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Shallow diffusion profile analysis of phosphorus in silicon at 1100 °C and an empirical fit

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A detailed study of a phosphorus diffusion profile in silicon at 1100 °C was made by repeated removal of silicon layers and resistivity measurements by observing the limitations of four-point probe voltage and currents [Solid-State Electron. **25**, 611 (1982)]. The results confirmed that the phosphorus diffusion profile is not always given by an error function and on the contrary, a distinct kink and tail structure occurs in the profile. The observed data seems to agree with the concept of two diffusion coefficients proposed by Tsai [Proc. IEEE **57**, 1499 (1969)] for temperatures below 1100 °C. Observed experimental data have been analyzed to give the values of the two diffusion coefficients and an empirical fit has been found. It is pointed out that two independent Gaussian profiles can be fitted for the phosphorus profiles by the two diffusion coefficients which lead to the apparent kink and tail structure of the profile.

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Simple theories of impurity diffusion in semiconductors assuming a constant diffusivity yield either complementary error function or Gaussian profiles. However, in most cases, especially at high surface concentrations, strong deviations of the experimental impurity profiles from theories are found to occur. Experimental profiles can be fitted by theoretical curves only by making a number of assumptions regarding diffusivity dependence on impurity concentration, surface effects, the influence of the electric field, the influence of the existence of vacancies in the host lattice, the effects of plastic deformation and the degeneracy of highly doped silicon, the effect of strain-induced band-gap narrowing, and the lattice contraction coefficient of the impurity diffused. For process control and for device characterization and optimization, an accurate knowledge of the diffusion profiles and especially the prediction of the diffusion depth from a knowledge of the diffusion and chip parameters is a necessity. This communication reports some results of the diffusion of phosphorus in silicon and clearly shows that the diffusion is not a simple complementary error function but, on the contrary, a distinct kink and tail structure occurs in the profile diffused at 1100 °C. Further, it is possible to obtain empirical fits for two distinct diffusion coefficients.

Tannenbaum¹ demonstrated experimentally that the distribution of phosphorus is not an error function complement for temperatures greater than 600 °C and for surface concentrations greater than $1.0 \times 10^{20} \text{ cm}^{-3}$. After her, a large number of investigators have studied the detailed features of phosphorus diffusion profiles by using some of the phosphorus-oxygen compounds like P_2O_5 and POCl_3 , and also by tracer methods. Some of the studies showed the phosphorus profiles in silicon to be much more complicated than observed by Tannenbaum.²⁻⁶

The electrical characteristics of semiconductor devices are primarily determined by the impurities incorporated into the body of the semiconductor and by their spatial dis-

tribution. Three basic methods are available to determine impurity profiles: spreading resistance, $C-V$ measurements, and successive removal of controlled amounts of semiconductor. Three basic techniques for sectioning exist: mechanical/chemical polishing, anodic oxidation, and chemical etching. In the present investigation we have adopted the combination of anodic oxidation^{7,8} and controlled chemical polishing for profile measurements.

To study the phosphorus diffusion profile we selected three silicon wafers, finely polished on one side and lapped on the other side, with a $1\text{-k}\Omega \text{ cm}$ resistivity p type, and a crystallographic orientation (111). About $0.6\text{-}\mu\text{m}$ -thick thermal oxide layers were grown on the lapped side to ensure that the diffusion would take place only on the finely polished side. The diffusion was carried out at 1100 °C for 1 h in a nitrogen ambient in an open tube furnace by using P_2O_5 as the impurity source. The silicon surface was then etched with buffer HF for all the wafers to make it free from the phosphosilicate glass. At each stage of anodic oxidation and chemical polishing the wafers were cleaned chemically and also with hot deionized water and vacuum dried. From the weight difference the amount of silicon removed was calculated. After each removal the sheet resistivity was measured by four-point probe technique taking the precaution suggested by the authors⁹ and by Huang and Ladbrooke.¹⁰

The conductivity of the removed silicon layer can be calculated from the relation

$$\sigma(w)\delta w = \frac{1}{4.5} \left(\frac{I_1}{V_1} - \frac{I_2}{V_2} \right), \quad (1)$$

where $\sigma(w)$ is the conductivity of the removed silicon layer of thickness δw , V_1 , I_1 and V_2 , I_2 are probe voltages and currents of the two successive measurements on the silicon surface. By repeating the process the variation of conductivity with depth $\sigma(z)$ can be plotted. This is related to the variation in electron concentration by the relation

$$\sigma(z) = n(z)B(z)e, \quad (2)$$

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where $B(z)$ is the mobility. Using the empirical relations given by Caughey and Thomas¹¹ as modified by Plunkett *et al.*¹² the value of $n(z)$ can be calculated.

