOS is a continuous function with respect to energy and is related to a square root of energy. For 2, 1 and 0 dimensions, the DOSs are the discrete function with respect to energy. The lower the dimension, the smaller the number of available energy values and the discrete function turns into a delta function at zero dimension.

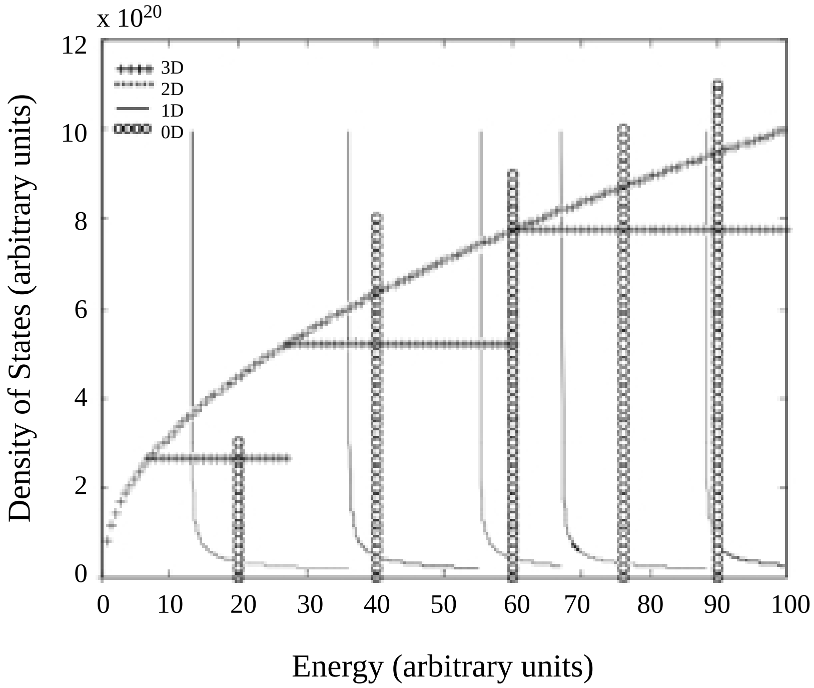

Figure 1. The function of density of state at 3, 2, 1 and 0 dimensions with respect to the energy.

Density of states and Fermi-Dirac distribution are the basic parameters for calculation of electrical properties such as intrinsic carrier concentration, heat capacity and conductivity, etc. Therefore, a change of dimension should have an effect on the electrical properties.

Bogacheck et al., (1996) have calculated the conductance of nanowire and demonstrated the quantization of conductance in the value $2e^2 / h$ of according to Landauer formula. The conductance quantization of gold nanowire has been experimentally confirmed by Takayanaki (2001). However, to our best knowledge, there has been no report on the intrinsic carrier concentration as a function of dimension.

In this paper, we report on dimension effect on intrinsic carrier concentration of semiconductor, calculated from density of state and Fermi-Dirac distribution. We will demonstrate that the intrinsic carrier concentration of semiconductor depends on the dimension and is proportional to $T^{D/2} \exp(-E_g / 2k_BT)$ where D is a dimension.

MATERIALS AND METHODS

Assumption and calculation method:

The electron and hole concentrations can be defined as in equation (1).

$$n = \int_{E_c}^{\infty} D_e(\varepsilon)\, f_e(\varepsilon)\, d\varepsilon \quad \text{and} \quad p = \int_{-\infty}^{E_v} D_h(\varepsilon)\, f_h(\varepsilon)\, d\varepsilon \tag{1}$$

For further calculation, the following assumptions are applied:

1. Fermi-Dirac distribution can be applied to all dimensions
2. All dimensions have conduction level and valence level
3. The thermal energy satisfies the condition $\varepsilon - \mu >> k_BT$
4. For all dimensions, intrinsic carrier concentration follows law of mass action $n_i^2 = np$.

