A simple expression for impurity distribution after multiple diffusion processes

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Abstract: There are several diffusion processes with different temperatures in modern semiconductor technology. The impurity distribution after these diffusion processes is analyzed and a simple expression for describing the distribution is given. It is found that the impurity distribution after multiple diffusion processes can be characterized with an effective diffusion length. The relation between this effective diffusion length and the diffusion lengths of each diffusion process is given and shows itself to be very simple and instructive. The results of the expression agree well with numerical simulations by using SUPREM Ⅳ. An example of the application of the expression is also shown.

Key words: impurity distribution; multiple diffusions; planar junction
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1. Introduction

There are several diffusion processes in modern semiconductor technology, especially in BCD technology, smart power IC technology and power device technology[1−4]. The implanted impurities will redistribute during every subsequent diffusion process. It is efficient for the technology design process to know the final impurity distribution in advance. This information can be obtained by using a proper EDA[5] but such results are not very instructive for designing a process. Kennedy and Brien[6] obtained an expression of the impurity distribution through a semi-finite mask window, indicating that the distribution can be characterized with the diffusion length $L = \sqrt{Dt}$, where D is the diffusion coefficient of the impurity atom and t is the time interval of the diffusion process. Kasley *et al.*[7] got the junction contours of DMOS and BJT using such an expression. However, in their discussions the diffusion coefficient is the same all the time. In modern technologies, the temperature of each diffusion process may not be the same and because of this the diffusion coefficient in each diffusion process is not the same. The impurity distribution cannot be calculated simply by adding the diffusion time.

This paper analyzes the impurity diffusion through multiple diffusion processes. It is indicated at the beginning that the diffusion of numerous impurity atoms can be calculated by starting from the diffusion of an impurity atom. An analytical expression for impurity distribution is given. Such information is sometimes important for estimation of technology parameters in advance in the design of a proper process of BCD, smart power IC or power device. The results of the expression agree well with numerical simulation and provide an example of the application of the expression.

2. Theory

The assumptions made in this paper are:

(1) A fixed amount of impurity atoms is involved in all the diffusion processes;

(2) The impurity atoms do not affect each other in the diffusions;

(3) The impurity atoms diffuse isotropically in the semiconductor material.

The reason for assumption (1) is that two-step diffusion processes of the impurity atoms are often used in modern planar technologies[8]. A fixed quantity of impurity atoms is predeposited upon the semiconductor material during the two-step diffusion process. Sometimes, impurity diffusion goes with oxidization. The oxidation layer will absorb boron and exclude phosphorus, decreasing or increasing the amount of impurity atoms. This happens near the surface, thus the calculation in this paper is sometimes not exact for describing the situations at the surface. Assumption (2) is true for most of the impurities[9]. Situations where the impurity atoms affect each other are not taken into consideration in this paper. The use of a single impurity atom diffusion coefficient is permitted for all directions in each diffusion process under assumption (3). This assumption is made for the convenience of analysis. The expression given also suits anisotropic diffusions, if using a different diffusion coefficient for each direction.

In each diffusion process, the impurity atoms diffuse based on the result of the previous diffusions. After the first diffusion, the impurity distribution can be characterized by a diffusion length $L_1 = \sqrt{D_1 t_1}$, where D_1 is the diffusion coefficient of the impurity atom and t_1 is the time interval in the first diffusion process. In the second diffusion, the impurity atoms diffuse from where they were after the first diffusion. The second diffusion can be characterized by a diffusion length $L_2 = \sqrt{D_2 t_2}$, if taking the place where impurity atoms were after the first diffusion as the coordinate origin, where D_2 is the diffusion coefficient of the impurity atom and t_2 is the time interval in the second diffusion process. Similarly, the n-th diffusion can be characterized by a diffusion length $L_n = \sqrt{D_n t_n}$, if taking the place where impurity atoms were after the $(n-1)$-th diffusion as the coordinate origin, where D_n is the diffusion coefficient of the impurity atom and t_n is the time interval in the n-th diffusion process. There should be an expression, which

