The Three-Dimensional Impurity Distribution of a Planar p-n Junction

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I. Introduction

In the fabrication of the modern silicon semiconductor device, such as the passivated planar transistor or the monolithic intergrated circuit, the p-n junction is formed by impurity diffusion through a finite diffusion mask opening. The diffusion mask is a layer of silicon dioxide thermally grown by steam oxidation technique. The diffusion opening may be a rectangular stripe or circular dot precisely revealed by photolithographic technique. (1)

The impurity atom distribution can not be approximated by an elementary one-dimensional diffusion process. (2) Instead, this distribution must be determined from a detailed solution of a boundary value problem for the structure under consideration. (3) The purpose of this paper is to present a full three-dimensional soution of diffusion problem by integral transform method. The solution is based upon an instantaneous source diffusion process. Two different diffusion openings are considered in the analysis. The rectangular coordinates and the multiple Fourier transform are used for the rectangular geometry. The cylindrical coordinates and the multiple Fourier-Bessel transform are used for the circular geometry.

II. Analysis

The entire semiconductor surface is assumed to be covered by a diffusion mask, except that portion of the surface from which diffusion is to take place. It should be recognized that the present mathematical analysisis based upon an idealization of the oxide masking technique. For analytical purposes, it is assumed that the diffusion mask is an impenetrable barrier for impurity atoms, thereby reducing to zero the impurity atom flux normal to the semiconductor surface.

The diffusion of impurity atoms within a homogeneous medium is governed by the differential equation

(1) $(\nabla^2 - \frac{1}{D}\frac{\partial}{\partial t})\, N(\bar{x}, t) = 0$

where $N(\bar{x}, t)$ is the impurity concentration, D is the impurity diffusion constant and ∇^2 is the Laplacian operator. In rectangular coordinates, $\bar{x} = (x, y, z)$

(2) $\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$

In cylindrical coordinates, $\bar{x} = (r, \phi, z)$

(3) $\nabla^2 = \frac{1}{r}\frac{\partial}{\partial r} r \frac{\partial}{r} + \frac{1}{r^2}\frac{\partial^2}{\partial \phi^2} + \frac{\partial^2}{\partial z^2}$

A two-step diffusion process is generally used in order to obtain a good impurity profile. A suitable amount of impurity atoms is deposited on the semiconductor surface during the first step in relatively low temperature, and, after the removal of impurity glass, the impurity atoms are drive in during the main diffusion process in high temperature.

For the case that the diffusion opening is a rectangle 2a wide 2b long and is predeposited with Q impurity atoms per unit area on the surface $z=0$, the initial condition for the main diffusion can be written by means of singularity functions $u_n(x)$[4]

(4) $N(x,y,z,o)$
$= 2Q[u_{-1}(x+a) - u_{-1}(x-a)][u_{-1}(y+b) - u_{-1}(y-b)]u_0(z)$

where $u_0(z)$ is the unit impulse function

(5) $u_0(z) = \begin{cases} \infty; z=0 \\ 0; z \neq 0 \end{cases}$ and $\int_{-\infty}^{\infty} u_0(z)dz = 1$

and $u_{-1}(z)$ is the unit step function

(6) $u_{-1}(z) = \int_{-\infty}^{z} u(z')\, dz' = \begin{cases} 1; z > 0 \\ 0; z < 0 \end{cases}$

For the circular surface geometry with radius a, the initial condition canbe written as

(7) $N(r,z,0) = 2Qu_{-1}(a-r)u_0(z)$

where the condition that the impurity concentration is constant in the angular direction is implied.

These boundary value problems can be solved easily by integral transform methods. By the use of integral transforms, both the differential equations and the boundary conditions can be transformed directly into simple forms. These simple equations can be solved by means of simple manipulation. Then the desired solutions can be obtained by taking inverse transformation.

In the rectangular coordinates, the multiple Fourier transform is used and is defined as

$$(8) \qquad n(k_1,k_2,k_3,t)=\iiint_{-\infty}^{\infty} N(x,y,z,t)\exp\left[-i(k_1x+k_2y+k^3z)\right]dxdydz$$

The most important formulas[5] and Fourier transforms of some special functions[4] are compiled in Table I.

The Fourier transform of the partial differential equation (1) in rectangular coordinates (2) can easily be obtained

$$(9) \qquad \left[-(k_1^2+k_2^2+k_3^2)-\frac{1}{D}\frac{\partial}{\partial t}\right]n(k_1,k_2,k_3,t)=0$$

where use has been made of (a) in Table I.