Then, the Fermi-Dirac distribution and density of state in 2, 1 and 0 dimension are substituted in Equation (1).

Thus, at room temperature $\varepsilon - \mu >> k_BT$, then Fermi-Dirac distribution can be written down as

$$f_e(\varepsilon) = \frac{1}{\exp\left(\frac{\varepsilon-\mu}{k_BT}\right) + 1} \approx \exp\left(\frac{\mu-\varepsilon}{k_BT}\right) \tag{2}$$

$$f_h(\varepsilon)\ 1-f_e(\varepsilon) = 1-\frac{1}{\exp\left(\frac{\varepsilon-\mu}{k_BT}\right) + 1} \approx \exp\left(\frac{\varepsilon-\mu}{k_BT}\right) \tag{3}$$

where $f_e(\varepsilon)$ is a electron distribution in the conduction band
$f_h(\varepsilon)$ is a hole distribution in the valence band.

For 2 dimension, density of state of electrons and holes are

$$D_{2D,e}(\varepsilon)\,d\varepsilon = \frac{m_e}{\pi\hbar^2} \sum_i \mathrm{H}\,(\varepsilon - \varepsilon_i)d\varepsilon \tag{4}$$

$$D_{2D,h}(\varepsilon)\,d\varepsilon = \frac{m_h}{\pi\hbar^2} \sum_i \mathrm{H}\,(\varepsilon - \varepsilon_i)d\varepsilon \tag{5}$$

Therefore, electron and hole concentrations in 2 dimension are

$$n_{2D} = \frac{m_e}{\pi\hbar^2}\ \exp(\mu / k_BT) \int_{E_c}^{\infty} \exp(-\varepsilon / k_BT) \sum_i H\,(\varepsilon - \varepsilon_i)d\varepsilon \tag{6}$$

$$p_{2D} = \frac{m_h}{\pi\hbar^2}\ \exp(-\mu / k_BT) \int_{-\infty}^{E_v} \exp(\varepsilon / k_BT) \sum_i H\,(\varepsilon - \varepsilon_i)d\varepsilon \tag{7}$$

For 1 dimension, density of state of electrons and holes are

$$D_{1D,e}(\varepsilon)\,d\varepsilon = \frac{1}{\pi}\left(\frac{2m_e}{\hbar^2}\right)^{1/2} \sum_i \frac{n_iH(\varepsilon - \varepsilon_i)}{(\varepsilon - \varepsilon_i)^{1/2}}\ d\varepsilon \tag{8}$$

$$D_{1D,h}(\varepsilon)\,d\varepsilon = \frac{1}{\pi}\left(\frac{2m_h}{\hbar^2}\right)^{1/2} \sum_i \frac{n_iH(\varepsilon - \varepsilon_i)}{(\varepsilon_i - \varepsilon)^{1/2}}\ d\varepsilon \tag{9}$$

Therefore, electron and hole concentrations in 1 dimension are

$$n_{1D} = \frac{1}{\pi}\left(\frac{2m_e}{\hbar^2}\right)^{1/2} \exp(\mu / k_BT) \int_{E_c}^{\infty} \exp(-\varepsilon / k_BT) \sum_i \frac{n_iH(\varepsilon - \varepsilon_i)}{(\varepsilon - \varepsilon_i)^{1/2}}\,d\varepsilon \tag{10}$$

$$p_{1D} = \frac{1}{\pi}\left(\frac{2m_h}{\hbar^2}\right)^{1/2} \exp(-\mu / k_BT) \int_{-\infty}^{E_v} \exp(\varepsilon / k_BT) \sum_i \frac{n_iH(\varepsilon - \varepsilon_i)}{(\varepsilon_i - \varepsilon)^{1/2}}\,d\varepsilon \tag{11}$$

