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Monte Carlo Analysis of Transistor Diffusion Techniques

This note concerns an analytical approach to the problem of base-width reproducibility in the construction of double-diffused transistors. Current gain, being dependent upon base width, is frequently distributed over a wide range of magnitudes for devices intended to be identical. Lack of adequate control in the diffusion process is suggested as a contributing factor in this problem. To investigate the influence of diffusion tolerances, Monte Carlo methods of statistical analysis are applied to an elementary equation characterizing the impurity distribution within a transistor.

From large statistical samples, base-width distribution diagrams are presented which illustrate the simultaneous influence of experimental tolerances for five parameters of the diffusion process. The relative contribution of each tolerance to variations in the emitter-collector distance is easily estimated, thereby providing fundamental information for process improvement.

This analytical investigation was conducted on the IBM 7090. With the aid of a number generator having suitable statistical properties (described in the Analysis section), independent variables within the impurity distribution equation were varied throughout a range representing their individual experimental tolerances. The emitter-collector junction distance was then computed for each new set of diffusion parameters and thus – with a sufficient quantity of such computations – statistical information was obtained on the base-width reproducibility for a particular diffusion process. Any number of diffusion parameters can be treated in this manner; five are simultaneously changed in this investigation to study the overall properties of a given process. If, on the other hand, a single parameter is modified by the number generator – while all others are held at their mean value – we obtain specific information applicable to process improvement.

Analysis

The distribution of donor and acceptor atoms in this type of transistor is assumed to be fully characterized by elementary diffusion theory. Impurity atoms enter the homogeneous semiconductor material under the influence of thermal excitation alone; this situation is represented by Fick's first law,

$$J = -D \operatorname{grad} [c] . \tag{1}$$

The proportionality constant D, having the dimensions of l^2t^{-1}, establishes the impurity atom flux density resulting from a unit concentration gradient. This parameter, which is the diffusion constant, is temperature dependent[1] and must, therefore, be considered in any statistical investigation of diffusion,

$$D = D_0 \exp(-\Delta H/RT) . \tag{2}$$

The flux distribution characterized by Eq. (1), being divergence free, results in a continuity equation of the form

$$\frac{\partial c}{\partial t} = D \operatorname{div}[\operatorname{grad} c] , \tag{3}$$

which is frequently called Fick's Second Law. Eq. (3) is assumed to fully characterize the distribution of impurity atoms within the diffused transistor and is, therefore, used throughout this analytical investigation.

Previous authors[2,3,4] have established solutions of the impurity atom continuity equation for a wide selection of physical situations. For this case we are interested in a one-dimensional solution of Eq. (3) for a semi-infinite solid which satisfies the boundary and initial conditions

$$c(x;t) = \begin{cases} 0 & 0 < x < \infty ;\ t = 0 \\ c_0 & x = 0 ;\ 0 < t < \infty . \end{cases} \tag{4}$$

It has been shown[2] that the required impurity distribution equation satisfying the condition of continuity, Eq. (3), and the above boundary equation are given by

$$c(x;t) = c_0 \operatorname{erfc}(x/2\sqrt{Dt}) . \tag{5}$$

In the construction of transistors by diffusion methods, a semiconductor material of specified impurity

Table 1

	D_0*	D_0	ΔH*	ΔH
Arsenic	0.71-12.7	0.71	51-53	51
Indium	0.45-20	1.552	62-69	62

*Published values.