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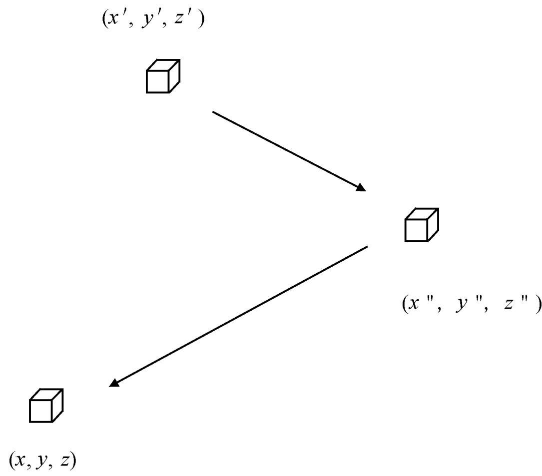

Fig. 1. Locations of impurity atom before and after diffusions; the atom locates at (x', y', z') before diffusions, at (x'', y'', z'') after the first diffusion, at (x, y, z) after the second diffusion.

takes all these diffusion lengths into consideration, to depict the impurity distribution after multiple diffusion processes, so that for designing a device, prediction and instruction can be obtained in advance.

2.1. Probability of an atom located at a place after multiple diffusion processes

The impurity distribution after diffusion processes is the result of random movements of numerous impurity atoms. According to statistical physics, the probability of an atom locating at a place is the average concentration of numerous impurity atoms at the same place. That is to say, if the impurity distribution profile is normalized with the amount of impurity atoms, the result is the same as the probability of an atom locating at places. The amount of impurity atoms located at a place P after one diffusion process can be found by integrating the product of amount of impurity atoms located at places in the semiconductor material before the diffusion and the probability of them moving to place P after the diffusion, through the semiconductor material. Based on assumption (2), we can start from an atom, calculating the probability of it moving from one place to another place after multiple diffusion processes. The impurity distribution can be found by integrating through the semiconductor material, according to distribution of impurity atoms in the initial conditions. The situation after two diffusions is analyzed first. The result for multiple diffusion processes can be derived from there.

The atom is assumed to be at place (x', y', z') in a Cartesian coordinate system before the diffusions, as seen in Fig. 1. After one diffusion process there is a probability of this atom being in the place (x'', y'', z''). At the end of two diffusions there is a probability of this atom being in the place (x, y, z).

The movement of an impurity atom can be described by a three-dimensional diffusion equation,

$$\frac{\partial^2 G}{\partial x^2}+\frac{\partial^2 G}{\partial y^2}+\frac{\partial^2 G}{\partial z^2}=\frac{1}{D}\frac{\partial G}{\partial t}, \tag{1}$$

where G describes the probability of an atom locating at a place, and D is the diffusion coefficient of the atom. There is an initial condition for the equation,

$$G(x, y, z, t=0)=\delta(x', y', z').$$

This represents the atom being at place (x', y', z') before the diffusions. After D, t, the equation is satisfied by

$$G(x, y, z, t; x', y', z')=\frac{(\pi Dt)^{-3/2}}{8}\left\{\exp\left[-\frac{(y-y')^2}{4Dt}\right]\right\}\times\left\{\exp\left[-\frac{(x-x')^2}{4Dt}\right]\right\}\left\{\exp\left[-\frac{(z-z')^2}{4Dt}\right]\right\}. \tag{2}$$

So after the first diffusion the probability of the atom moving to (x'', y'', z'') is

$$G(x'', y'', z'', t_1; x', y', z')=\frac{(\pi D_1t_1)^{-3/2}}{8}\left\{\exp\left[-\frac{(y''-y')^2}{4D_1t_1}\right]\right\}\times\left\{\exp\left[-\frac{(x''-x')^2}{4D_1t_1}\right]\right\}\left\{\exp\left[-\frac{(z''-z')^2}{4D_1t_1}\right]\right\}. \tag{3}$$

The probability of the atom moving from (x'', y'', z'') to (x, y, z) in the second diffusion is

$$G(x, y, z, t_2; x'', y'', z'')=\frac{(\pi D_2t_2)^{-3/2}}{8}\left\{\exp\left[-\frac{(y-y'')^2}{4D_2t_2}\right]\right\}\times\left\{\exp\left[-\frac{(x-x'')^2}{4D_2t_2}\right]\right\}\left\{\exp\left[-\frac{(z-z'')^2}{4D_2t_2}\right]\right\}. \tag{4}$$

Then, the probability of the atom moving from (x', y', z') to (x, y, z) after two diffusion processes can be obtained by integrating the product of Eqs. (3) and (4) on x'', y'', z'' through the semiconductor material, as shown in Eq. (5).

