Model Calculation for Ion Implantation

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Abstract

In this paper, the diffusion of gas atoms that injected by ion implantation into a layer of certain thickness is studied and investigated by using the equation for the local gas atom concentration. The ion implantation in to multilayer membrane will be investigated and parameterized, with various situations will be discussed.

Notablly, we assume that the implanted ion flux up on the surface dose not sputter the target atomes or in other words the coefficient of sputtering is small which means that the incident ions are light.

الخلاصة

في هذا البحث تمت دراسة عملية انتشار غاز ذري تم حقنه بالزرع الايوني في طبقة ما بسمك معين اذ تم فحصها باستخدام معادلة التركيز الموقعي لذرات الغاز. فحصت عملية زرع الايونات في غشاء متعدد الطبقات وتمت مغايرتها ونوقشت لحالات مختلفة. لقد افترضنا ان الفيض الايوني المزوع على السطح لا يحدث عملية سبترة لذرات الهدف او بكلمات اخرى ان معامل السبترة يكون صغير والذي يعني ان الايونات الساقطة خفية.

Introduction

In the last few years there have been rapid advances in the technology and understanding of electronic devices prepared by ion implantation (G.Carter & W.A. Grant, 1976), which can be defined as the doping of a substrate by a flux of energetic ions. Ions, that accelerated to high energy, enter the substrate (target) with high energy (velocity) and lose energy through collisions with target nuclei and target electrons.

So ion implantation was developed as a means of doping the semiconductor elements of integrated circuits (J.F.Ziegler, 1988). And because of the apeep, accuracy, cleanliness and controllability of the process, it has become the standard for this type of work.

Ion implantation offers the advantages (comparing with thermal diffusion(G.Carter, D.G. Armour & U.Z. Funuli, 1995)) of permitting the doping of semiconductor with a large variety of elements and to concentrations exceeding the solubility limit. The depth and distribution of dopant atoms can be flexibly controlled by adjusting the bombarding energy, incident beam direction and temperature.

The chief disadvantage associated with the technique is the radiation damage (G.Hobler, 1995) accompanying the implantation. This damage can be easily produce a high enough concentration of electrically active defects to completely mask the effects due to the implanted ions. Thus some annealing treatment (J. Tzeng Lue, 1982)is almost invariably required in order to reduce the defect concentration to an acceptable level.

On the theoretical side, many physically based simulation techniques for ion implantation have been used and investigated (K. Wimmer, 1994), These techniques will be summarized by:-

1-Monte-Carlo Simulation (MCS)

In this technique (M.T. Robinson O.S. Oen, 1963), the ion is assumed to change direction with each elastic binary nuclear collision and to move in a free path between collesion . Between these elastic collisions, the ion is slowed down continuously by the electrons of the lattice atoms. When the ion's energy drops below some threshold E_{min} (10 eV), it stops and the end point of the trajectory (x,y,z) is included in the doping profile. The trajectory of one ion as simulated by the Monte Carlo technique is shown in fig.(1)

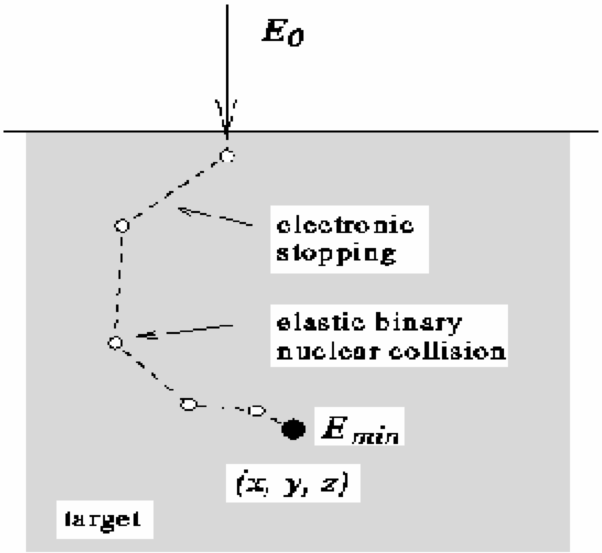


Fig.(1) shows the trajectory of one ion as simulated by the Monte-Carlo technique

2-Boltzmann Transport Equation Method (BTE)

The Boltzmann transport equation describes the scattering processes of the ions in the target by changes in the statistical momentum's distribution f(p,x).The momentum p can be substituted by energy E and θ the angle between the direction of the ion motion and the x-axis $(\theta \leq \text{Л}/2)$.