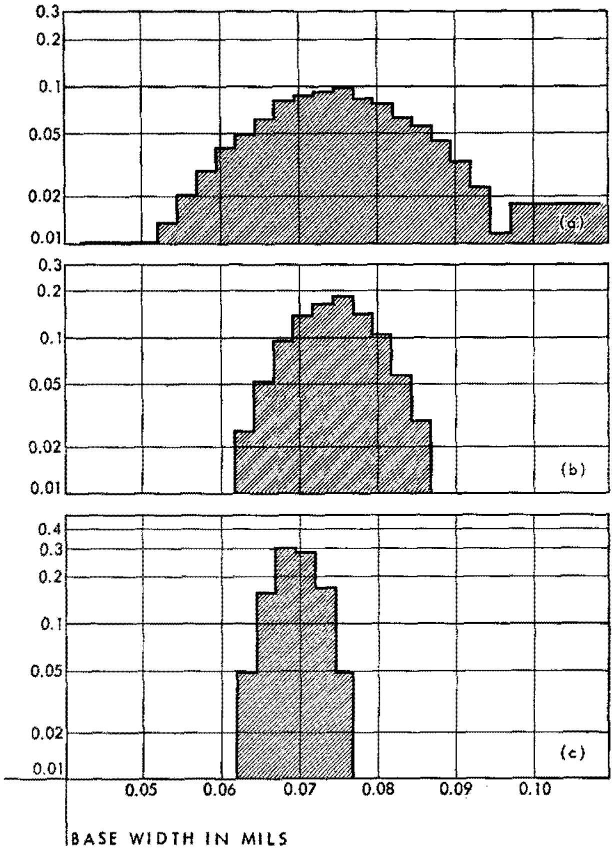


Figure 1 **Base-width distribution for three degrees of control upon diffusion process.**

concentration, C_b, is subject to two independent diffusion cycles. The first diffusion cycle forms the collector junction by introducing sufficient impurity atoms to overcompensate bulk properties of the semiconductor material. The second diffusion forms an emitter junction by overcompensating the impurity atoms of the first diffusion; this emitter junction formation is assumed to be accomplished by experimental techniques which leave the two diffusions independent of each other. From Eq. (5), and with these assumptions, we can express the total impurity distribution within a double-diffused transistor by the relation

$$c(x;\,t)=c_b+c_{01}\,\mathrm{erfc}(x/2\sqrt{D_1t_1})-c_{02}\,\mathrm{erfc}(x/2\sqrt{D_2t_2})\,. \tag{6}$$

Equation (6) is the fundamental expression used in this investigation to characterize the impurity distribution within a double-diffused transistor. The collector and emitter junctions are established by the two roots of Eq. (6): their relative distance is assumed to be the transistor base width. From Eq. (6) – and also Eq. (2) – we have five parameters which are subject to experimental tolerances and, therefore, contribute to a decreased reproducibility of the transistor base width.

To simulate experimental variations within this diffusion process, a number generator has been used whose output is a normal distribution about a mean value. This distribution was adjusted so that 90 per cent of all numbers, for each variable, were within the specified experimental tolerances; 99 per cent of all numbers were accepted.

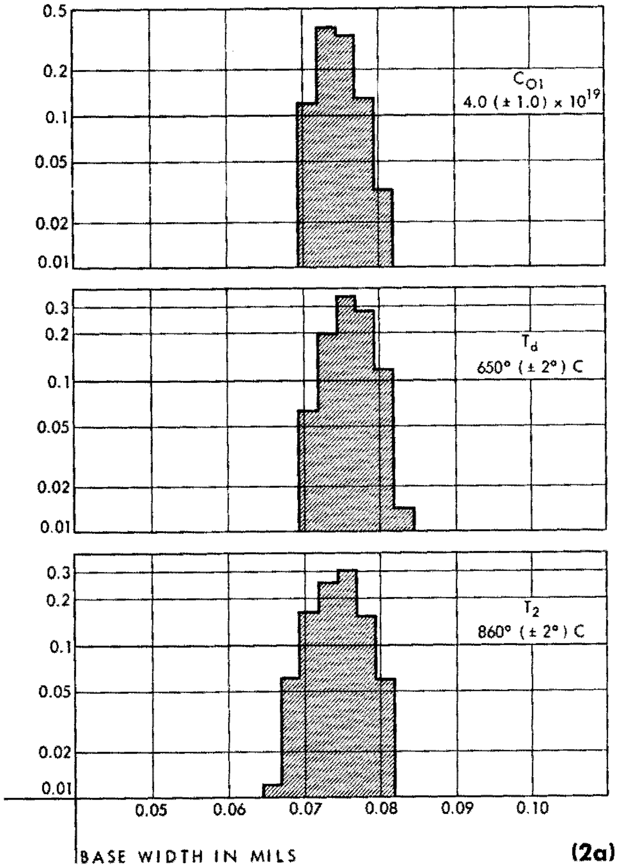
Base-width distribution of an *n-p-n* transistor

A difficult problem arises when attempting to establish the physical constants of a particular diffusion process. Published values for the diffusion coefficients (D_0) and activation energies (ΔH), for example, will often have a range so large as to be of little practical value. Further, experimental differences between the diffusion methods used in a laboratory and those represented by the ideal impurity distribution of Eq. (6) may not permit the use of other than experimentally determined physical constants. In this analysis of an *n-p-n* transistor, some of the required parameters were obtained from the literature[1] while others were established from measurements upon actual devices.