$$G(x, y, z, t_1+t_2; x', y', z')=\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}G(x'', y'', z'', t_1; x', y', z')\times G(x, y, z, t_2; x'', y'', z'')\mathrm{d}x''\mathrm{d}y''\mathrm{d}z''. \tag{5}$$

The result of the integration above is given as follows,

$$G(x, y, z, t_1+t_2; x', y', z')=\frac{(\pi L_\mathrm{a}^2)^{-3/2}}{8}\left\{\exp\left[-\frac{(y-y')^2}{4L_\mathrm{a}^2}\right]\right\}\times\left\{\exp\left[-\frac{(x-x')^2}{4L_\mathrm{a}^2}\right]\right\}\left\{\exp\left[-\frac{(z-z')^2}{4L_\mathrm{a}^2}\right]\right\}, \tag{6}$$

where

$$L_\mathrm{a}^2=L_1^2+L_2^2, L_1=\sqrt{D_1t_1}, L_2=\sqrt{D_2t_2}.$$

Obviously, the probability of an atom moving from (x', y', z') to (x, y, z) after n times diffusion processes is

$$G(x, y, z, \sum t_n; x', y', z')=\frac{(\pi L_\mathrm{e}^2)^{-3/2}}{8}\left\{\exp\left[-\frac{(y-y')^2}{4L_\mathrm{e}^2}\right]\right\}\times\left\{\exp\left[-\frac{(x-x')^2}{4L_\mathrm{e}^2}\right]\right\}\left\{\exp\left[-\frac{(z-z')^2}{4L_\mathrm{e}^2}\right]\right\}, \tag{7}$$

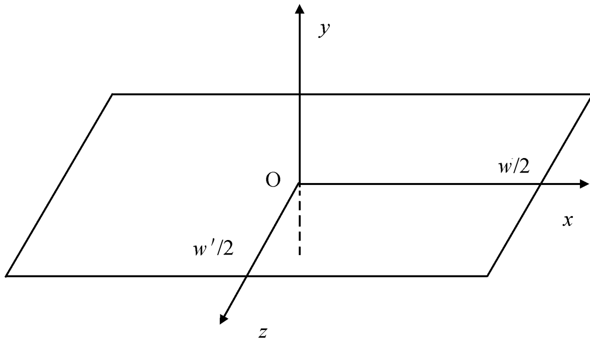

Fig. 2. Mask window used in the diffusion.

where $L_e^2 = \sum L_n^2$, $L_n = \sqrt{D_n t_n}$, L_n is the diffusion length of the n-th diffusion process, and L_e is called the effective diffusion length of multiple diffusion processes in this paper.

It can be seen from Eq. (7) that the probability of the atom being located in a place after multiple diffusion processes is related to an effective diffusion length L_e. The square of L_e equals the sum of the square of diffusion lengths in each diffusion process.

2.2. Impurity distribution through a mask window

The diffusion window considered here is shown in Fig. 2, with a length of w and a width of w'. The pre-deposited impurity atoms with density N_s upon the surface in the window produce a concentration $N(x, y, z)$ after multiple diffusion processes. There is no flux of impurity atoms through plane $y = 0$, required by assumption (a). This is satisfied by locating two instantaneous point sources symmetrically about $y = 0$, as shown in Eq. (8).

$$G(x, y, z, \sum t_n; x', y', z')$$
$$= \frac{(\pi L_e^2)^{-3/2}}{8} \left\{ \exp\left[-\frac{(y-y')^2}{4L_e^2} \right] + \exp\left[-\frac{(y+y')^2}{4L_e^2} \right] \right\}$$
$$\times \left\{ \exp\left[-\frac{(x-x')^2}{4L_e^2} \right] \right\} \left\{ \exp\left[-\frac{(z-z')^2}{4L_e^2} \right] \right\}, \quad (8)$$

where $L_e^2 = \sum L_n^2 N(x, y, z)$ can be obtained by integrating Eq. (8) along the window area, then

$$N(x, y, z) = \frac{N_s}{4\sqrt{\pi L_e^2}} \exp\left(-\frac{y^2}{4L_e^2} \right) \left[\mathrm{erf}\left(\frac{x + w/2}{2L_e} \right) + \right.$$
$$\left. \mathrm{erf}\left(\frac{w/2 - x}{2L_e} \right) \right] \left[\mathrm{erf}\left(\frac{z + w'/2}{2L_e} \right) + \mathrm{erf}\left(\frac{w'/2 - z}{2L_e} \right) \right], \quad (9)$$

where $L_e^2 = \sum L_n^2$.