At each step in this method (L.A. Christel, J.F. Gibbons, S. Mylroie, 1980), the redistribution of the particles in the momentum space at depth x in a depth element dx can be obtained from the following equation:-

$$\frac{\partial f(\vec{p},x)}{\partial x} = N \int_{0}^{E_o} \left(\frac{f(\vec{p}\,',x) \bullet d\sigma}{\cos\theta'} - \frac{f(\vec{p},x) \bullet d\sigma}{\cos\theta} \right) \tag{1}$$

dσ represents the probability of a collision.

The two terms between brakets represent the scattering from state p into a final state p and the scattering out of p′ in to p respectively. N is target atoms per unit volume. E_o is the ion's energy in the initial state.

3-Lindhard-Scharff-Schiott (LSS) Theory

Lindhard,Scharff and Schiott (J. Lindhard, M. Scharff, H.E. & eth., 1963) calculated the moments of the implantation profile by the following integro-differential equation using spherical coordinates:-

$$\frac{dp}{d\vec{r}} = N \int_{0}^{E_{\max}} [p(r, E - E_{\ell}, \theta) - p(e, E, \theta)] d\sigma(E_{\ell}) \qquad (2)$$

They defined p(r,E,θ) as the probability that an ion with energy E will come to rest at a distance r and angle θ. And if the ion moves a small (vector) distance dr then the differential scattering cross section $d\sigma(E_\ell)$ describes the probability that a collision will occur resulting in an energy loss E_ℓ. E_{max} represents the maximum possible energy transfer in a collision.

Note that, eq.(2) represents recurrence relations for the moments of p in terms of Legendre polynomials, These calculations are available in form of tables for various ion/target combinations in ref.(J.F. Gibbons, W.S. Johnson, & eth., 1975).

4- Molecular Dynamics Simulation (MDS)

One of the best ways to study damage formation (during ion implantation) theoretically is the molecular dynamics simulations (K. Nordlund, J. Keinonen, & eth.1994) in which the time evolution of a system of atoms is calculated by solving the equations of motion numerically. Since the movement of each atom involved in a collisions cascade can be followed in MDS. It is the most realistic way of examining defect formation during ion implantation.

The MDS process starts by calculating the force F_i acting on each atom i in the system.The epuations of motion for the system are:-

$$\overline{F}_i(\vec{r}_i) = \sum_{j \neq i} \overline{F}_{ij}(r_{ij}) = -\sum_{j \neq i} \nabla V_{ij}(r_{ij}) \qquad (3)$$

where F_{ij} is the force acting between atom i and j, r_{ij} is the distance between atoms and $V_{ij}(r_{ij})$ is the potential energy function which is divided into a repulsive part govering high energetic collisions and the potential well that govering equilibrium phenomena.

Thus the repulsive potential can be described by multiplying the Coulombic repulsion between nuclei with a screening function Φ(r) (J.F.Ziegler, J.P. Biersak, & eth, 1985),

$$V(r) = \frac{1}{4\Pi\varepsilon_o} \frac{Z_1 Z_2}{r} \Phi(r) \qquad (4)$$

where Φ(r)→1 when r → 0. Here z_1 and z_2 are the charges of the interacting nuclei and r the distance between them.

In the present work, the diffusion of gas atoms that injected by ion implantation in to a layer (of certain thickness) will be studied and investigated by using the equation for the local gas atom concentration Z. A. Iskanderova, T. D. Radjabov,& eth,1985). The ion implantation in to multilayer membrane also will be investigated and various situations will be analysed and discussed.

Theory

In the time-independent (stationary) regime, the diffusion of gas atoms that injected by ion implantation into the membrane (of thickness ℓ) can be described by the equation for the local gas atom concentration C (z) at a depth z,

$$D\frac{d^2C(z)}{dz^2}+\frac{1}{r}qe^{-z/r}=0 \tag{5}$$

with boundary condition,

$$\begin{aligned} C(z=0)&=0 \\ C(z=\ell)&=0 \end{aligned} \tag{6}$$

The second term in eq.(1) represents the ion range destribution function with q is the current density, r is the mean ion range (T. T. Fang, W. T. C. Fang, & eth, 1996) and D is diffusion coefficient of the injected impurity.

