

Calculations of Impurity Atom Diffusion Through a Narrow Diffusion Mask Opening*

Abstract: Relaxation methods have been used to solve a mixed boundary value problem arising in the fabrication of junction transistors: impurity atom diffusion through a narrow diffusion mask opening. This particular problem is encountered in the fabrication of very narrow diffused p - n junctions. It is shown that the depth of a very narrow junction cannot always be determined from an elementary one-dimensional analysis of this diffusion process. If the width of a diffusion mask opening is less than two impurity atom diffusion lengths, the junction depth becomes geometry dependent. Normalized graphs are presented to illustrate the impurity atom distribution resulting from this particular geometric configuration.

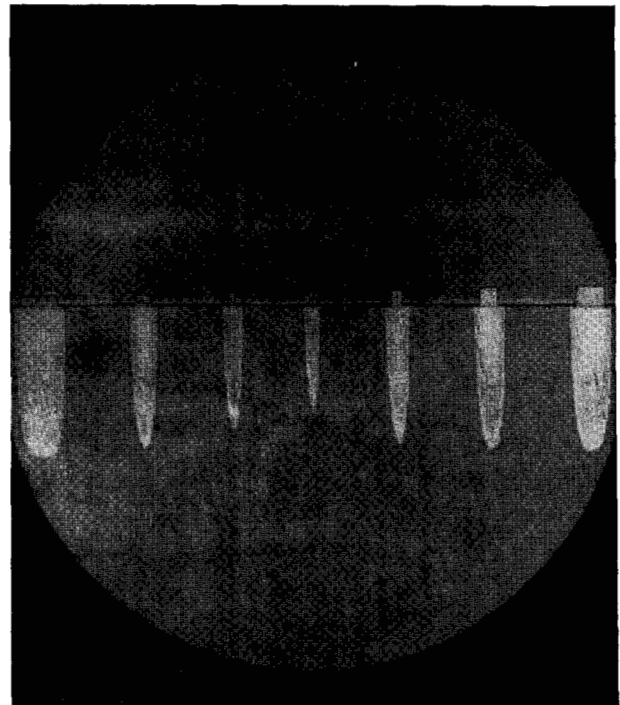
Introduction

In the design and fabrication of diffused semiconductor devices, the stripe geometry has become widely accepted. This type of structure is well suited to the photolithographic techniques used in transistor and integrated circuit fabrication. Furthermore, the stripe configuration has many advantages in the operation of junction transistors; for example, it reduces emitter current crowding, which is a frequent problem in high power devices. Although many such advantages are derived from a stripe geometry, important fabrication difficulties frequently arise because a very narrow diffusion mask opening will sometimes limit impurity atom penetration into the semiconductor material. In this type of structure the impurity atom distribution is no longer described by an elementary one-dimensional diffusion process. Instead, this distribution must be determined from a detailed solution of a boundary value problem approximating the structure under consideration.

Figure 1 shows an experimental demonstration¹ of the diffusion problem considered in this mathematical investigation. Several stripe-shaped openings were made in an oxide diffusion mask, each stripe of a different width. Next, impurity atoms were simultaneously diffused through these openings and into the semiconductor material. After the material had been beveled and stained a substantial difference could be observed in the penetration depth of each p - n junction. An important characteristic was observed by repeating this type of diffu-

sion process throughout a wide range of experimental conditions. The minimum width for a diffusion mask opening (before junction penetration becomes geometry

Figure 1 Photograph of the p - n junction profiles resulting from various size openings in a diffusion mask.



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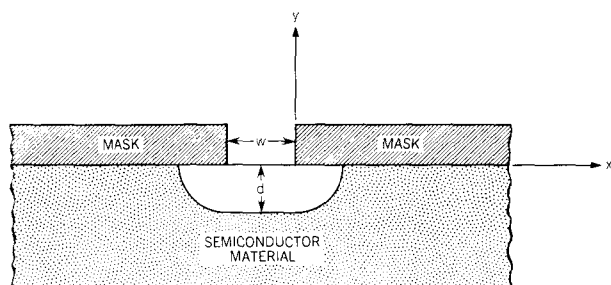


Figure 2 Mathematical model of the diffusion mask used for narrow *p-n* junction fabrication.

dependent) is not a constant; the minimum stripe width increases with an increase in impurity atom diffusion length.

