ION IMPLANT PROFILE CALCULATIONS

An initial ion implant follows the Gaussian or normal distribution, with a distribution center and scattering parameter being given in the literature for a stated energy of implant. Subsequent heat treatments will cause an alteration of the profile so as to broaden the distribution and to reduce the peak concentration. If the ion implant were deep enough in silicon so that the total distribution were well within the silicon material (as shown in Figure 1), the subsequent behavior with heat treatments for each half of the distribution would correspond exactly to a pre-deposition followed by a drive-in diffusion. This is due to the fact that no charge can cross the plane through the center of the distribution. Instead, the charge moves away from the center plane in each direction, thereby corresponding exactly to the situation of a pre-dep into the silicon, which subsequently cannot out-gas from the silicon (because an oxide is formed immediately at the silicon surface) and must therefore diffuse deeper into the silicon. The design task therefore is to use the data for the ion implant initial profile in such a manner that the drive-in diffusion calculations can be performed and a new profile calculated.

Even if a shallower implant is used, as shown in Figure 2, the drive-in diffusion calculation is useful as some measure of the spreading that subsequent heat treatments can impose on the initial profile. Clearly, the center of the distribution must move somewhat deeper into the silicon (representing a deviation from the drive-in model), since that portion of the implant moving toward the surface encounters an obstacle that prevents the spreading which is available to that portion of the implant moving toward the interior of the silicon. In fact, the profile behavior starting from Figure 2 is qualitatively shown in Figure 3. For some duration of heat treatment, the surface concentration increases while the peak distribution is decreasing, although ultimately even the surface concentration can decrease below the initial value. However, for some intermediate time period the "drive-in diffusion" experiences a source of additional charge near the surface in a manner analogous to a pre-deposition action so that the ultimate profile is, in some uncalculable fashion, a compromise between a Gaussian distribution and a complementary error function distribution.

Next, the drive-in diffusion of a sheet charge Q behaves according to*

$$C(x,t) = \frac{Q}{\sqrt{\pi Dt}} e^{-\frac{x^2}{4 Dt}}$$

This can be put into a form analogous to the normal distribution by making use of the substitution

$$y^2 = \frac{x^2}{2 Dt}$$

so that

$$C(y,t) = \frac{Q}{\sqrt{\pi Dt}} e^{-y^2/2}$$

For the normal distribution, the standard deviation and half-value occur at $y = 1$ and $y = \boxed{1.177}$, respectively. (Note that the $y = 0$ value for the normal distribution is 0.3989, so that the half-value, for example, is taken <u>relative</u> to the zero value.) $\left\} \frac{1}{\sqrt{2\pi}} = .3989 \right.$ Thus, for the drive-in diffusion model, the equivalent initial value $(Dt)_0$ is found from

$$\frac{\sigma^2}{2(Dt)_0} = 1$$

---

*Andrew S. Grove, <u>Physics and Technology of Semiconductor Devices</u>, 2nd ed., 1967, p. 50, equation 3.21.

or

$$\frac{(x_{1/2})^2}{2(Dt)_0} = (1.177)^2$$

so that, either

$$(Dt)_0 = \frac{\sigma^2}{2}$$

or

$$(Dt)_0 = \frac{(x_{1/2})^2}{2.77}$$

To this initial value $(Dt)_0$ must be added the Dt product of all subsequent high-temperature processing steps to arrive at a total $(Dt)_1$. Then, since any point on the initial normal distribution increases proportional to the square-root of the Dt product, we can calculate the new standard deviation or the new half-value or any other value x by using

$$\frac{\sigma_1}{\sigma_0} = \frac{(x_{1/2})_1}{(x_{1/2})_0} = \frac{x_1}{x_0} = \frac{\sqrt{(Dt)_1}}{\sqrt{(Dt)_0}}$$

Correspondingly, the peak concentration has decreased inversely proportional to the square-root of the Dt product so that

$$\frac{(C_{peak})_1}{(C_{peak})_0} = \frac{\sqrt{(Dt)_0}}{\sqrt{(Dt)_1}}$$

where the initial peak value $(C_{peak})_0$ was calculated from the total charge and a given standard deviation or a given half-value range according to (see Appendix 1):

$$(C_{peak})_0 = 0.3989 \frac{Q}{\sigma}$$

$$\left[(C_{peak})_0 = .7978 \frac{Q}{\sigma} \right]$$

and

$$(C_{peak})_0 = 0.4695 \frac{Q}{x_{1/2}}$$

~~$\left[(C_{peak})_0 = .9390 \frac{Q}{X_{1/2}}\right]$~~

This sequence of calculations is summarized for easy reference in Appendix 2 under the title, "Ion Implant Spreading Calculations."