Extentions to multilayer structures mostly give acceptable results (H. Ryssel, W. Krüger, J. Lorenz, 1987) But it still suffer from lacking underlying physic since each layer usually has adifferent stopping power for the implanted ions, so the first layer has a strong influence on the (velocity, energy, …) distribution of the ions at the interface to the underneath layer. As an approach to model the implanted ions concentrations in multilayer structures, we will for simplicity assume a two-layer target composed of thin film (layer 1) and a substrate (layer 2), see fig.2. Accordingly, the time independent regime for the two-layer membrane can be considered by a system of equations:-

$$D_1\frac{d^2C_1}{dz^2}+\frac{q_1}{r_1}e^{-z/r_1}=0 \tag{7}$$

$$D_2\frac{d^2C_2}{dz^2}+\frac{q_2}{r_2}e^{-z/r_2}=0 \tag{8}$$

with,

a-The assumption of partial trapping of the implanted ions in the first layer (in to the film with thickness ℓ_1) and penetration in to the second layer in to the substrate with thickness ℓ_2 (see fig.2).

The diffusion coefficients for implanted impurites in the first and second layers are D_1 and D_2 respectively.

b-The following boundary conditions:

1- $C_1(z=0)=0$

2- $C_2(z=\ell_1+\ell_2)=0$

3- $$D_1 \left.\frac{dC_1}{dz}\right|_{z=\ell_1} = D_2 \left.\frac{dC_2}{dz}\right|_{z=\ell_1} \tag{9}$$

4- $$C_1(z=\ell_1) = kC_2(z=\ell_1)$$

here k is the segregation coefficient at the interference between the two layers.

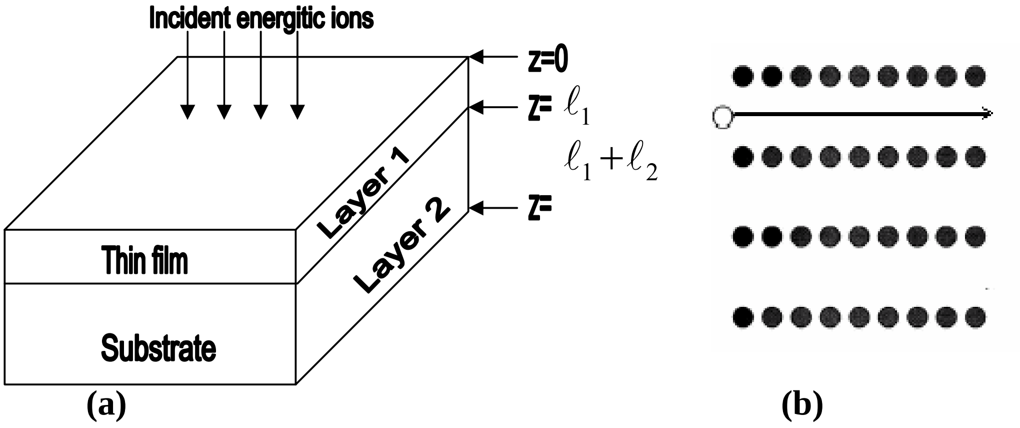


Fig.(2) **a.** shows two-layer target composed of a film and substrate
b. the target atoe implanted ion flux up on the surface does not sputter ms.Filled circles represent the target atoms while empty one represents the implanted ion.

The solution of eq.(7) and (8) are,

$$C_1(z) = \frac{-q_1 r_1}{D_1} e^{-z/r_1} + \frac{a_1 z}{D_1} + \frac{b_1}{D_1} \tag{10}$$

$$C_2(z) = \frac{-q_2 r_2}{D_2} e^{-z/r_2} + \frac{a_2 z}{D_2} + \frac{b_2}{D_2} \tag{11}$$

Equations (10) and (11) can be solved analytically for certain values of the gas atoms concentration in the first and second layers, as a function of depth z, diffusion coefficients D_i , the thickness ℓ_i , the mean ion range r_i , the segregation coefficient as well as the current density q_i .