It is shown in Eq. (9) that the impurity distribution after multiple diffusion processes can be characterized with an effective diffusion length, the square of which equals the sum of the square of diffusion lengths of each diffusion process.

3. Results and discussion

3.1. Numerical results

Using Eq. (9), it is possible to calculate the impurity distribution after multiple diffusion processes. Several conditions

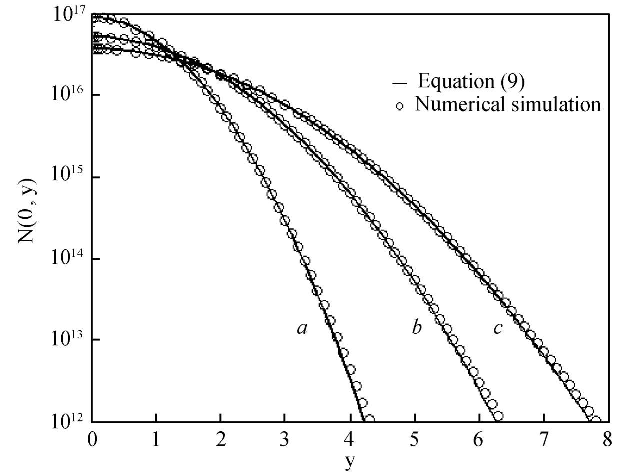

Fig. 3. Impurity distribution along the y direction in Fig. 2 in different conditions. The impurity atoms diffuse for (a) 210 min at 1100 °C and then 30 min at 1200 °C, (b) 120 min at 1100 °C and then 120 min at 1200 °C, (c) 30 min at 1100 °C and then 210 min at 1200 °C.

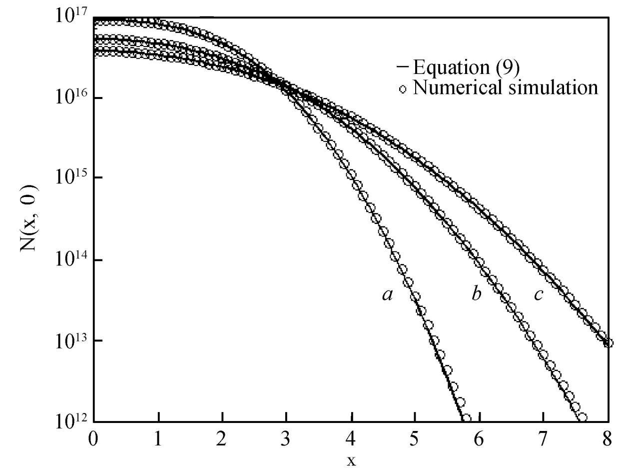

Fig. 4. Impurity distribution along the x direction in Fig. 2. The impurity atoms diffuse for (a) 210 min under 1100 °C and then 30 min under 1200 °C, (b) 120 min under 1100 °C and then 120 min under 1200 °C, (c) 30 min under 1100 °C and then 210 min under 1200 °C.

have been considered and the results are presented here. Numerical simulations by using SUPREM Ⅳ are also taken to verify the accuracy of the expression.

The impurity atoms diffuse in a two-dimensional plane here, setting w' in Eq. (9) ∞. The window considered here is 4 μm wide. Before the diffusions, a fixed amount of impurity atoms is pre-deposited upon the plane. The conditions considered here are: (a) the impurity atoms diffuse for 210 min at 1100 °C and then 30 min at 1200 °C; (b) the impurity atoms diffuse for 120 min at 1100 °C and then 120 min at 1200 °C; (c) the impurity atoms diffuse for 30 min at 1100 °C and then 210 min at 1200 °C. The density N_s of pre-deposited impurity atoms is 1×10^{13} cm^{-2}. The diffusion coefficient of impurity atom is 1.54×10^{-13} cm^2/s at 1100 °C, 1.1×10^{-12} cm^2/s at 1200 °C respectively. The results of numerical simulations and Equation (9) are shown in Figs. 3 and 4. Figure 3 shows the impurity distribution along the y direction in Fig. 2 start-

