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# Analytical Modeling of Nonlinear Diffusion of Arsenic in Silicon

## Kjell O. Jeppson and Dan Anderson

*Department of Electrical and Computer Engineering, Chalmers University of Technology, S-412 96 Göteborg, Sweden*

## Gehan Amaratunga[1]

*Department of Electronics and Information Engineering, University of Southampton, England*

## Colin P. Please[2]

*Department of Mathematics, University of Reading, Reading, England*

## ABSTRACT

An analytical model is given for the nonlinear evolution of the diffusion profile of implanted arsenic in silicon. Special emphasis is given to the study of the front region of the diffusing impurity profile where the concentration falls steeply and previously given approximate investigations fail to apply. In particular, explicit expressions are found for the junction depth and the steepness of the profile at the junction, both important parameters in semiconductor device fabrication.

It is well known that at high impurity concentrations, $C$, the diffusion of arsenic in silicon results in much more abrupt impurity profiles than the classical (gaussian and erf functions) profiles described by linear diffusion theory. These high concentration impurity profiles can be described by solving the diffusion equation using a nonlinear diffusion coefficient (1)

$$D = h[D^0 + D^-(n/n_i)] \qquad [1]$$

where $n$ is the electron concentration

$$n = \frac{C}{2} \left\{ 1 + \left[ 1 + \left( \frac{2n_i}{C} \right)^2 \right]^{1/2} \right\} \qquad [2]$$

$n_i$ is the intrinsic concentration and $h$ is the self-electric field enhancement factor

$$h = 1 + \frac{C}{2n_i} \left[ \left( \frac{C}{2n_i} \right)^2 + 1 \right]^{-1/2} \qquad [3]$$

$D^0$ and $D^-$ represent the effective diffusivities under intrinsic conditions. This nonlinear diffusion coefficient has been verified from experimentally measured impurity profiles obtained, *e.g.*, by secondary ion mass spectroscopy (SIMS). The physical mechanism causing nonlinear diffusion in silicon has recently been summarized by Fair (2, 3).

The nonlinear diffusion equation is usually solved numerically as analytical approaches to nonlinear diffusion are very limited. Usually, attempts to analytically study diffusion at high impurity concentrations neglect the linear diffusion and approximate the diffusion coefficient in Eq. [1] by

$$D = 2D^-(C/n_i) \qquad [4]$$

For this approximation there exist exact solutions in the variable $x/\sqrt[3]{t}$ for the case of redistributive diffusion of high-dose shallow implants (4-6) and accurate approximations based on Chebyshev polynomials in the variable $x/\sqrt{t}$ for the case of constant surface concentration (1, 7). These solutions provide excellent approximations of the impurity profile down to about two orders of magnitude below the surface concentration where the concentration approaches the intrinsic value. However, they fail to accurately describe the impurity profile for lower

concentrations and to predict the junction depth for low background concentrations.

The purpose of the present work is to generalize the above solution for redistributive diffusion of high-dose shallow implants by expanding it into the low concentration tail region where the linear and nonlinear contributions to the diffusion coefficient are of the same order of magnitude. As in earlier work by Anderson and Jeppson (5, 8) and King and Please (9, 10), this work is based on similarity methods which provide a powerful and flexible tool for studies of nonlinear diffusion. Furthermore, the analytical solutions which are obtained are attractively simple and provide accurate approximations in excellent agreement with both numerical simulations and experimental results.

## Analysis

The present analysis will consider the case of a two-step diffusion process, where in the first step a shallow high dose, $Q_0$, ion implantation (represented by a delta function at the surface) is made. The second diffusive drive-in step redistributes the implanted impurities according to the diffusion equation

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x} \left[ D(C) \frac{\partial C}{\partial x} \right] \qquad [5]$$

At high concentrations, $C >> n_i$, the diffusion coefficient in Eq. [1] can be simplified according to Eq. [4] as discussed in the introduction. This reduces the diffusion equation to

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x} \left( 2D^- \frac{C}{n_i} \frac{\partial C}{\partial x} \right) \qquad [6]$$

which has been investigated extensively in several recent papers (5, 6). The solution of Eq. [6] describing the redistributive diffusion of an initially delta function shaped dose, $Q_0$, located at $x = 0$ is

$$C(x, t) = C_S(t)[1 - x^2/x_F^2(t)] \qquad [7]$$

where

$$x_F(t) = (18Q_0 D^- t/n_i)^{1/3} \qquad [8]$$

$$C_S(t) = 3/2 \, Q_0/x_F(t)$$

The solution of Eq. [6] is given by Eq. [7] and [8] displays the well-known diffusive behavior in the sense that the

[1]Present address: Cambridge University, Cambridge, England.
[2]Present address: University of Southampton, Southampton, England.

impurity profile flattens and become successively broader. However, an important difference as compared to linear diffusion is the fact that the solution [7] has compact support, *i.e.*, is zero outside a finite region at all times, which implies a well-defined diffusion front at $x = x_F(t) \sim t^{1/3}$.