The constants a_i and b_i (i =1,2) can be evaluated by getting use of eq.(9),

$$b_1 = q_1 r_1 \tag{12}$$

$$b_2 = q_2 r_2 e^{-(\ell_1+\ell_2)/r_2} - a_2(\ell_1+\ell_2) \tag{13}$$

$$a_2 = a_1 + q_1 e^{-\ell_1/r_1} - q_2 e^{-\ell_1/\ell_2} \tag{14}$$

and

$$\frac{-q_1 r_1}{D_1} e^{-\ell_1/r_1} + \frac{a_1}{D_1}\ell_1 + \frac{b_1}{D_1} = k[\frac{-q_2 r_2}{D_2} e^{-\ell_1/r_2} + \frac{a_2}{D_2}\ell_1 + \frac{b_2}{D_2}] \tag{15}$$

The above system of equations can be solved analytically for certain values of D_i, ℓ_i, r_i, q_i, and k.

The process of impurity implantation and diffusion in a three-layer system, where relative quantity of impurity is injected in to the third layer after passing through the first and the second layers, can be studied through out the following system of equations:

$$D_i \frac{d^2 C_i}{dz^2} + \frac{q_i}{r_i} e^{-z/r_i} = 0 \qquad (i=1\rightarrow 3) \tag{16}$$

with the boundary conditions,

$$\begin{aligned}
&C_1(z=0)=0\\
&C_3(z=\ell_1+\ell_2+\ell_3)=0\\
&C_1(z=\ell_1)=k_1 C_2(z=\ell_1)\\
&C_2(z=\ell_1+\ell_2)=k_2 C_3(z=\ell_1+\ell_2)\\
&D_1 \left.\frac{dC_1}{dz}\right|_{z=\ell_1} = D_2 \left.\frac{dC_2}{dz}\right|_{z=\ell_1}\\
&D_2 \left.\frac{dC_2}{dz}\right|_{z=\ell_1+\ell_2} = D_3 \left.\frac{dC_3}{dz}\right|_{z=\ell_1+\ell_2}
\end{aligned} \tag{17}$$

The solutions of eq.(16) are,

$$C_i = \frac{-q_i r_i}{D_i} e^{-z/r_i} + \frac{a_i z}{D_i} + \frac{b_i}{D_i} \qquad (i=1\rightarrow 3) \tag{18}$$

With ℓ_3 , D_3 and C_3 are the thickness, the diffusion coefficient and the impurity concentration of the third layer respectively. While k_1 and k_2 are segregation coefficients of the first and the second interferences. Similarly, we get use of eqs. (17)

to get a system of linear equations for a_i and b_i ($i=1\rightarrow3$) which we solve analytically. Notably, we assume that the implanted ion flux up on the surface does not sputter the target atomes or in other words the coefficient of sputtering is small which means that the incident ions are light. The coefficient of sputtering can be very significant in certain metals at high dose values and especially when the ion beam is incident at a small angle to the surface.

Results and Conclusions

In this section many situations will be parametrised. In fig.(3), the concentration is shown as a function of z for the case were $r_2 > r_1$, $d_1 < d_2$ while $q_2 = q_1/4$ For different values of k.

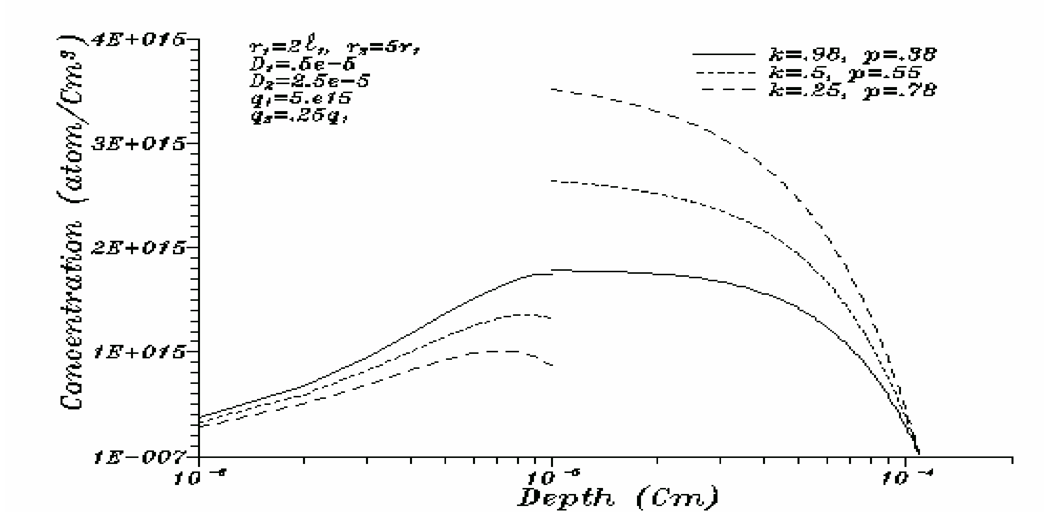


Fig.(3) shows the concentration of implanted ions as a function of depth with $r_2 > r_1$, $d_1 < d_2$ and $q_2=q_1/4$ for different values of k.