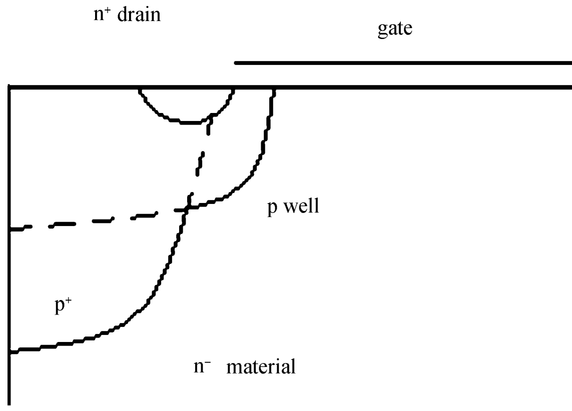

Fig. 5. Structure of an IGBT cell.

ing from the middle of the window. Figure 4 shows the impurity distribution along the x direction in Fig. 2 starting from the middle of the window. The impurity distributions given by Eq. (9) agree well with the results of numerical simulations. The total diffusion time of each condition is the same but the impurity distribution in the end is not the same. So the impurity distribution after multiple diffusion processes cannot be got simply by adding all the diffusion times.

3.2. Application of the expression

In vertical IGBT, a high dose of p-type impurity is used to decrease the base resistance of a parasitic npn transistor. A lower dose of p-type impurity is diffused into the n^--material later to form the channel, as seen in Fig. 5. If the hole current flowing under the n^+-drain is large enough to forward bias the p-well/n^+-drain junction, latch-up occurs. So it is important to calculate the p-well resistance under the n^+-drain.

The impurities under the n^+-drain are partly from p^+-diffusion, partly from p-well diffusion. Assuming that the effective diffusion length of p^+-distribution before p-well diffusion is L_{e1}, the effective diffusion length for the p-type impurity is L_{e2} in the p-well diffusion process.

Then the p-type impurity distribution can be described as:

$$N(x,y,z) = \frac{N_{s1}}{4\sqrt{\pi L_{ef}^2}}\exp\Big(-\frac{y^2}{4L_{ef}^2}\Big)\Big[\mathrm{erf}\Big(\frac{x+w_1/2}{2L_{ef}}\Big) + \mathrm{erf}\Big(\frac{w_1/2-x}{2L_{ef}}\Big)\Big]\Big[\mathrm{erf}\Big(\frac{z+w_1'/2}{2L_{ef}}\Big)+\mathrm{erf}\Big(\frac{w_1'/2-z}{2L_{ef}}\Big)\Big] + \frac{N_{s2}}{4\sqrt{\pi L_{e2}^2}}\exp\Big(-\frac{y^2}{4L_{e2}^2}\Big)\Big[\mathrm{erf}\Big(\frac{x+w_2/2}{2L_{e2}}\Big)+\mathrm{erf}\Big(\frac{w_2/2-x}{2L_{e2}}\Big)\Big] \times\Big[\mathrm{erf}\Big(\frac{z+w_2'/2}{2L_{e2}}\Big)+\mathrm{erf}\Big(\frac{w_2'/2-z}{2L_{e2}}\Big)\Big], \tag{10}$$

where $L_{ef}^2 = L_{e1}^2 + L_{e2}^2$, N_{s1} is the amount of impurity in the p^+-diffusion, w_1, w_1' are the length and width of the window for p^+-diffusion respectively. N_{s2} is the amount of impurity in the p^+-diffusion, w_2, w_2' are the length and width of the window for p-well diffusion respectively.

The first part at the right of Eq. (10) describes the impurity distribution due to p^+-diffusion, the second part describes the impurity distribution due to p-well diffusion. The resistance under the n^+-drain can be calculated using Eq. (10) for different sizes of IGBT cell and different process conditions, thus estimating the latch-up current for IGBT devices. Gaussian functions may be used to simplify the error functions in Eq. (10), as has been previously proposed in Ref. [10].

4. Conclusion

This paper analyzes the impurity distribution after multiple diffusion processes. It is proved that the distribution in the end can be characterized with an effective diffusion length L_e. The square of L_e equals the sum of the square of diffusion lengths in each high temperature process. The results agree well with numerical simulations by using SUPREM Ⅳ. An example of the application of the expression for impurity distribution is proposed. Software can also tell what the impurity distribution is, but it requires efficient simulation codes with a considerable amount of computing time and effort. The simulation results are not instructive and cannot tell the effect of each diffusion process in the final impurity distribution. The effect of subsequent processes on the already formed junctions can be estimated in advance with the help of the expressions given in this paper. The results are helpful and instructive in the design and fabrication of devices.

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