Table I Foruier Transform Pairs

	$f(t)=\frac{1}{2\pi}\int_{-\infty}^{\infty}F(w)\exp(jwt)dw$	$F(w)=\int_{-\infty}^{\infty}f(t)\exp(-jwt)dt$
a	$\frac{d^n}{dt^n}f(t)$	$(jw)^nF(w)$
b	$\int_{-\infty}^{t}f(x)dx$	$\frac{1}{jw}F(w)$
c	$f(t\pm T)$	$F(w)\exp(\pm jwT)$
d	$f(t)\exp(\pm jw_0t)$	$F(w\mp w_0)$
e	$u_n(t)$	$(jw)^n$
f	$\frac{1}{\sqrt{4\pi a^2}}\exp\left(\frac{-t^2}{4a^2}\right)$	$\exp(-a^2w^2)$

The transform of the initial condition (4) is

(10) $$n(k_1,k_2,k_3,0) = 8Q \frac{\sin k_1 a}{k_1} \frac{\sin k_2 b}{k_2}$$

where use is made of (c) and(e) in Table I.

The solution of the first order differential equation (9) satisfied with the initial condition (10) is

(11) $$n(k_1,k_2,k_3,t) = 8Q \frac{\sin k_1 a}{k_1} \frac{\sin k_2 b}{k_2} \exp[-(k_1^2 + k_2^2 + k_3^2)Dt]$$

The desired impurity distribution can be obtained by taking the inverse Fourier transform of $n(k_1,k_2,k_3,t)$ of (11)

(12) $$N(x,y,z,t) = \frac{1}{(2\pi)^3} \iiint_{-\infty}^{\infty} n(k_1,k_2,k_3,t) \exp[j(k_1 x + k_2 y + {}_3 z)] dk_1 dk_2 dk_3$$

The inverse transform of $\exp(-k_3^2 Dt)$ is followed directly from (f) in Table I.

(13) $$\frac{1}{2\pi} \int_{-\infty}^{\infty} \exp(-k_3^2 Dt) \exp(jx_3 z) dk_3 = \frac{1}{\sqrt{4\pi Dt}} \exp\left(\frac{-z^2}{4Dt}\right)$$

The inverse transform of $\frac{\sin k_1 a}{k_1} \exp(-k_3^2 Dt)$ can be derived by means of (f), (b) and (c) in Table I.

(14) $$\frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{\sin k_1 a}{k_1} \exp(-k_1^2 Dt) \exp(jk_1 x) dk_1$$

$$= \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{\exp(jk_1 a) - \exp(-jk_1 a)}{2jk_1} \exp(-k_1^2 Dt) \exp(jk_1 x) dk_1$$

$$= \frac{1}{2} \int_{-\infty}^{x+a} \frac{1}{\sqrt{4\pi Dt}} \exp\left(\frac{-x'^2}{4Dt}\right) dx' - \int_{-\infty}^{x-a} \frac{1}{\sqrt{4\pi Dt}} \exp\left(\frac{-x'^2}{4Dt}\right) dx'$$

$$= \frac{1}{4} \left[\frac{2}{\sqrt{\pi}} \int_{x-a}^{x+a} \frac{1}{4Dt} \exp\left(\frac{-x'^2}{4Dt}\right) dx' \right]$$

$$= \frac{1}{4} \left[\mathrm{erf}\left(\frac{x+a}{2\sqrt{Dt}}\right) - \mathrm{erf}\left(\frac{x-a}{2\sqrt{Dt}}\right) \right]$$

Similarly

$$(15) \qquad \frac{1}{2\pi}\int_{-\infty}^{\infty} \frac{\sin k_2 b}{k_2} \exp(-k_2^2 Dt)\exp(jk_2 y)\, dk_2$$

$$= \frac{1}{4}\left[\operatorname{erf}\left(\frac{y+b}{2\sqrt{Dt}}\right) - \operatorname{erf}\left(\frac{y-b}{2\sqrt{Dt}}\right)\right]$$