One of the most important characteristics of the impurity profile is the junction depth, $x_J$, defined by

$$C(x_J, t) = C_J \qquad [9]$$

where generally the background concentration, $C_J$, is much smaller than the intrinsic concentration, $n_i$. As a first approximation of the junction depth one could take it equal to the width of the nonlinear diffusion profile, $x_F$, *i.e.*, $x_J \approx x_F$, *cf.* (5). However, in the vicinity of the front of the solution in Eq. [7], the concentration falls and ultimately the assumption $C >> n_i$ becomes violated. This implies that a more careful determination of the junction depth must consider in more detail the tail region of the diffusion profile and in particular the transition between nonlinear and linear diffusive behavior. Such an analysis is the purpose of the present investigation.

In order to improve on the nonlinear solution given by Eq. [7] and [8], we perform a tail analysis as follows: close to the front at $x = x_F(t)$ it is convenient to analyze the evolution of $C(x, t)$ in terms of the variables $t$ and $\eta = x - x_F(t)$, *i.e.*, $C = C(\eta, t)$. This procedure follows that given by King and Please (9, 10). In these variables Eq. [5] becomes

$$\frac{\partial C}{\partial t} + \frac{\partial C}{\partial \eta} \frac{\partial \eta}{\partial t} = \frac{\partial}{\partial \eta}\left( D \frac{\partial C}{\partial \eta} \right) \qquad [10]$$

where

$$\frac{\partial \eta}{\partial t} = -\frac{\partial x_F}{\partial t} = -\frac{x_F}{3t} \qquad [11]$$

and the diffusion coefficient $D$ is given by Eq. [1].

In the steep front region, the left-hand side of Eq. [10] is dominated by the $\partial C/\partial \eta$-term and we can neglect the term $\partial C/\partial t$. This is justified in the Appendix. This yields the following simplified equation, viz.

$$-\frac{x_F}{3t} \frac{\partial C}{\partial \eta} = \frac{\partial}{\partial \eta}\left( D \frac{\partial C}{\partial \eta} \right) \qquad [12]$$

Although Eq. [12] is still a partial differential equation, it only contains time as a parameter. Thus we can directly integrate [12] twice to obtain a closed form solution as shown by King and Please (10). However, in order to arrive at a simplified explicit result we choose to use an approximate diffusion coefficient given by, *cf.* (3)

$$D(C) = D_i + 2D^-(C/n_i) \qquad [13]$$

where $D_i = D^0 + D^-$ is the linear diffusion coefficient under intrinsic conditions. In this approximation, the self-electric field enhancement, $h$, is chosen one under intrinsic conditions and two for high concentration diffusion. This yields the following approximate solution

$$-\frac{x_F}{3t}\eta = D_i \ln \frac{C}{n_i} + 2D^- \frac{C}{n_i} + B(t) \qquad [14]$$

where $B(t)$ is a function of $t$ as yet to be determined. In deriving Eq. [14] we have also used the fact that $C$ and $\partial C/\partial \eta \to 0$ as $\eta \to \infty$ for every $t$.

It is easily seen that the high concentration limit of Eq. [14], viz.

$$\frac{C}{n_i} = -\frac{x_F}{6D^-t}\eta \qquad [15]$$

asymptotically joins the nonlinear solution [7] (assuming $C/C_S << 1$). However, the impurity profile for low concentrations develops an extended exponential tail given by

$$C \sim n_i \exp\left( -\frac{x_F}{3tD_i}\eta \right) \qquad [16]$$

It now remains to connect the tail solution [14] to the fully nonlinear solution given by Eq. [7]. A rigorous mathematical treatment of this problem using matched asymptotic expansions of the two solutions has recently been presented by King and Please (9, 10). Since the mathematical analysis used in (9, 10) is rather complicated, we adopt an alternative approximate procedure which has the advantage of being inherently simple but still provides basically the same information about the front behavior of the impurity profile. This procedure consists of choosing $B(t)$ so that both $C$ and $\partial C/\partial x$ are continuous at a matching-point $x$. which is also to be determined.