This paper presents the results of a two-dimensional mathematical solution for a boundary value problem approximating the above experiment; such information is not presently available in the literature. Two different diffusion processes are considered in the mathematical analysis. The first solution is based upon a constant- C_0 diffusion process; i.e., during diffusion, a constant impurity atom concentration is maintained upon the exposed semiconductor surface. In addition, a solution is presented for this boundary value problem assuming the use of a two-step diffusion technique.² The two-step technique consists of maintaining a constant impurity atom surface concentration for a relatively small portion of the total diffusion time; thereafter the impurity atom source is removed and diffusion is continued.

Analysis

Figure 2 illustrates the mathematical model used in this investigation. 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 analysis is 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. It is further assumed that the diffusion mask does not provide an easy diffusion path along the mask and semiconductor boundary.

In rectangular Cartesian coordinates, the diffusion of impurity atoms within homogeneous media is given by the differential equation

$$\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} = \frac{1}{D} \frac{\partial C}{\partial t}, \quad (1)$$

where $C(x, y)$ represents the concentration density of impurity atoms, and D is their diffusion constant.

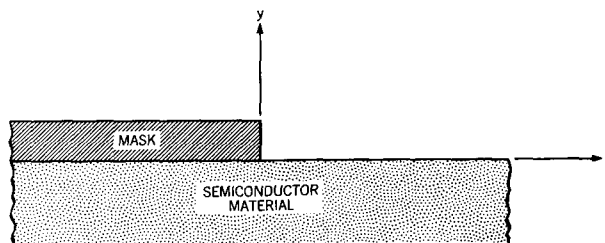


Figure 3 Semi-infinite analytical model of a planar junction diffusion mask.

There is no known analytical solution for Eq. (1) that is consistent with the boundary conditions shown in Fig. 2. In fact, this particular type of mixed boundary value problem is one of recognized mathematical difficulty.³ For this reason, relaxation methods⁴ have been used to obtain the required impurity atom distribution. The entire two-dimensional analytical model (Fig. 2) was approximated by a symmetrical matrix array of 4225 nodes. The boundary conditions of this structure (Fig. 2) were approximated by maintaining a specified impurity atom density upon the matrix nodes representing the semiconductor surface. Thereafter, the impurity atom density within this array was relaxed in a fashion consistent with a finite-difference approximation for Laplace's equation; thereby the diffusion process was synthesized. After a prescribed number of relaxation cycles through this matrix array, the resulting impurity atom distribution was taken to be the required solution of the boundary value problem.

Solving problems by relaxation is a numerical method rather than an analytical method. An important part of this numerical method is to estimate the resulting computational accuracy. The computation time required to complete this type of analysis is often excessive, and a relatively small nodal matrix must therefore be used to approximate the boundary value problem under consideration. For this reason, the computational accuracy becomes limited. In the present analysis an estimate of the accuracy is obtained by numerically calculating the impurity atom distribution within a structure similar to that shown in Fig. 2, yet this test structure differs sufficiently from Fig. 2 to represent a mathematically tractable boundary value problem. Thereafter, a direct comparison is made between the numerically determined impurity atom distribution, and the distribution obtained from an analytical solution of this same test problem.