The multiple integral (12) is therefore reduced to the product of the error functions (14), (15) and the Gaussian function (13)

$$(16) \qquad N(x,y,z,t) = \frac{Q}{4\sqrt{\pi Dt}}\left[\operatorname{erf}\left(\frac{x+a}{2\sqrt{Dt}}\right) - \operatorname{erf}\left(\frac{x-a}{2\sqrt{Dt}}\right)\right] \cdot$$

$$\left[\operatorname{erf}\left(\frac{y+b}{2\sqrt{Dt}}\right) - \operatorname{erf}\left(\frac{y-b}{2\sqrt{Dt}}\right)\right] \exp\left(\frac{-z^2}{4Dt}\right)$$

In the cylindrical coordinates, the Fourier-Bessel integral must be used[6], and the transform of a function $N(r,z,t)$ can be defined as

$$(17) \qquad n(k,k_3,t) = \int_0^{\infty} r dr \int_{-\infty}^{\infty} dz\ N(r,z,t)\ J_0(kr)\exp(-jk_3 z)$$

where

$$(18) \qquad n(k,z,t) = \int_0^{\infty} r dr\ N(r,z,t)\ J_0(kr)$$

is known as zero-order Hankel transform.[5] It is easy to show that[7]

$$(19) \qquad \int_0^{\infty} r dr \left[\frac{1}{r} \frac{\partial}{\partial r} r \frac{\partial}{\partial r} N(r,z,t)\ J_0(kr) = -k^2 n(k,z,t)\right]$$

and

$$(20) \qquad \int_0^{\infty} r dr\ u_{-1}(a-r)\ J_0(kr) = \frac{a}{k} J_1(ka)$$

The Fourier-Bessel integral transform (17) of the differential equation (1) with operator (3) is simply

$$(21) \qquad k\left(-k^2 - \frac{2}{3} - \frac{1}{D} \frac{\partial}{\partial t}\right) n(k,k_3,t) = 0$$

where use is made of (a) in Table I and (19). The Fourier-Bessel integral transform of the boundary condition (7) is

$$(22) \qquad n(k,k_3,0) = 2Q\frac{a}{k} J_1(ka)$$

where use is made of (e) in Table I and (20)

The solution of the first order differential equation (21) satisfied with the initial condition (22) is

$$(23)\qquad n(k,k_3,t) = 2Q\frac{a}{k}J_1(ka)\exp\left[-(k^2+k_3^2)Dt\right]$$

The desired impurity distribution $N(r,z,t)$ can be obtained by taking the inverse transform of $n(k,k_3,t)$

$$(24)\qquad N(r,z,t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dk_3 \int_0^{\infty} kdk\ n(k,k_3,t)\ J_0(kr)\exp(jk_3z)$$

It is easy to show that

$$(25)\qquad \int_0^{\infty} kdk\frac{a}{k}J_1(ka)\exp(-k^2Dt)\ J_0(kr)$$

$$= -\sum_{m=0}^{\infty}\sum_{\ell=0}^{\infty}\frac{(m+\ell)!}{(m+1)!m!(\ell!)^2}\left(\frac{-a}{4Dt}\right)^{m+1}\left(\frac{-r^2}{4Dt}\right)^{\ell}$$

where use is made of the series expansion of the Bessel functions $J_1(ka)$ and $J_0(kr)$and the definition of the Gamma function. By means of (f) in Table I and(25), the multiple integral (24) becomes

$$(26)\qquad N(r,z,t)$$

$$= \frac{-Q}{\sqrt{\pi Dt}}\sum_{m=0}^{\infty}\sum_{\ell=0}^{\infty}\frac{(m+\ell)!}{(m+1)!m!(\ell!)^2}\left(\frac{-a^2}{4Dt}\right)^{m+1}\left(\frac{-r^2}{4Dt}\right)^{\ell}\exp\left(\frac{-z^2}{4Dt}\right)$$

or

$$(27)\qquad N(r,z,t)$$

$$= \frac{-Q}{\sqrt{\pi Dt}}\sum_{m=0}^{\infty}\frac{1}{(m+1)!}\left(\frac{-a^2}{4Dt}\right)^{m+1}{}_1F_1\left(m+1;1;\frac{-r^2}{4Dt}\right)\exp\left(\frac{-z^2}{4Dt}\right)$$

where

$$(28)\qquad {}_1F_1(g;h;x) = \sum_{i=0}^{\infty}\frac{g_i}{h_i}\frac{x^i}{i!};\qquad g_i = \frac{(g+i-1)!}{(g-1)!}$$

is the confluent hypergeometry function.[8]

III. Discussion

From the rigorous mathematical solution in the rectangular coordinates (16), it is interesting to note that the surface concentration at the center of the diffusion window

(30) $$N(o,o,o,t)=\frac{Q}{\sqrt{\pi Dt}}\operatorname{erf}\frac{a}{2\sqrt{Dt}}\operatorname{erf}\frac{b}{2\sqrt{Dt}}$$

depends upon the dimension of the rectangle, if a and b are comparable with the diffusion length $2\sqrt{Dt}$.