For the derivative we obtain from Eq. [7] by expanding in $C/C_S$ together with Eq. [14]

$$\frac{\partial C}{\partial x}\bigg|_x = -\frac{2C_S}{x_F}\left( 1 - \frac{1}{2}\frac{C_.}{C_S} \right)$$

$$= -\frac{x_F}{3t}\left( \frac{D_i}{C} + \frac{2D^-}{n_i} \right)^{-1} \qquad [17]$$

which implies

$$\frac{C}{n_i} = \left( \frac{D_i}{D^-}\frac{C_S}{n_i} \right)^{1/2} \qquad [18]$$

or equivalently

$$\frac{C}{C_S} = \left( \frac{D_i}{D^-}\frac{n_i}{C_S} \right)^{1/2} \qquad [19]$$

Note that $C_./n_i \sim t^{1/6}$, but $C_./C_S \sim t^{-1/6}$, *i.e.*, the matching will occur at successively lower values of concentration but higher up the front slope. Having found $C$ , the integration function $B(t)$ is determined from the continuity conditions and is found to be

$$B(t) = D_i\left[ 0.5 - \ln \frac{C}{n_i} \right] \qquad [20]$$

This value should be compared with the value obtained in (9), which after some manipulations leads to $B(t) = D_i [1.17\text{-}\ln(C_S/n_i)]$. The difference is fairly small in practice and the value in Eq. [20] compares well with numerical simulations.

Collecting our results we now obtain the solution for $C > C_.$

$$C = C_S\left( 1 - \frac{x^2}{x_F^2} \right) \qquad [21]$$

for $C < C_.$

$$\ln \frac{C}{n_i} + \frac{2D^-}{D_i}\frac{C}{n_i} = -\frac{x_F}{3tD_i}(x - x_F)$$

$$- \frac{1}{2}\left[ 1 - \ln\left( \frac{D_i}{D^-}\frac{C_S}{n_i} \right) \right] \qquad [22]$$

The smooth matching between the high concentration and the tail solutions is shown in Fig. 1 for the case of a total dose of $5 \times 10^{15}$ cm$^{-2}$ after 30 min of diffusion.

Of particular interest in the fabrication of semiconductor devices is the junction depth, which is found as

$$x_J = x_F + \frac{3tD_i}{x_F}\left\{ -\frac{2D^-}{D_i}\frac{C_J}{n_i} + \ln \frac{n_i}{C_J} \right.$$

$$\left. -\frac{1}{2}\left[ 1 - \ln\left( \frac{D_i}{D^-}\frac{C_S}{n_i} \right) \right] \right\}$$

$$\approx x_F + \frac{3tD_i}{x_F}\ln \frac{n_i}{C_J} \qquad [23]$$

For small times (shallow junctions and high background concentrations) the junction depth $x_J \approx x_F \sim t^{1/3}$ as earlier pointed out (5) and experimentally verified by Fair and Tsai (11). However, for longer diffusion times deviations
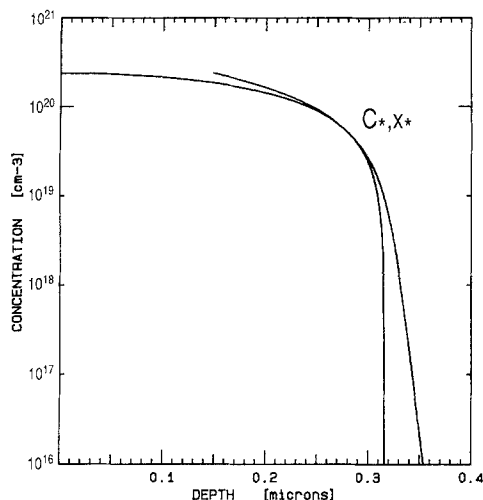
**Fig. 1.** Arsenic doping profile showing the match [at $(C, x)$] between the high concentration solution and the tail region solution.



**Fig. 3.** Comparison between doping profiles from analytical model (solid lines) and numerical simulations (dashed) after 20, 30, 40, and 60 min of diffusion.

from this simple relation become important, particularly at low background concentrations when the junction depth increases more rapidly.

Another important consequence of the tail analysis is its ability to provide information about the gradient of the impurity profile at the junction. By differentiating Eq. [16] at the junction we get

$$\left.\frac{\partial C}{\partial x}\right|_{x_J} \approx \frac{x_F}{3D_i t} C_J \qquad [24]$$

This indicates that the gradient decreases with the diffusion time as $t^{2/3}$. It is also worth noting that when plotted in a logarithmic scale the profile appears linear in the low concentration region as shown in Fig. 1.

