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Arsenic Diffusivity Study by Comparison of Post-Surface and Post-Implant Diffusion in Silicon with Local Density Diffusion (LDD-) Model Approximation

Frank Wirbeleit
GLOBALFOUNDRIES, D-01109 Dresden, Germany
Email: Frank.Wirbeleit@globalfoundries.com

Abstract

The LDD model was first applied to Arsenic concentration profiles determined in surface diffusion experiments by Yoshida and Arai [1]. The new method presented is based on a mathematical convolution with a delta-function-like concentration profile. By comparing the LDD approximation of post-surface diffusion with post-implant diffusion experiments, the same LDD model parameter r is found to hold for both experimental arrangements. This work found that post-implant diffusivity is concentration dependant and this might indicate an anomalous diffusion mechanism for Arsenic.

Keywords: Arsenic, Silicon, implant, diffusion, non-Gaussian diffusion model

Introduction

Arsenic is a key donor impurity for ultra shallow junction engineering in today's microelectronic technology. For high performance FET devices in the sub 100nm range it is critical to balance thermal dopant activation with the diffusion distance. The diffusion behavior of Arsenic was studied by surface diffusion experiments and described in terms of the dual pair diffusion model by Yoshida and Arai [1]. Arsenic implant and diffusion in Silicon is investigated by numerous teams and also part of the investigation in Ref. [2] for example. In many cases in the literature, numerical simulations are applied to model Arsenic diffusion by *ab initio* or kinetic Monte Carlo simulations [3]. With the LDD model the understanding of diffusion diverges by introducing both forward (towards the penetration direction) and backward (or reflected) diffusion current density. Since the LDD model was created and applied to Arsenic surface diffusion experimental results first time in Ref. [4], the model has been improved with focus on impurity post-implant and post-epitaxial diffusion profiles and clustering effects of Boron [5]. Based on the mathematical convolution approach [6] the same diffusivity function holds under different experimental conditions. This work details LDD approximation results, obtained by SIMS profile approximations either post Arsenic implant or post-surface diffusion by the same convolution approach [6]. Surface diffusion is modeled by convoluting the LDD diffusivity function with a delta-function-like surface profile, as explained in the following section.

A. Convolution with delta function like surface profile

To describe Arsenic impurity diffusion post-surface and post-implant diffusion, both the initial impurity profile $c_0(x)$ and the diffusivity model $D(x)$ have to be considered. In this approach, the final concentration profile $c(x)$ is obtained by the mathematical convolution given in Equ. 1 ([6]).

$$c(x) = [c_0 * D](x) = \int_{-\infty}^{\infty} c_0(r)\, D(x-r)\, dr \qquad (1)$$

In the case of impurity diffusion from a vapor atmosphere through the sample surface into the volume (positive x direction), the initial concentration slope $c_0(x)$ prior to diffusion is assumed to be a single surface concentration constant value c_0:

$$c_0(x) = \begin{cases} c_0 & x = 0 \\ 0 & else \end{cases} \qquad (2)$$

Based on this assumption (see Equ. 2), the convolution integral of the initial concentration slope $c_0(x)$ and diffusivity model $D(x)$ as given in Equ. 1 is solved by partial integration in Equ. 3:

$$\int_{-\infty}^{\infty} c_0(r)\, D(x-r)\, dr = \int_{-\infty}^{\infty} c_0(r)\, D'(x-r) dr - \underbrace{\int_{-\infty}^{\infty} c_0{}'(r)\, D(x-r) dr}_{=0} \qquad (3)$$

Considering Equ. 2, the integral in Equ. 3 simplifies further in Equ. 4 (ξ is an infinitesimal small environment around zero):

$$
\begin{aligned}
\int_{-\infty}^{\infty} c_0(r)\,D'(x-r)\,dr &= \underbrace{\int_{-\infty}^{-\xi} c_0(r)\,D'(x-r)\,dr}_{=0} + \int_{-\xi}^{+\xi} c_0(r)\,D'(x-r)\,dr \\
&\quad + \underbrace{\int_{+\xi}^{\infty} c_0(r)\,D'(x-r)\,dr}_{=0} \\
&= c_0 \int_{-\xi}^{+\xi} D'(x-r)\,dr = c_0\left[D(x-r)\right]_{-\xi}^{+\xi} \\
&\quad \textit{with } \xi \to +0 \qquad D(x-\xi) = D(x) \\
&\quad \textit{and } \xi \to -0 \qquad D(x+\xi) = 0 \\
&= \underline{\underline{c_0 D(x)}}
\end{aligned}
\tag{4}
$$