Finally, to simplify the computation of the amount of charge that has entered the silicon compared to the total charge measured by the ion implanter, attached hereto is a cumulative probability distribution with one abscissa in units of standard deviation, plus a second abscissa in units of half-value. Depending upon which parameter is known, the percentage of charge in the silicon can be read directly from the curve. That is, if the center of the distribution is one half-value within the silicon, 88% of the measured charge is in the silicon: if the center of the distribution is two half-values within the silicon, 99% of the measured charge is within the silicon.

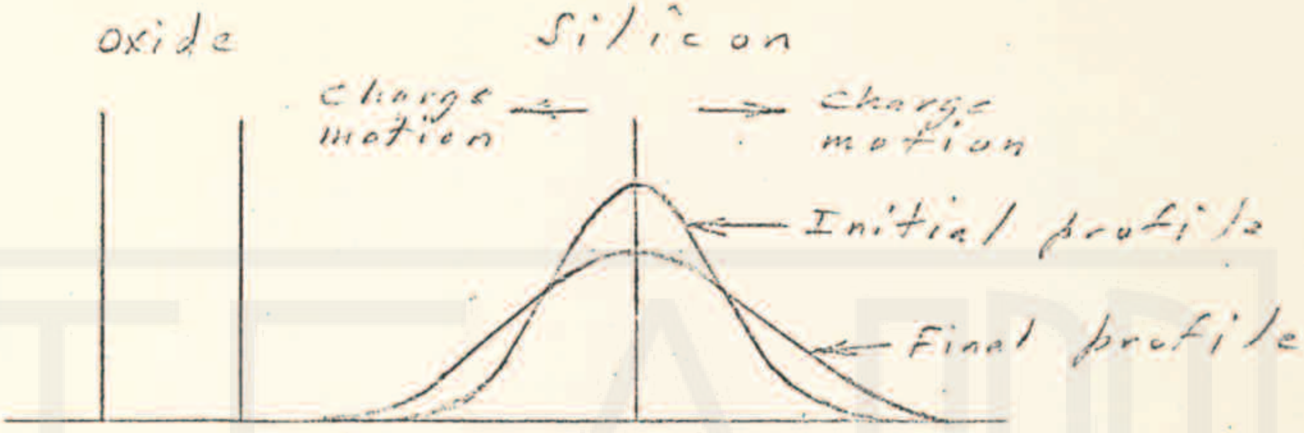


Figure 1

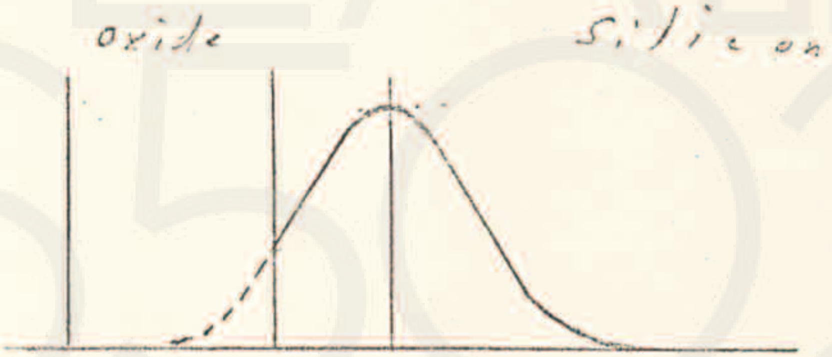


Figure 2

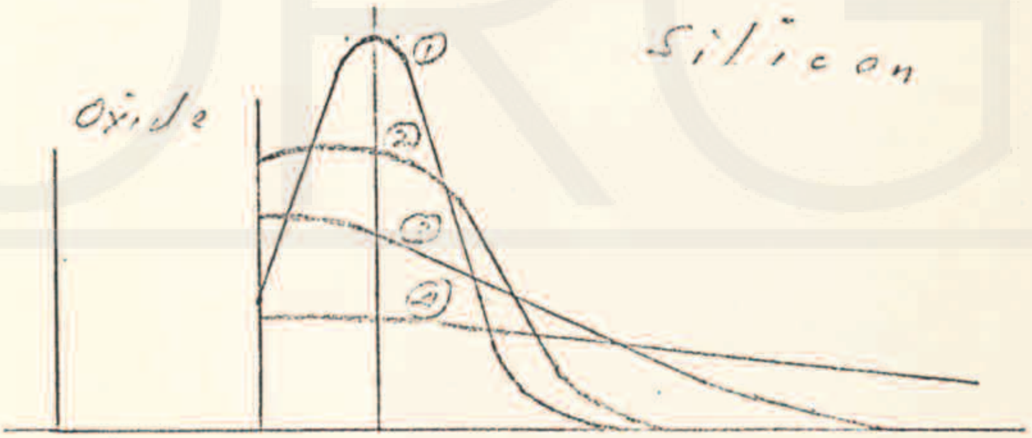
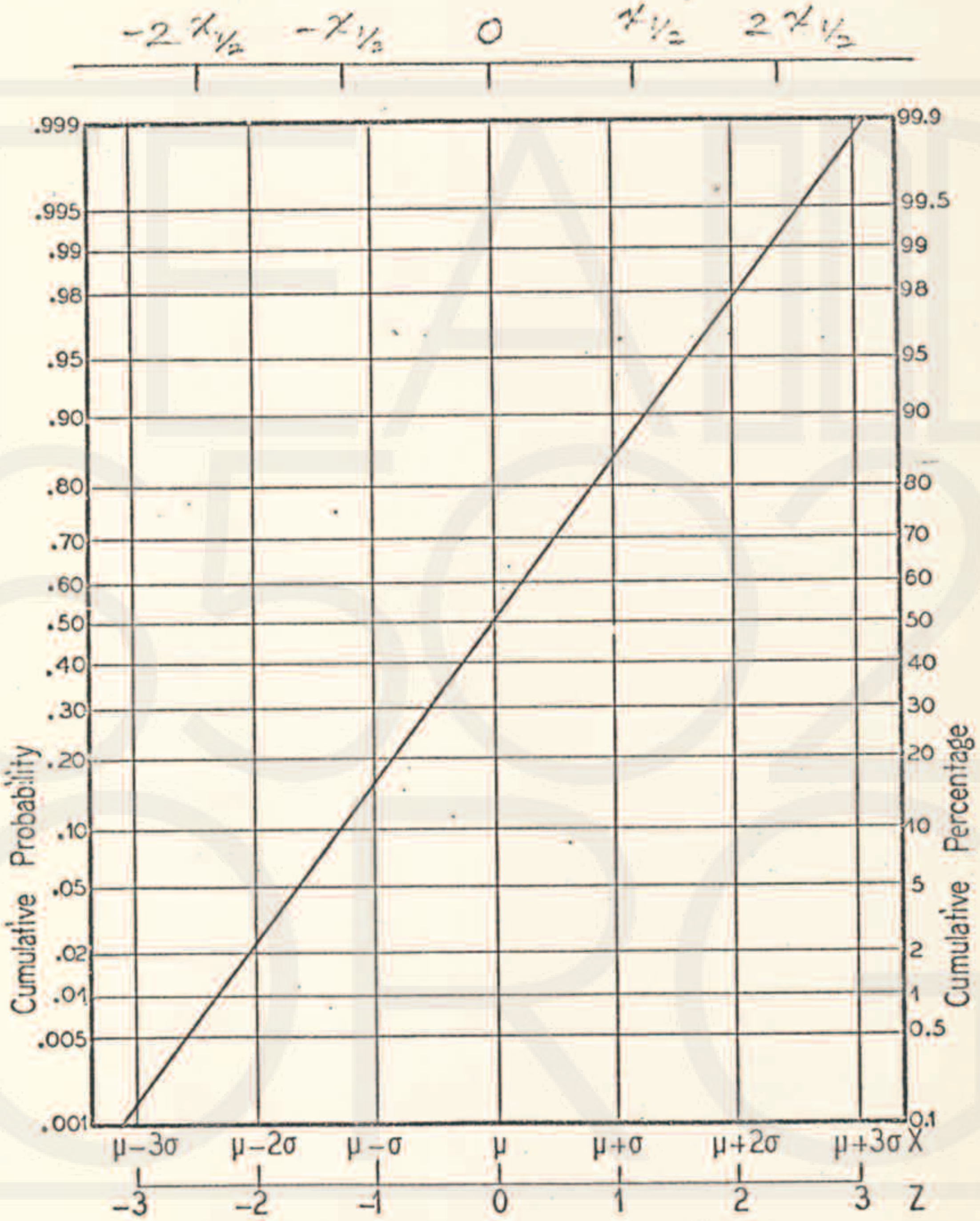