For 0 dimension, density of state of electrons and holes are

$$D_{0D,e}(\varepsilon)\,d\varepsilon = D_{0D,h}(\varepsilon)d\varepsilon = A \sum_i n_i\delta(\varepsilon - \varepsilon_i)d\varepsilon\,;\ \text{A is constant} \tag{12}$$

Therefore, electron and hole concentrations in 0 dimension are

$$n_{0D} = \int_{E_c}^{\infty} D_{0D}\,(\varepsilon)_{e,d}\, f_e\,(\varepsilon)d\varepsilon = \exp(\mu / \mathrm{k_BT}) \int_{E_c}^{\infty} A \sum_i n_i\delta(\varepsilon - \varepsilon_i)\exp(-\varepsilon / k_BT)\mathrm{d}\varepsilon \tag{13}$$

$$p_{0D} = \int_{-\infty}^{E_v} D_{0D}(\varepsilon)_{h,d}\, f_h(\varepsilon)\, d\varepsilon = \exp(-\mu / \mathrm{k_B T}) \int_{-\infty}^{E_v} A \sum_j n_j \delta(\varepsilon - \varepsilon_j) \exp(-\varepsilon / k_B T)\, \mathrm{d}\varepsilon \qquad (14)$$

Finally, the intrinsic carrier concentration can be obtained from law of mass action.

RESULTS AND DISCUSSION

The general solution of the product of electron and hole concentrations in 3, 2, 1 and 0 dimensions, calculated from density of state, are summarized in Table 1. In order to simply calculate the intrinsic carrier concentration, we considered the special cases for two cases. For the first case, electrons are considered to have energy only E_c and holes are considered to have energy only E_v. The calculated intrinsic carrier concentration for the first case is summarized in Table 2. It was found that the intrinsic carrier concentration is related to dimension as

$$n_{iD} \; \alpha \; T^{D/2} \, exp(-E_g / 2k_B T) \quad ;D{=}3,2,1 \textit{ and } 0 \qquad (15)$$

Table 1. The general solution of the product of electron and hole concentrations in 3, 2, 1 and 0 dimensions calculated from density of state.

Dimension	**General solution of the product of electron and hole concentration** ($n_i^2 = np$)
3	$n_{3D} p_{3D} = 4 \left(\frac{k_B T}{2\pi\hbar^2}\right)^3 (m_e m_h)^{3/2} \exp(-E_g / k_B T)$
2	$n_{2D} p_{2D} = \frac{m_e m_h (k_B T)^2}{\pi^2 \hbar^4} \left[\sum_{n=1}^{\infty} \exp(-E_{c_n} / k_B T)\right]\left[\sum_{n=1}^{\infty} \exp(-E_{v_n} / k_B T)\right]$
1	$n_{1D} p_{1D} = \frac{2(m_e m_h)^{1/2} k_B T}{\pi\hbar^2} \left[\sum_{n=1}^{\infty} n_{c_n} \exp(-E_{c_n} / k_B T)\right]\left[\sum_{n=1}^{\infty} n_{v_n} \exp(E_{v_n} / k_B T)\right]$
0	$n_{0D} p_{0D} = A^2 \left[\sum_{n=1}^{\infty} n_{c_n} \exp(-E_{c_n} / k_B T)\right]\left[\sum_{n=1}^{\infty} n_{v_n} \exp(E_{v_n} / k_B T)\right]$

where

E_{c_n} is an energy level in conduction level of order n and $E_{c_1}{=}E_c$
E_{v_n} is an energy level in valence level of order n and $E_{v_1} = \mathrm{E}_v$.

The plot of intrinsic carrier concentration as a function of temperature for the first case is shown in Figure 2. It can be seen that the curves are different at different dimension.

Table 2. The first case of intrinsic carrier concentration in 3, 2, 1 and 0 dimensions.