The constant concentration surfaces can be calculated from (16). The contour in the y-z plane is

(31) $$\frac{N(o,y,z,t)}{N(o,o,o,t)}=\frac{\operatorname{erf}\left(\frac{y+b}{2\sqrt{Dt}}\right)-\operatorname{erf}\left(\frac{y-b}{2\sqrt{Dt}}\right)}{2\operatorname{erf}\left(\frac{b}{2\sqrt{Dt}}\right)}\exp\left(\frac{-z^2}{4Dt}\right)=\text{const.}$$

and is shown in Fig. 1, and the contour in the surface z=o is

(32) $$\frac{N(x,y,o,t)}{N(o,o,o,t)}$$

$$=\left[\frac{\operatorname{erf}\left(\frac{x+a}{2\sqrt{Dt}}\right)-\operatorname{erf}\left(\frac{x-a}{2\sqrt{Dt}}\right)}{2\operatorname{erf}\left(\frac{a}{2\sqrt{Dt}}\right)}\right]\left[\frac{\operatorname{erf}\left(\frac{y+b}{2\sqrt{Dt}}\right)-\operatorname{erf}\left(\frac{y-b}{2\sqrt{Dt}}\right)}{2\operatorname{erf}\left(\frac{b}{2\sqrt{Dt}}\right)}\right]$$

$$=\text{const.}$$

and are shown in Fig. 2. These two configurations illustrate the ina dequacy of the one-dimensional approximation for the deep diffusch as the isolation process in the fabrication of integrated circuits.[9]

The impurity distribution along x-axis is

(33) $$\frac{N(x,o,o,t)}{N(o,o,o,t)}=\frac{\operatorname{erf}\left(\frac{x+a}{2\sqrt{Dt}}\right)-\operatorname{erf}\left(\frac{x-a}{2\sqrt{Dt}}\right)}{2\operatorname{erf}\left(\frac{a}{2\sqrt{Dt}}\right)}$$

and is shown in Fig. 3, and the distribution along z-axis is

(34) $$\frac{N(o,o,z,t)}{N(o,o,o,t)}=\exp\left(\frac{-z^2}{4Dt}\right)$$

and is the Gaussian distribution and is shown in Fig. 4.

The constant concentration contours for the circular geometry can be calculated from (28). Using the fact that

(35) $${}_1F_1(g;h;o)=1$$

it is easy to show that the concentration at the center of the diffusion opening is

(36) $$N(o,o,t)=\frac{Q}{\sqrt{\pi Dt}}\ 1-\exp\left(\frac{-a^2}{4Dt}\right)$$

and the impurity distridution along z-axis is

(37) $$N(o,z,t)=N(o,o,t)=N(o,o,t)\exp\left(\frac{-z^2}{4Dt}\right)$$

and is identical with (34).

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V. References

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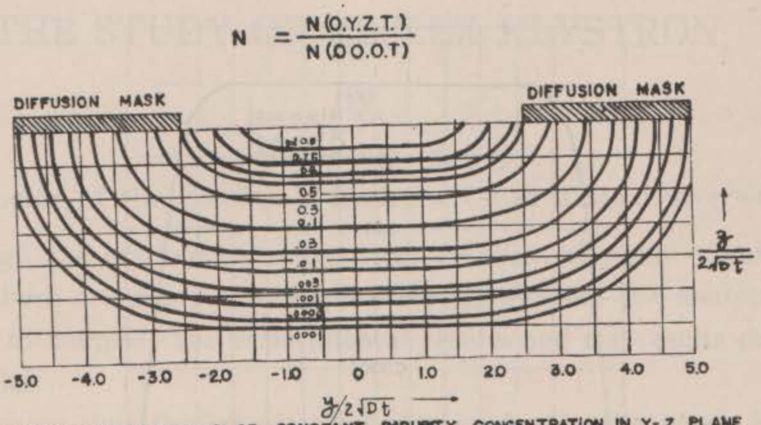