Figure 3



Graph of Cumulative Normal Distribution $F_N(x)$ on Probability Graph Paper

Appendix 1
Ion Implant Peak-Concentration-to-Total-Charge Ratio

The probability density function $f_N(x)$ for a normal distribution having mean μ and standard deviation σ is given by the formula

$$f_N(x) = \frac{1}{\sqrt{2\pi}\,\sigma}\, e^{-\frac{1}{2\sigma^2}(x-\mu)^2}$$

The corresponding cumulative distribution function is given by

$$F_N(x) = \frac{1}{\sqrt{2\pi}\,\sigma} \int_{-\infty}^{x} e^{-\frac{1}{2\sigma^2}(x-\mu)^2}\, dx.$$

(Numerical values for both of these functions are usually tabulated under the assumptions that $\mu = 0$, $\sigma = 1$.)

From the first equation above, the peak value of the normal distribution is found at the center of the distribution, that is, for $x = \mu$. This is given by

$$f_N(\mu) = \frac{1}{\sqrt{2\pi}\,\sigma}.$$

If we substitute this in the second equation, we obtain

$$F_N(x) = f_N(\mu) \int_{-\infty}^{x} e^{-\frac{1}{2\sigma^2}(x-\mu)^2}\, dx.$$

Next, we can obtain from integral tables the relationship that

$$\int_{-\infty}^{+\infty} e^{-\frac{1}{2\sigma^2}(x-\mu)^2}\, dx = \sqrt{2\pi}\,\sigma$$

so that

$$F_N(\infty) = f_N(\mu)\sqrt{2\pi}\,\sigma$$

which relates the integral of a normal distribution function to the peak value found at the center of the distribution. Thus, for an ion implant with a known total charge, Q, with a standard deviation σ the peak concentration is given by

$$C_{peak} = \frac{Q}{\sqrt{2\pi}\,\sigma}$$

$$= 0.3989\,\frac{Q}{\sigma}$$

If we know the range at which the distribution has fallen to one half of the peak, rather than knowing the standard deviation, we can substitute from

$$1.177\sigma = x_{1/2}$$

to obtain

$$C_{peak} = \frac{1.177\ Q}{\sqrt{2\pi}\,x_{1/2}}$$

$$= 0.4696\,\frac{Q}{x_{1/2}}$$

These relationships defining the peak concentration are valid even though some of the ion implant is located in the gate oxide rather than being in the silicon. As a subsequent calculation, the cumulative probability distribution can be used to identify what portion of the total charge actually has been deposited into the silicon itself.

Appendix 2

Ion Implant Spreading Calculations

1) Find the equivalent $(Dt)_0$ for the initial distribution from either

$$(Dt)_0 = \frac{\sigma^2}{2}$$

or

$$(Dt)_0 = \frac{(x_{1/2})^2}{2.77}$$

2) Compute any subsequent process Dt and add to $(Dt)_0$ for total $(Dt)_1$.

3) Calculate the new profile using

$$\frac{\sigma_1}{\sigma_0} = \frac{(x_{1/2})_1}{(x_{1/2})_0} = \frac{x_1}{x_0} = \frac{\sqrt{(Dt)_1}}{\sqrt{(Dt)_0}}$$

and the new peak concentration using

$$\frac{(C_{peak})_1}{(C_{peak})_0} = \frac{\sqrt{(Dt)_0}}{\sqrt{(Dt)_1}}$$

where

$$(C_{peak})_0 = 0.3989 \frac{Q}{\sigma_0}$$

or

$$(C_{peak})_0 = 0.4695 \frac{Q}{(x_{1/2})_0}$$

For reference, in the normal distribution,

$$x_{1/2} = 1.177\,\sigma$$

$$x_{1/10} = 2.146\,\sigma$$

$$x_{1/100} = 3.04\,\sigma$$

so that

$$x_{1/10} = 1.823\ x_{1/2}$$

$$x_{1/100} = 2.583\ x_{1/2}$$