Dimension	**First case of intrinsic carrier concentration** (n_i)
3	$n_{i,3D} = 2\left(\frac{k_B T}{2\pi\hbar^2}\right)^{3/2} (m_e m_h)^{3/4} \exp(-E_g / 2k_B T)$
2	$n_{i,2D} = \left(\frac{k_B T}{\pi\hbar^2}\right) (m_e m_h)^{1/2} \exp(-E_g / 2k_B T)$
1	$n_{i,1D} = \left(\frac{2k_B T}{\pi\hbar^2}\right)^{1/2} (m_e m_p)^{1/4} \exp(-E_g / 2k_B T)$
0	$n_{i,0D} = A \exp(-E_g / 2k_B T)$

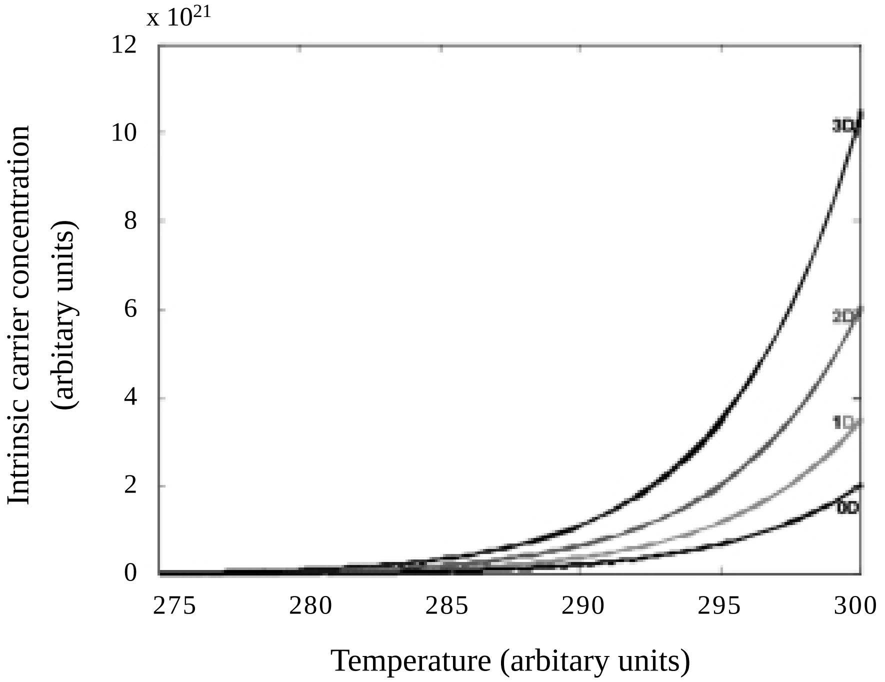

Figure 2. Plot of intrinsic carrier concentration as a function of temperature for the first case.

For the second case, energy level of electrons in upper conduction level and energy level of holes in lower valence level are considered to be symmetrical, behave as the free electron and then, follow the relation

$$E_{c_n} = n^2 E_c \text{ and } E_{v_n} = E_v - (n^2 - 1)E_c \,;\, n_{c_n} = n_{v_n} \tag{16}$$

The calculated intrinsic carrier concentration for the second case is summarized in Table 3.

Table 3. The second case of intrinsic carrier concentration in 3, 2, 1 and 0 dimensions.

Dimension	Second case of intrinsic carrier concentration (n_i)
3	$n_{i,3D} = 2\left(\frac{k_BT}{2\pi\hbar^2}\right)^{3/2}(m_em_h)^{3/4}\exp(-E_g/2k_BT)$
2	$n_{i,2D} = \frac{(m_em_h)^{1/2}k_BT}{\pi\hbar^2}\exp((E_c+Ev)/2k_BT)\left[\sum_{n=1}^{\infty}\exp(-n^2E_c/k_BT)\right]$
1	$n_{i,1D} = \left(\frac{2k_BT}{\pi\hbar^2}\right)^{1/2}(m_em_h)^{1/4}\exp((E_c+Ev)/2k_BT)\left[\sum_{n=1}^{\infty}n_{c_n}\exp(-n^2E_c/k_BT)\right]$
0	$n_{i,0D} = A\exp((E_c+Ev)/2k_BT)\left[\sum_{n=1}^{\infty}n_{c_n}\exp(-n^2E_c/k_BT)\right]$