Before discussing the obtained results, we would like to emphasize the following points: (*i*) the validity of the approximation leading to Eq. [13], *i.e.*, the neglect of the $\partial C/\partial t$-term, is justified *a posteriori* in the Appendix; (*ii*) the use of the high concentration solution in Eq. [7] for concentrations down to $C$ is justified in Eq. [18]. This greatly simplifies the analysis as compared to the rigorous mathematical expansion in (9, 10). The advantage of the present approach and its results is then the simple form emphasizing the physical understanding without any significant loss in accuracy.

### Discussion

In Fig. 2 the doping profile of a shallow arsenic implant after 30 min of diffusion in argon at 1000°C [measured by Hill (12)], has been compared to the analytical solution
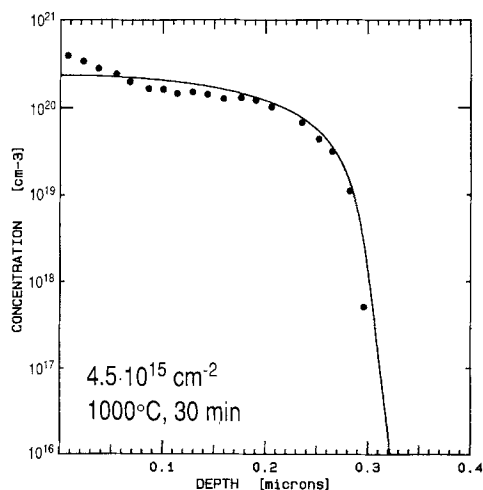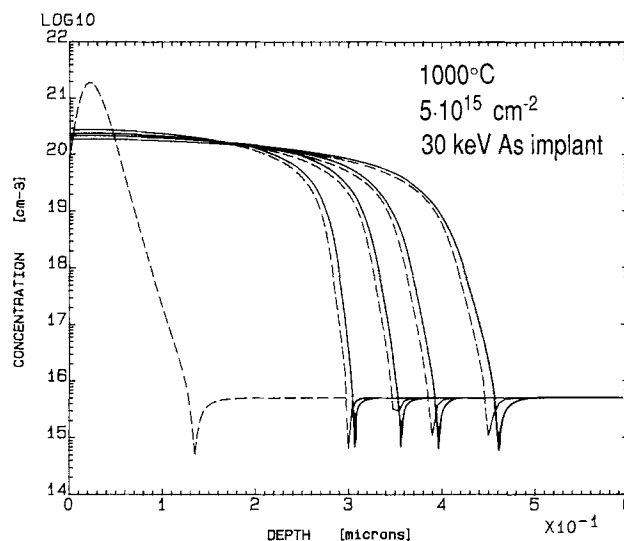


**Fig. 2.** Doping profile for a shallow arsenic implant after 30 min of diffusion compared with experimental data from Hill (12).

given by Eq. [21] and [22]. Excellent agreement is found between the theoretical curve and experimental data. A clear improvement has been obtained by adding the tail analysis in Eq. [22] as compared to the fitting of experimental data to the high impurity concentration theory of Eq. [7] only, which was given in an earlier paper (5). In this plot the widely accepted values of $D'' = 0.066$ exp-$(3.44/kT)$ and $D^- = 12$ exp-$(4.05/kT)$ has been used together with

$$n_i = 3.1 \cdot 10^{16} \, T^{3/2} \exp - (E_G/2kT) \qquad [25]$$

for the intrinsic concentration.

The analytical model has also been compared with numerical solutions of arsenic diffusion using finite difference based numerical simulations. In the numerical simulation a shallow 30 keV As implant with a dose of $5 \times 10^{15}$ cm$^{-2}$ was represented by a Pearson IV distribution. This implanted profile was then allowed to diffuse for 20, 30, 40, and 60 min, and compared to the analytical model. As can be seen from Fig. 3 there is excellent agreement. The difference in initial conditions (Pearson IV distribution *vs.* a surface delta function) is of minor importance even after very short diffusion times. This is because of the negligible time before the Pearson IV distribution assumes a similarity profile.

Neither the analytical nor the numerical solutions shown in Fig. 3, include a model for clustering of impurities. It is, however, observed from numerical simulations that clustering effects do not affect the shape of the tail region but merely alter its position. In this paper we have presented an extended analysis of impurity diffusion resulting in an analytical solution for this tail region.

The main result of this paper is then the possibility of accurately predicting the gradient of the impurity profile near the junction in device fabrication. The information provided by the tail region analysis in Eq. [24] is of great importance in semiconductor device models.