Table 1 establishes the published ranges for each physical constant of this system and also the magnitude used in this investigation. The diffusion coefficient (D_0) and activation energy (ΔH) for arsenic were taken from published values. For indium, on the other hand, the diffusion coefficient was obtained from junction depth measurements and therefore is probably applicable only to this particular diffusion process.

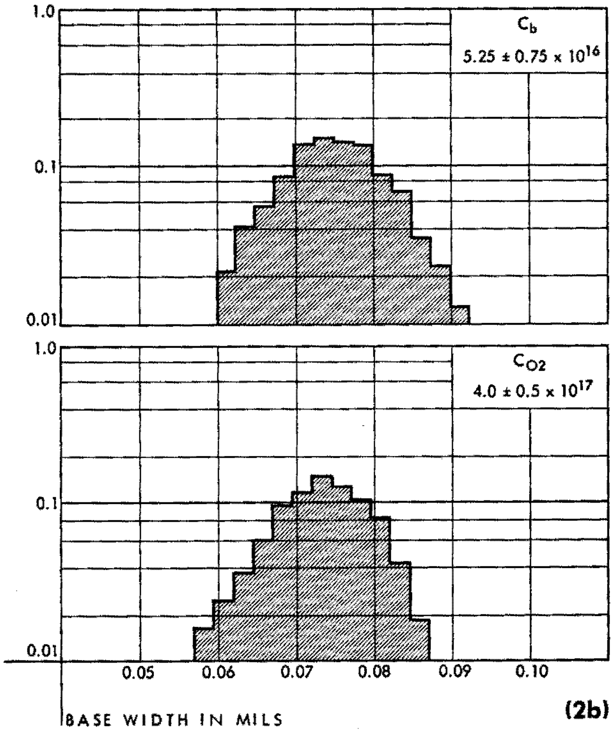
Table 2

	$T(°C)$	t	C_b	C_{01}	C_{02}
Antimony			$5.25(\pm 0.75)\times 10^{16}$		
Arsenic	$650(\pm 2)$	150(min)		$4(\pm 1.0)\times 10^{19}$	
Indium	$860(\pm 2)$	9.25(hrs)			$4.0(\pm 0.5)\times 10^{17}$

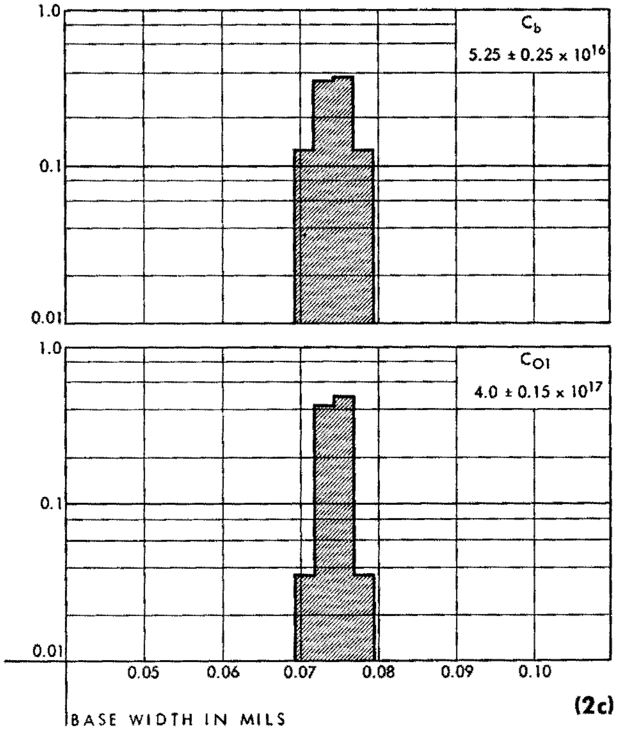


(2a)