To investigate in more detail, ZnO was used as a study case. For ZnO at room temperature about 300 K, it was found that the first term of series in all dimensions was greater than the other term of series. Thus, the first case and the second case have the same function. Then, the intrinsic carrier concentration can be related to dimension as

$$n_{i,D}\alpha\ \ T^{D/2}\ exp(-E_g/2k_BT)\quad ; D = 3,2,1\ and\ 0.$$

Moreover, if we plotted the graph between $1\mathrm{n}n+E_g/2k_BT$ *and* $1\mathrm{n}T$, the slope of the graph would correspond to $D/2$ as shown in Figure 3. This plot could be used to determine the dimension of the sample by comparing with the experimental results.

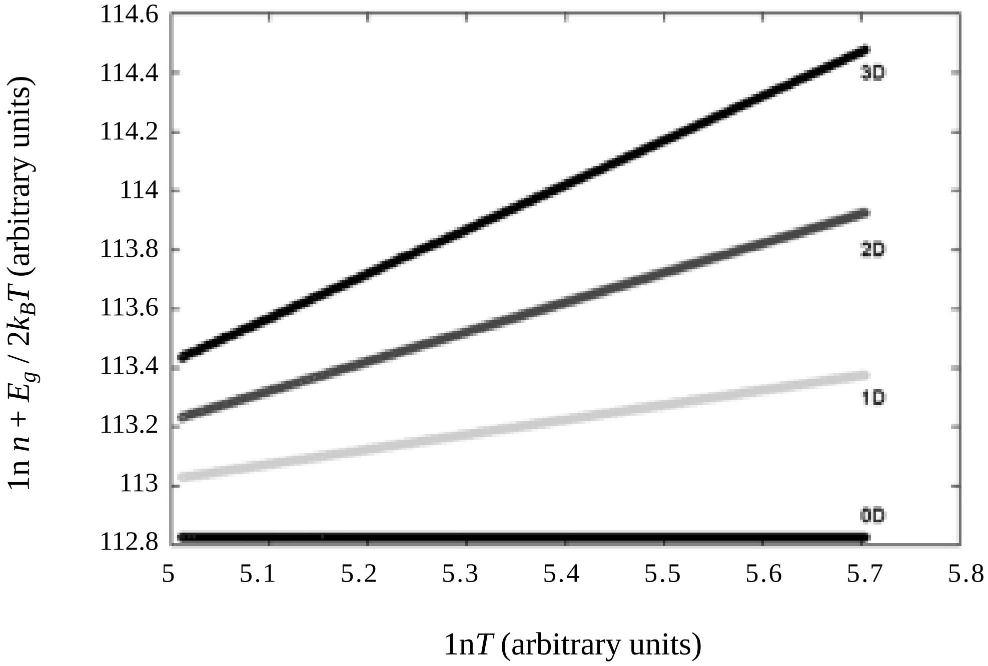

Figure 3. Plot between and for ZnO.

CONCLUSION

The dimension effect on intrinsic carrier concentration of semiconductor has been studied. The study is based on the calculation from the density of state at 3, 2, 1 and 0 dimensions at temperature $k_BT << \frac{E_g}{2}$ where E_g is energy gap. From the calculation, it was found that the intrinsic carrier concentration of semiconductor depends on the dimension and it is proportional to $T^{D/2}\exp(-E_g / 2k_BT)$ where D is a dimension. Moreover, the slope of the plot between $1\mathrm{n}n+E_g / 2k_BT$ and $1\mathrm{n}T$ would correspond to D/2 and could be used to determine the dimension of the sample by comparing with the experimental results.

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