The concentration in the second layer is higher than that in the first one nearly for all k. This may be explained by the fact that for low coefficient of ion implanted impurity diffusion in the first layer, its diffusive movement in the reverse direction is retarded.

The efficiency is also calculated for each condition since additional increase of efficiency is possible under the condition k=0.25 i.e. the gas solubility in the first layer (film) must be lower than in the second layer (substrate). More interesting

possibility is presented in fig.(4) where $r_2=r_1$, $D_1<D_2$, and $q_2 = q_1$

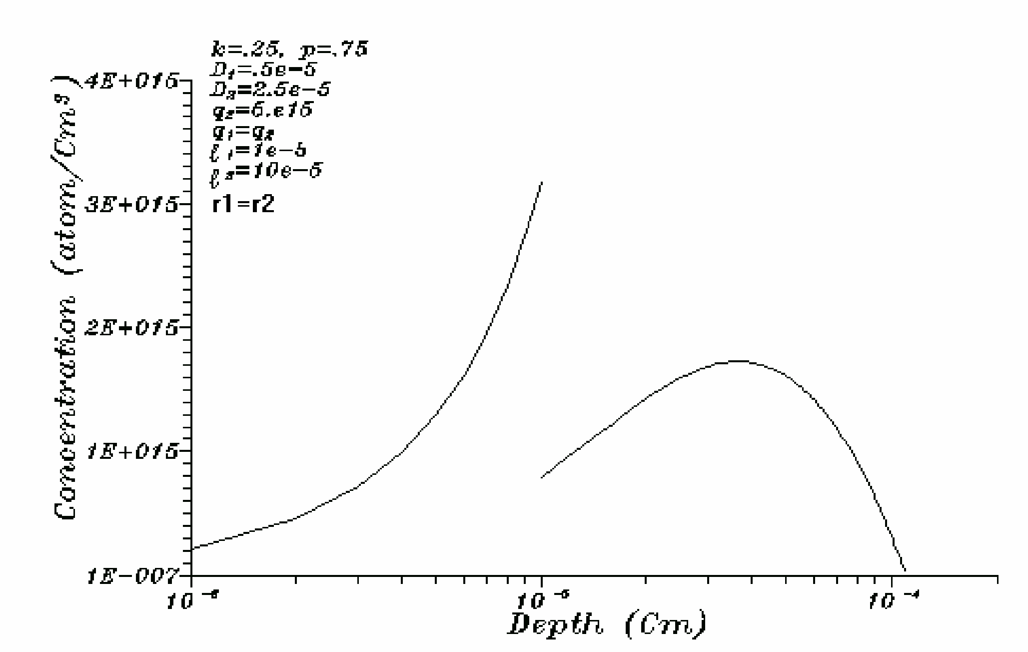
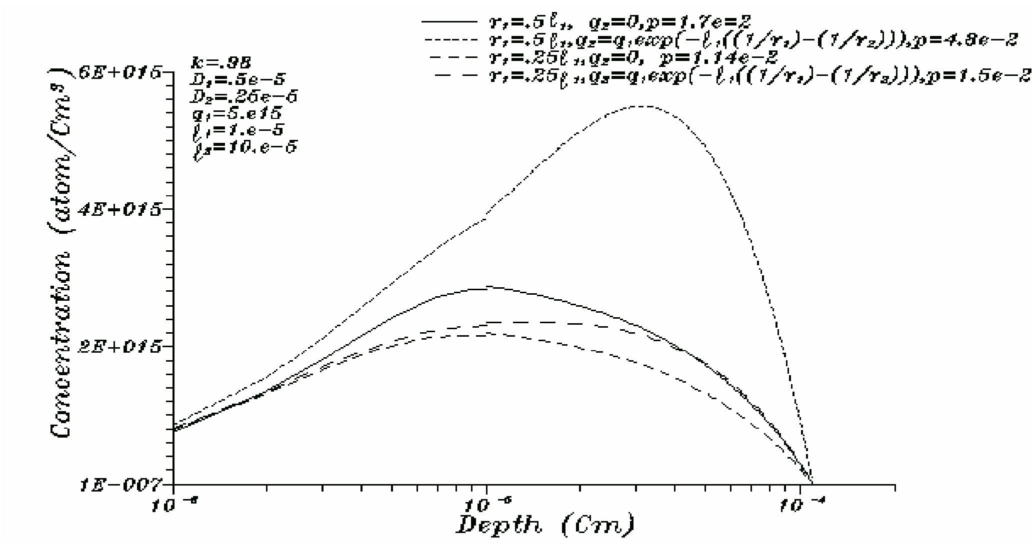