Because the diffusivity model *D(x)* is always defined independently from the absolute concentration level as given in Equ. 5, the scaling factor c_0 in Equ. 4 represents the integral value of the post diffusion impurity slope, as shown in Equ. 6.

$$
\int_{-\infty}^{+\infty} D(x)\,dx = 1 \tag{5}
$$

$$
\int_{-\infty}^{\infty} c(x)\,dx = c_0 \int_{-\infty}^{\infty} D(x)\,dx \;\rightarrow\; \underline{\underline{c_0 = \int_{-\infty}^{\infty} c(x)\,dx}} \tag{6}
$$

Equ. 6 proves that c_0 is equal to the integral of the LDD approximation post-surface diffusion. Fig. 1 illustrates Equ. 6 schematically, by convoluting a diffusivity function *D(x)* with delta-function-like surface concentration profile $c_0(x)$. If we set parameter $c_0=1$ (see Fig. 1a) or to a value according to Equ. 6 (see Fig. 1b) it can be seen in Fig. 1, that the convolution result *c(x)* in Fig. 1b is perfect aligned with *D(x)*. This is expected from calculus mathematics point of view also.

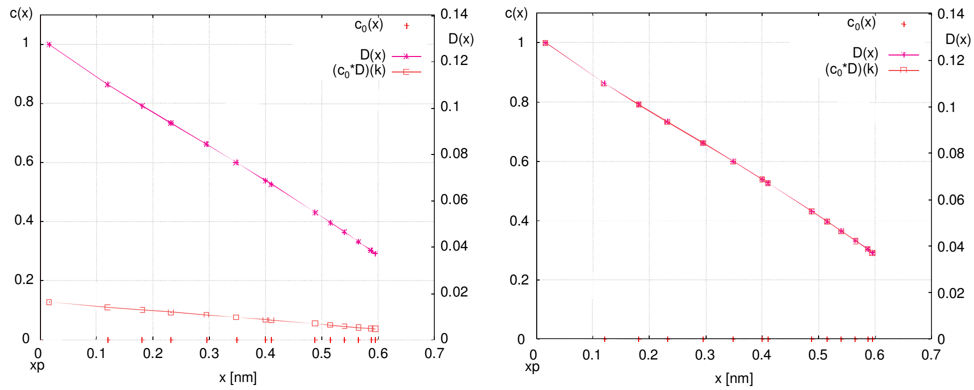

Figure 1: Mathematical convolution result of delta function like $c_0(x)$ profile according to Equ. 2 with diffusivity function $D(x)$ (Equ. 6) of LDD model for a) $c_0=1$ and b) c_0 =5.45 according to Equ. 6 ($D(0)$ =0.1835, see Equ. 4).

B. LDD model

As introduced earlier [5], the Local Density Diffusion (LDD-) model, given in Equ. 7 for delta-function-like profile $c_0(x)=c_0$ (e.g. $c_0*D(x) \Rightarrow c_0\times D(x)$), is based on Equ. 8 in a one dimensional frame. Equ. 7 consist of a quadratic term for forward and a logarithmic term for backward diffusivity, as well as the zero diffusion term ZD. Zero diffusion (ZD) is used for Boron diffusion in Silicon and Silicon-Germanium alloys [5], but is not seen for Arsenic diffusion in Silicon so far and is therefore not considered in this work.

$$c_0 \times D(x) = c_0\left[2-\frac{1}{4}\left(\frac{x}{x_i}+r\right)^2-\frac{1}{2}\log\left(\frac{x}{x_i}+r\right)\right]+ZD(\ldots) \qquad (7)$$

$$\Delta c+\frac{1}{x}\nabla c+c_0=0 \qquad (8)$$

Equ. 8 originates from Fick's 2[nd] law given in Equ. 9 by replacing the total diffusion current density j from Equ 10. Equ. 8 is further extended by adding the concentration constant c_0 in agreement with former work (see Ref. [5]):

$$k\Delta c-\dot{c}=0 \qquad (9)$$

$$j=\frac{1}{A}\dot{n}=\frac{1}{A}V\ \dot{c}=x\ \dot{c} \qquad (10)$$

Considering Fick's 1[st] law in Equ. 11, Equ. 8 is derived under the assumption of a constant volume over time.

$$j=-k\nabla c \qquad (11)$$