It has been shown⁵ that a limited form of the present boundary value problem (Fig. 3) can be solved in an analytical fashion. After transforming the diffusion equation, Eq. (1), to polar coordinates,

$$\frac{\partial^2 C}{\partial r^2} + \frac{1}{r} \frac{\partial C}{\partial r} + \frac{1}{r^2} \frac{\partial^2 C}{\partial \theta^2} = \frac{1}{D} \frac{\partial C}{\partial t}, \quad (2)$$

and thereafter solving for the impurity atom distribution in Fig. 3, we obtain

$$C(r, \theta, t) = C_0 \left\{ 1 - \frac{2}{\pi} \sum_{n=0}^{\infty} \sin(s_n \theta) \times \frac{(r/2\sqrt{Dt})^{s_n} \Gamma(s_n/2)}{2\Gamma(s_n + 1)} {}_1F_1\left[\frac{s_n}{2}; s_n + 1; -\frac{r^2}{4Dt}\right] \right\}, \quad (3)$$

where the hypergeometric series ${}_1F_1[\alpha; \beta; \gamma]$ is given by

$${}_1F_1[\alpha; \beta; \gamma] = \sum_{k=0}^{\infty} \frac{\alpha_k}{k! \beta_k} \gamma^k, \quad (4)$$

and

$$h_k = h(h+1)(h+2)(h+3) \cdots (h+k-1), \quad h_0 = 1, \quad (5a)$$

$$s_n = (n + \frac{1}{2}). \quad (5b)$$

Although Eq. (3) is not directly applicable to the boundary value problem under discussion (Fig. 2), this equation provides a means of estimating the computational accuracy obtained by the numerical analysis. From calculations of the impurity atom distribution in Fig. 3, using Eq. (3), it can be shown that negligible change will be observed in the impurity atom distribution of Fig. 2 when the diffusion mask opening is four impurity atom diffusion lengths, or larger. For structures containing a diffusion mask opening of four impurity atom diffusion lengths (Fig. 2), an estimate of the computational accuracy is obtained by a direct comparison between Eq. (3) and a numerical solution of the boundary value problem.

Equation (3) is applicable only when the diffusion process maintains a constant impurity atom concentration (C_0) upon the semiconductor surface. During recent years, transistor fabrication techniques have been directed toward a two-step diffusion process. In a two-step process, diffusion is first accomplished by the constant surface concentration method, although this initial diffusion is intentionally of limited penetration depth. The second part of this two-step process is accomplished without an impurity atom source. During this second diffusion, impurity atoms are permitted to penetrate deeply into the structure, with the presumed limitation that additional impurity atoms can neither enter nor leave the semiconductor material.

There is no known analytical two-dimensional solution for this two-step process. In one dimension, an integral solution has been obtained for the impurity atom distribution,²

$$C(x, t) = \frac{C_0}{2\sqrt{\pi D_2 t_2}} \int_0^{\infty} \left\{ \exp \left[-\frac{(x+x')^2}{4D_2 t_2} \right] + \exp \left[-\frac{(x-x')^2}{4D_2 t_2} \right] \right\} \text{Erfc}(x'/2\sqrt{D_1 t_1}) dx', \quad (6)$$

where t_1 and t_2 are the first and second diffusion times, respectively; D_1 and D_2 are the respective impurity atom diffusion constants during these intervals; and C_0 is the impurity atom surface concentration during the first diffusion.

The two-step diffusion represents a combination of two frequently used processes that are mathematically tractable in one dimension. If in Eq. (6) $D_2 t_2 \ll D_1 t_1$, we obtain the familiar complementary error function type of impurity atom distribution. If in Eq. (6) $D_1 t_1 \ll D_2 t_2$, this expression becomes a Gaussian distribution (instantaneous source). For Fig. 2, an instantaneous-source diffusion yields the two-dimensional impurity atom distribution

$$C(x, y, t) = \frac{C_0}{2\sqrt{\pi D_2 t_2}} e^{-(y^2)/4D_2 t_2} \times \left\{ \text{Erfc} \left(\frac{x-w}{2\sqrt{D_2 t_2}} \right) - \text{Erfc} \left(\frac{x+w}{2\sqrt{D_2 t_2}} \right) \right\}. \quad (7)$$

Equation (7) provides a means of evaluating the computational accuracy resulting from a relaxation solution of Fig. 2 when $D_1 t_1 \ll D_2 t_2$; this is accomplished in the same manner as described for Eq. (3).