Figure 2 **Base-width distribution from individual diffusion parameters.**



(2b)



(2c)

Figure 1 illustrates the theoretical base-width distribution for three different degrees of control upon the parameters of a diffusion process. Figure 1a presents the distribution for 5000 transistors which results from the conditions outlined in Table 2; this is typical of a practical diffusion process. Since many parameters are simultaneously changed when computing Fig. 1a, process improvement is best obtained by decreasing tolerance limits on selected parameters rather than on all five.

Figures 2a and 2b illustrate the relative contribution of the individual parameters in this diffusion process to Fig. 1a. In these distribution diagrams the indicated parameter was varied within its tolerance limits – from Table 2 – while all others were held at their mean value. From Fig. 3 the principal contribution to this base-width distribution results from the surface concentration of indium and the bulk impurity concentration of germanium. Upon decreasing the tolerance limits for these two parameters, Fig. 2c, a significant improvement is obtained in the base-width distribution, Fig. 1b.

The final base-width distribution diagram, Fig. 1c, results from an over-all decrease of tolerance limits for all diffusion parameters, Table 3. Here each tolerance has been decreased sufficiently to permit 80 per cent of the transistors to exhibit a base-width range of from 0.062 to 0.077 mil for the individual parameter under consideration.

Thus far, only the control of the diffusion process has been shown as a means of improving transistor reproducibility. In this investigation, shallow diffusions are found

Table 3

	$T(°C)$	t	C_b	C_{01}	C_{02}
Antimony			$5.25(\pm 0.15) \times 10^{16}$		
Arsenic	$650(\pm 1)$	150(min)		$4(\pm 0.5) \times 10^{19}$	
Indium	$860(\pm 1)$	9.25(hrs)			$4.0(\pm 0.1) \times 10^{17}$

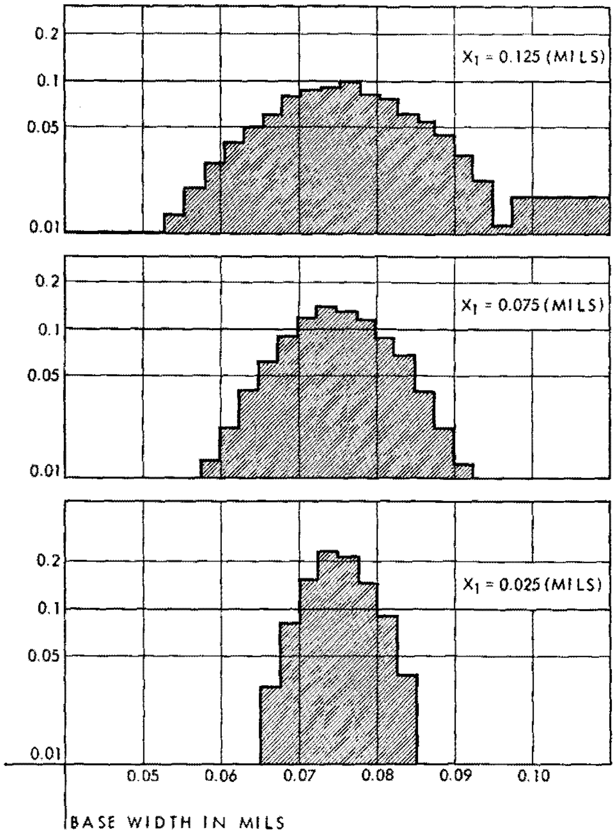


Figure 3 **Base-width distributions for parameters of Table 2 with decreased emitter junction depth.**

to yield a decreased sensitivity to the experimental tolerances of a system. Using the parameters of Table 2, the diffusion times were adjusted to maintain a constant base width with decreasing junction depths, Fig. 3. Here the shallow diffusion is shown to result in a decreased spread in transistor base width, thereby improving the reproducibility of this semiconductor device.

An IBM 7090 program is available[5] and will be sent upon request.

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