The junction depth of a nonlinearly diffused implanted impurity profile in high background concentration material (more than 1% of the surface concentration) has been shown by Fair (5) to increase as $t^{1/3}$ as predicted by Eq. [8]. However, when the background concentration is much lower, which is normally encountered in device fabrication, the junction depth may be considerably greater than predicted by this model. Therefore, a more accurate analytical model for junction depth prediction is desirable. The derivation of such a model is complicated by the lack of an analytical model which includes clustering in the high concentration region. However, the present analysis is useful even in the case of clustering effects if we accept the position of the diffusion front in Eq. [8] as a guideline for the junction depth at the
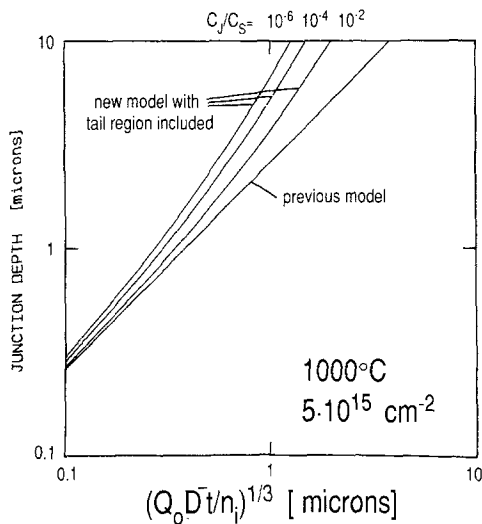
**Fig. 4.** Theoretical dependence of the junction depth on diffusion time, temperature, and dose (Eq. [23]) for three different background concentrations ($C_J/C_S = 10^{-2}$, $10^{-4}$, and $10^{-6}$) compared to the high concentration diffusion front approximation (Eq. [9]).

intrinsic concentration level. The tail analysis included in this paper then accounts for the increase in junction depth when the background concentration is lowered. As shown in Eq. [23], and illustrated in Fig. 4 the junction depth is increased $(3D_i t/x_F) \ln 10$ for every order of magnitude decrease in background concentration.

## Acknowledgments

## APPENDIX

There remains to verify, *a posteriori*, that we were justified in neglecting $\partial C/\partial t$ in Eq. [11]. For this purpose we take the derivatives of Eq. [22] $\partial/\partial t$

$$\left( \frac{1}{C} + \frac{2D^-}{D_i} \frac{1}{n_i} \right) \frac{\partial C}{\partial t}$$

$$= \frac{2}{9} \frac{x_F^2}{t^2 D_i} (x - x_F) + \frac{1}{6t} \qquad [A\text{-}1]$$

$$\frac{\partial}{\partial \eta}$$

$$\left( \frac{1}{C} + \frac{2D^-}{D_i} \frac{1}{n_i} \right) \frac{\partial C}{\partial \eta} = -\frac{x_F}{3tD_i} \qquad [A\text{-}2]$$

Our approximation is justified if

$$\left| \frac{\partial C}{\partial t} \right| << \left| \frac{\partial C}{\partial \eta} \frac{\partial n}{\partial t} \right| \qquad [A\text{-}3]$$

*i.e.*

$$\left| \frac{\dfrac{\partial C}{\partial t}}{\dfrac{\partial C}{\partial \eta} \dfrac{\partial \eta}{dt}} \right| = \left| \frac{\dfrac{2}{9} \dfrac{x_F^2}{t^2 D_i} (x - x_F) + \dfrac{1}{6t}}{x_F^2/(9t^2 D_i)} \right| << 1$$

$$[A\text{-}4]$$

A sufficient condition is

$$\frac{2}{9} \frac{x_F}{t^2} (x - x_F) << \frac{x_F^2}{9t^2 D_i} \qquad [A\text{-}5]$$

together with

$$\frac{1}{6t} << \frac{x_F^2}{9t^2 D_i} \qquad [A\text{-}6]$$

Equation [A-5] is satisfied if $|x - x_F| << x_F/2$ for the tail region. In particular this means that both the matching point and the junction should be close to the diffusion front, *i.e.*, $x_F - x << x_F/2$ and $x_J - x_F << x_F/2$ which is true as long as

$$C_S >> \frac{D_i}{D^-} n_i \qquad [A\text{-}7]$$

and

$$\ln (n_i/C_J) << \frac{2D^-}{D_i} \frac{C_S}{n_i} \qquad [A\text{-}8]$$

Equation [A-6] leads to a similar condition which is more relaxed than [A-7].

Our approximate solution should thus be a good one as long as $C_S >> (D_i/D^-)n_i$, *i.e.*, as long as the major part of the diffusion profile is governed by nonlinear diffusion effects and the matching point is close to the diffusion front.

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