Application

Figure 4 illustrates a series of calculated p - n junction profiles resulting from various size diffusion mask openings. This particular illustration was obtained from numerous relaxation solutions for the boundary value problem shown in Fig. 2. Although these calculated junction profiles (Fig. 4) are intended to approximate the accompanying photograph (Fig. 1), it should be mentioned that the photograph contains substantial distortion. This distortion arises from the use of a low angle bevel which magnifies the dimension perpendicular to the semiconductor surface, but the bevel permits greater accuracy to be obtained in the measurement of junction penetration depth.

It is impractical to present a detailed illustration of the impurity atom distribution resulting from calculations similar to those plotted in Fig. 4. For this reason, such information is given only along two important geometrical dimensions of a planar p - n junction: in a direction perpendicular to the semiconductor surface, at the center of the diffusion mask opening (Fig. 5); and in a direction parallel to the semiconductor surface, along the semiconductor-diffusion mask boundary (Fig. 6). Because

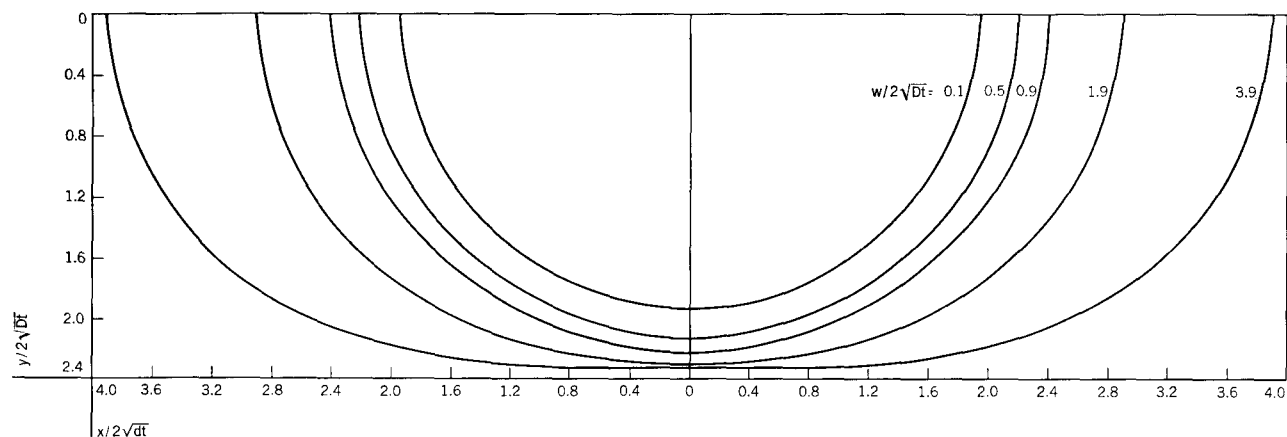


Figure 4 Calculated p - n junction profiles resulting from various size openings in a diffusion mask when $C_b/C_0 = 10^{-3}$. This calculation is based upon a constant- C_0 diffusion process.

both of these illustrations (Figs. 5 and 6) were obtained from relaxation solutions of the associated boundary value problem, an estimate must be made for the computational accuracy of the numerical technique. This estimate is obtained from Figs. 7 and 8.

Assuming a diffusion mask width of at least four impurity atom diffusion lengths (where $L_0 = 2\sqrt{Dt}$), it can be shown⁵ that Eq. (3) provides a valid description of the required impurity atom distribution. For this type of structure, a direct comparison has been made between Eq. (3) and the numerically determined impurity atom density. Figure 7 presents such a comparison along a line perpendicular to the semiconductor surface. Similarly,

Fig. 8 presents a comparison along the semiconductor-diffusion mask boundary.

From Figs. 7 and 8, when the diffusion mask opening has a width of at least four impurity atom diffusion lengths ($8\sqrt{Dt} \leq w$), the numerical method provides sufficient accuracy for most engineering purposes. A negligible error is observed in Fig. 7 along a line perpendicular to the semiconductor surface and at the center of this mask opening. In contrast, the numerical method introduces an error of about 15% in the calculated impurity atom density along the semiconductor-diffusion mask boundary (Fig. 8). The source of this error is readily seen. The density of a four thousand (4225) node relaxation

Figure 5 Calculated junction depth perpendicular to the semiconductor surface and at the center of the diffusion mask opening (constant- C_0 diffusion process).