FIG. 1 CALCULATED CONTOURS OF CONSTANT IMPURITY CONCENTRATION IN Y-Z PLANE

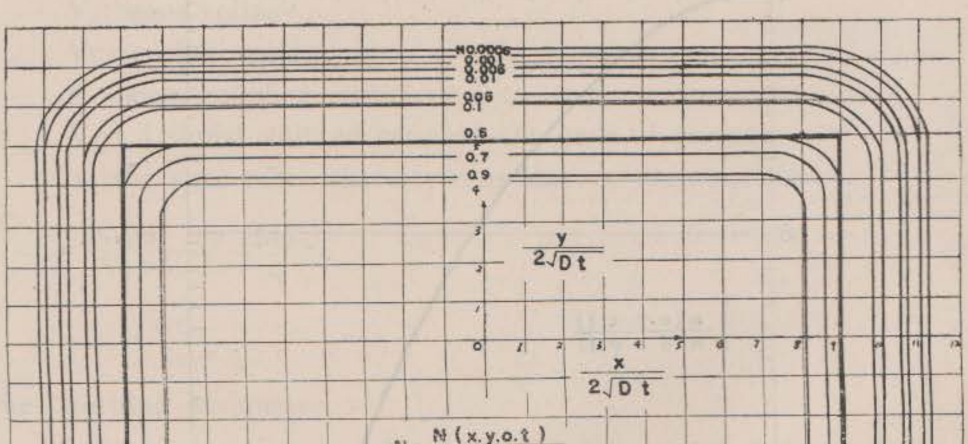

FIG. 2 CALCULATED CONTOURS OF CONSTANT IMPURITY CONCENTRATION AT THE SURFACE.

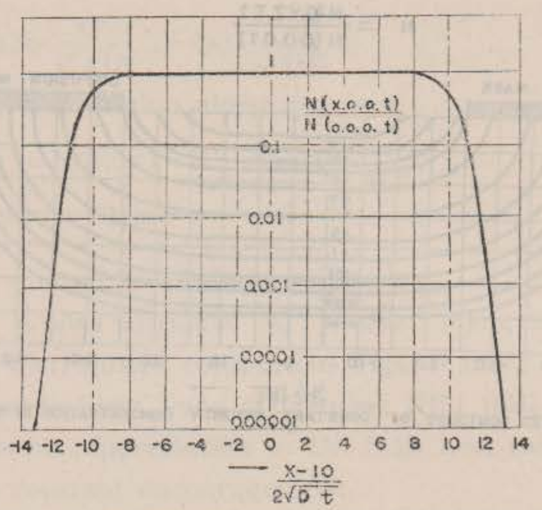

FIG.3 CALCULATED IMPURITY ATOM DISTRIBUTION ALONG X-AXIS

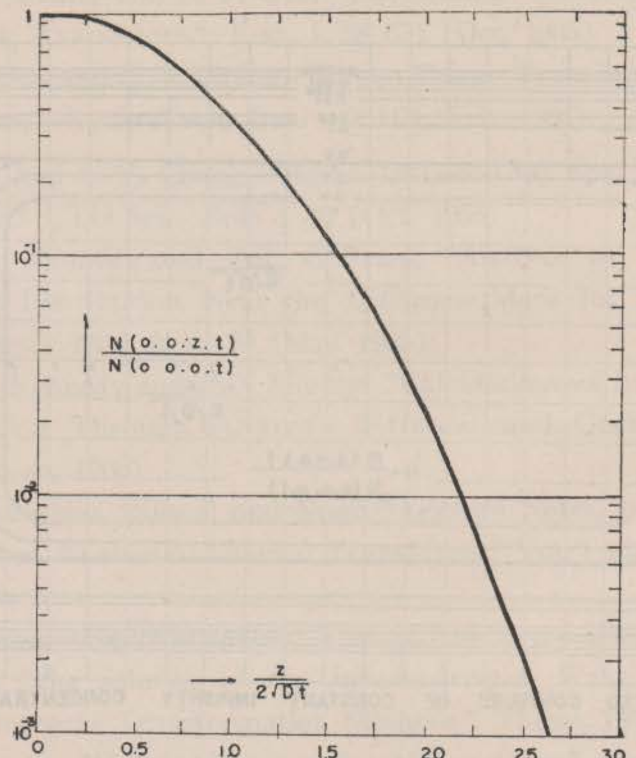

FIG.4 CALCULATED IMPURITY CONCENTRATION ALONG Z-AXIS