Fig.(4) shows the concentration of implanted ions as a function of depth with $r_2 = r_1$, $d_1 < d_2$ and $q_2 = q_1$ with k=0.25.

In fig.(5), two conditions are represented for different values of r_1 and $k \approx 1$, $d_1 > d_2$.

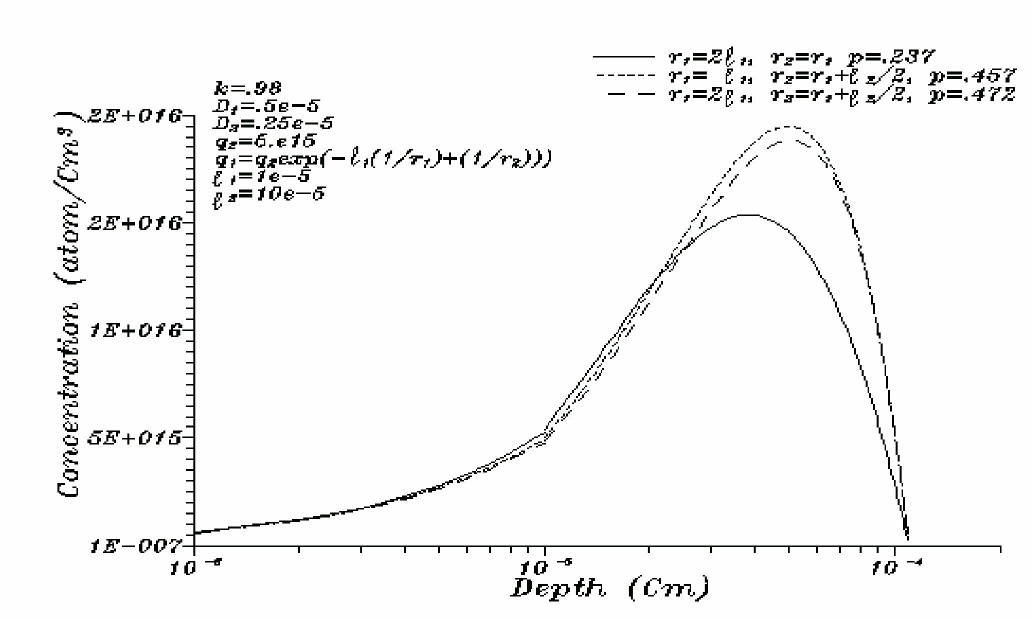
In the first one $q_2 = 0$ which means that the ion implanted is stopped in the second layer, in other words with the assumption of complete trapping of the implanted ions in the first layer. In the second one, q_1 and q_2 are related by,

$$q_2 = q_1 \exp[-\ell_1\{(1/r_1) - (1/r_2)\}] \tag{19}$$



Fig(5) Shows the concentration of implanted ions as a function of depth with $r_1 < \ell_1$, $D_1 > D_2$, k=.98 for two different relations between q_1,and q_2.

The calculated efficiency are all very small if we compare them with that calculated in fig.(6), in which $d_1 > d_2$ and $k \approx 1$ also but $r_1 > \ell_1$ and $r_2 \geq r_1$.



Fig(6) Shows the concentration of implanted ions as a function of depth with $r_1 > \ell_1$, $r_2 \geq r_1$, $D_1 > D_2$, k=.98 for certain relation between q_1,and q_2.

Finally, from these figures one can conclude that an increase of efficiency is revealed in two conditions,

1- $d_1 > d_2$, $k \approx 1$, $r_2 > r_1$

2- $d_2 > d_1$, $k = .25$, $r_2 > r_1$

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