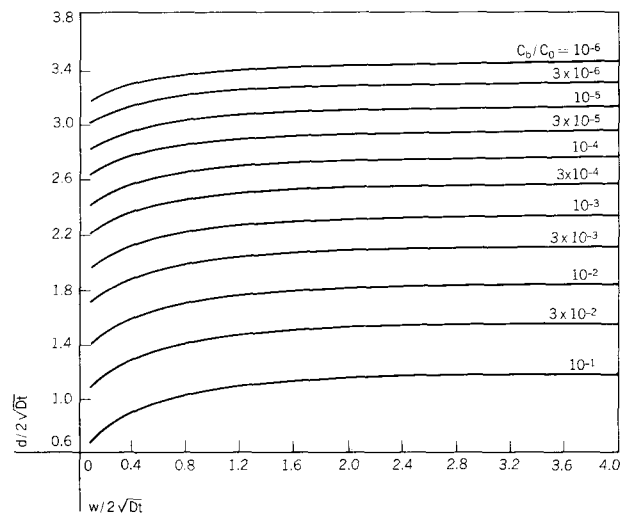
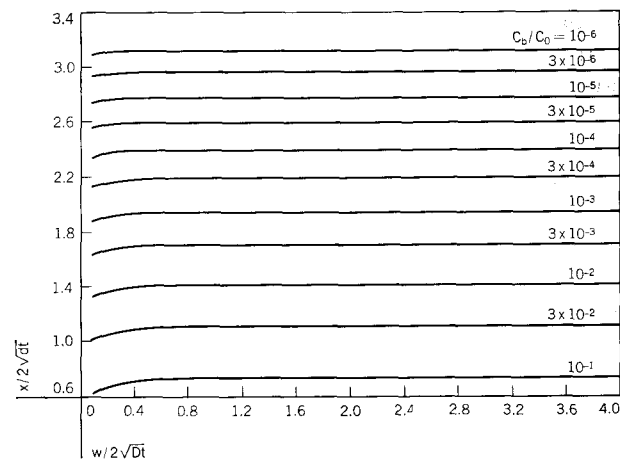


Figure 6 Calculated junction location along the semiconductor-diffusion mask boundary (constant- C_0 diffusion process).



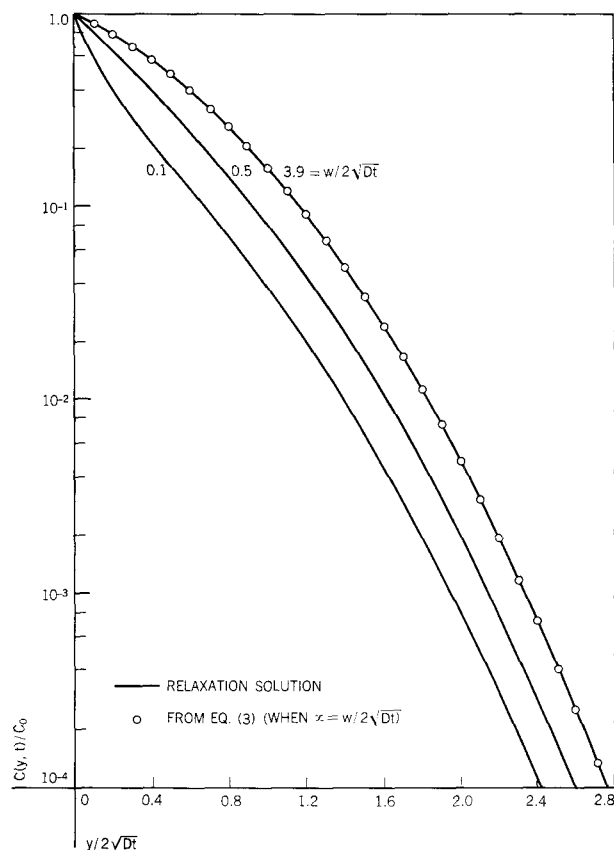


Figure 7 Impurity atom profile perpendicular to semiconductor surface and at the center of the diffusion mask opening (constant- C_0 diffusion process).

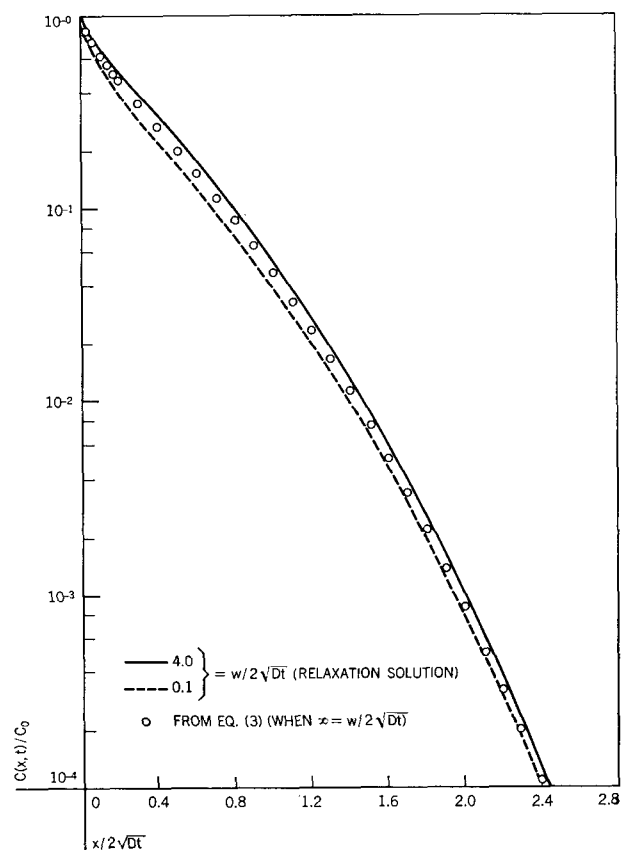


Figure 8 Impurity atom profile along the semiconductor-diffusion mask boundary (constant- C_0 diffusion process).

matrix is not sufficient to resolve a large impurity atom gradient, particularly when this gradient exists only within a small region of the semiconductor material. In Fig. 8, such a gradient is observed near the diffusion mask edge ($y = 0$).

An estimate of the computational accuracy has been made for narrow diffusion mask openings ($w \approx 0.2\sqrt{Dt}$). A decrease of opening width introduces no basic change in the impurity atom distribution along the semiconductor-diffusion mask boundary (Fig. 8). At this location we can therefore expect little increase (or decrease) in the computational error. The numerically determined concentration density should always remain slightly larger than its correct value, although this error should not exceed 15%.

It can be observed (Fig. 7) that a narrow diffusion mask opening introduces fundamental changes in the impurity atom distribution perpendicular to the semiconductor surface. In fact, a close comparison of Figs. 7 and 8 shows that the distributions become identical in these two illustrations when $w = 0.2\sqrt{Dt}$. This implies that a narrow mask opening results in the same impurity

atom distribution parallel and perpendicular to the semiconductor surface; an identical computational error will therefore exist in these two directions.

Figures 9 and 10 present the results of similar calculations, assuming the use of a two-step diffusion process. Figure 9 shows the calculated penetration depth of a p - n junction in a direction perpendicular to the semiconductor surface (at the center of the diffusion mask opening). Figure 10 shows the calculated junction penetration depth along the semiconductor-diffusion mask boundary. Both of these illustrations indicate an increased dependence upon the width of a diffusion mask opening, with a decrease in the ratio of the impurity atom diffusion lengths during the two parts of the two-step process (D_1t_1/D_2t_2).

Again, as in the constant- C_0 calculations (Figs. 5 and 6), it is necessary to evaluate the computational accuracy attained by these numerical techniques. For the two-step diffusion process, this evaluation has been conducted for values of the ratio (D_1t_1/D_2t_2) that yield an impurity atom distribution lying between the Gaussian (instantaneous source) and the complementary error function

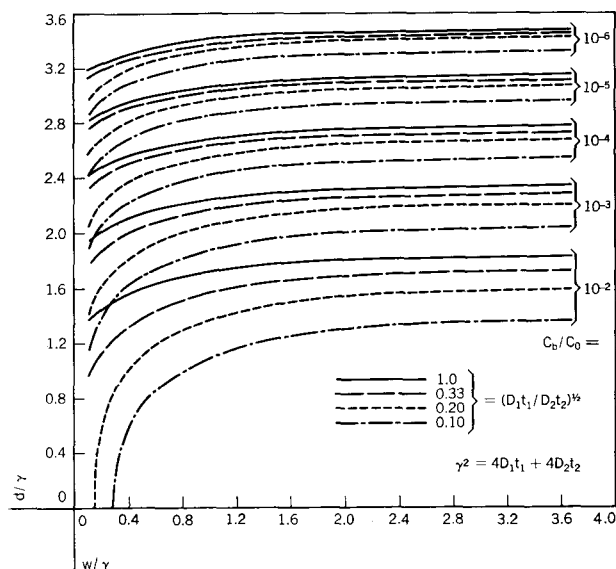


Figure 9 Calculated junction depth perpendicular to the semiconductor surface and at the center of the diffusion mask opening. This calculation is based upon a two-step diffusion process.

(constant C_0) types of distribution. Figure 11 (Curve A) presents the results of this evaluation. From a numerical calculation of the distribution perpendicular to the semiconductor surface and (at the center of the diffusion mask opening, Fig. 2), satisfactory agreement is obtained with the analytical one-dimensional equation for this distribution. This numerical calculation was conducted for a diffusion mask opening that is four diffusion lengths wide ($4.0 = w/\gamma$).

Because the boundary value problem of Fig. 2 is mathematically tractable for an instantaneous-source diffusion process, a means is available for estimating the accuracy of the numerical analysis at small values (.01) of (D_1t_1/D_2t_2) . This comparison is presented in Fig. 11 (Curves B and C). Satisfactory agreement is shown to exist between these two analytical techniques, thereby implying that the numerical solutions (Figs. 9 and 10) are adequate for most engineering purposes.

Conclusions

Figures 5 and 6 (constant- C_0 diffusion), and Figs. 9 and 10 (two-step diffusion), illustrate the p - n junction location within semiconductor material when diffusion takes place through a narrow diffusion mask opening. These junction locations are influenced negligibly by the width of the mask opening, assuming this width is two impurity atom diffusion lengths or larger ($4.0\sqrt{Dt} \leq w$). When the width of a diffusion mask opening becomes smaller than two impurity atom diffusion lengths ($w < 4\sqrt{Dt}$), a substantial reduction occurs in the p - n junction penetration depth. This reduced penetration depth is

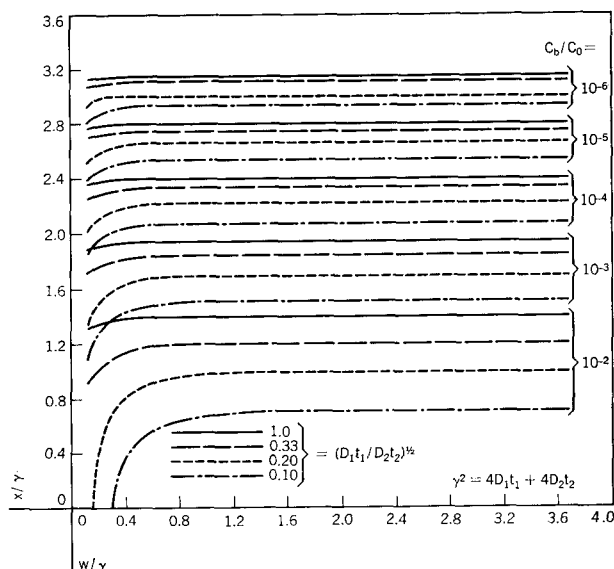
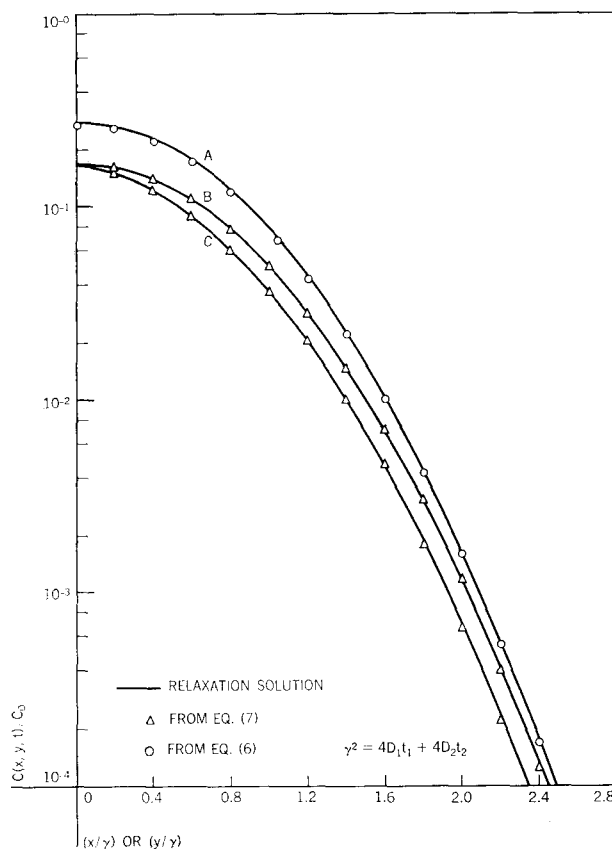


Figure 10 Calculated junction location along the semiconductor-diffusion mask boundary (two-step diffusion process).

Figure 11 Calculated impurity atom distributions after diffusion through narrow diffusion mask openings. Curve A perpendicular to surface when $w/\gamma = 4.0$ and $(D_1t_1/D_2t_2)^{1/2} = 0.33$; curve B perpendicular to surface when $w/\gamma = 0.30$ and $(D_1t_1/D_2t_2)^{1/2} = 0.10$; curve C along boundary when $w/\gamma = 0.30$ and $(D_1t_1/D_2t_2)^{1/2} = 0.10$.



shown to result from geometrical considerations alone, if no modifications are introduced into the diffusion process.

Figures 9 and 10 establish that at small values of the parameter ($D_1 t_1 / D_2 t_2$), the junction penetration depth becomes more dependent upon the width of the diffusion mask opening. In practice, one encounters such a situation when the initial step (t_1) in a two-step diffusion (holding constant C_0) becomes small as compared to the second step (diffusion after removal of the impurity atom source).

The results of this analysis have also established that impurity atom diffusion through a narrow mask opening ($w < 4.0 \sqrt{Dt}$) cannot be accurately described by an elementary one-dimensional analytical model. For a narrow stripe geometry, the one-dimensional approximation substantially overestimates the junction penetration depth.

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References

1. M. Duffy, private communication.
2. D. P. Kennedy and P. C. Murley, *Proc. IEEE* **52**, 620 (1964).
3. L. V. Kantorovich and V. I. Krylov, *Approximate Methods in Higher Analysis*, Interscience Publishing Co., New York, 1958.
4. R. V. Southwell, *Relaxation Methods in Engineering Science*, Oxford University Press, London, 1940.
R. V. Southwell, *Relaxation Methods in Theoretical Physics, Vol. I*, Oxford University Press, London, 1946.
R. V. Southwell, *Relaxation Methods in Theoretical Physics, Vol. II*, Oxford University Press, London, 1956.
R. V. Southwell, *An Introduction to the Theory of Elasticity*, Oxford University Press, London, 1941.
G. E. Forsythe and W. R. Wasow, *Finite-Difference Methods for Partial Differential Equations*, John Wiley and Sons, Inc., New York, 1960.
5. D. P. Kennedy and R. R. O'Brien, *IBM Journal* **9**, 179 (1965).

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