From the measured values of I_1 , I_2 and V_1 and V_2 the concentration of phosphorus was calculated for the three wafers. Figure 1 shows the impurity concentration and the depth from the silicon surface. The open circle (O) values are obtained by anodic oxidation and closed circles (●) by chemical polishing. The curve shows that there are two effective diffusion sources with two different diffusivity values. The one at lower concentrations is moving faster than the one at higher concentrations. The two values calculated from the experimental results are

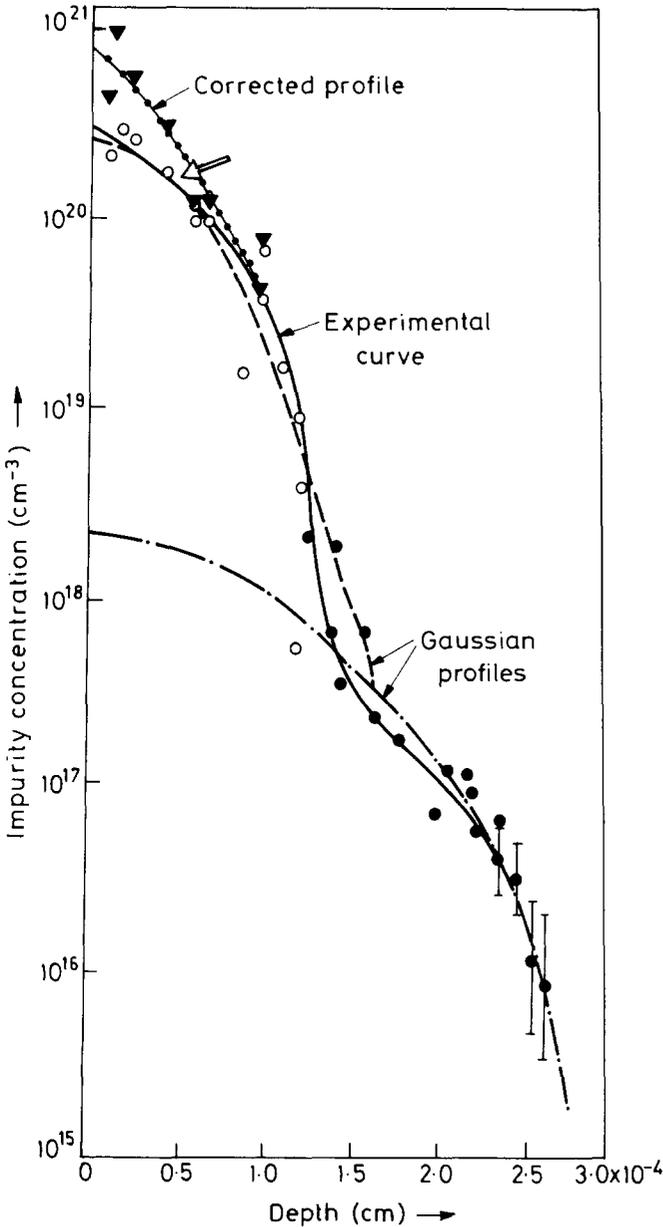


FIG. 1. Experimentally determined phosphorus diffusion profile in silicon. The smooth curve drawn to the experimental points shows kink and tail structure. The broken lines corresponds to two Gaussian curves to fit the experimental data. Open circles (O) obtained by anodic oxidation and closed circles (●) by chemical polishing technique. Triangles (▲) correspond to the actual phosphorus concentration as discussed in the text. The arrow mark indicates the kink position predicted by Fair and Tsai.¹⁴

$$D_1 = 2.850 \times 10^{-13} \text{ cm}^2/\text{S (slow)},$$

$$D_2 = 9.964 \times 10^{-13} \text{ cm}^2/\text{S (fast)}. \quad (3)$$

Several theoretical models have been proposed to explain the anomalous diffusion profiles for silicon viz. moving phase boundary by Tsai,² E -center model by Yoshida,⁴ strain induced band gap narrowing by Fair,⁵ effects of plastic deformation and degeneracy of highly doped silicon by Thai⁶ and the retardation of P diffusion as a result of the precipitation at moving dislocations by Lawrence.¹³

The kink formation in phosphorus diffusion in silicon is an established phenomenon in high concentration (extrinsic) diffusion and becomes more and more pronounced with decreasing temperatures lower than 1000 °C. It was predicted by Tsai² that as the diffusion temperature increases the diffusion constants for the slow and fast diffusants, approach each other, and at 1100 °C the diffusion profile can be represented by a single diffusion constant. In our experiments however the slow and fast diffusants are clearly distinguishable even at 1100 °C.

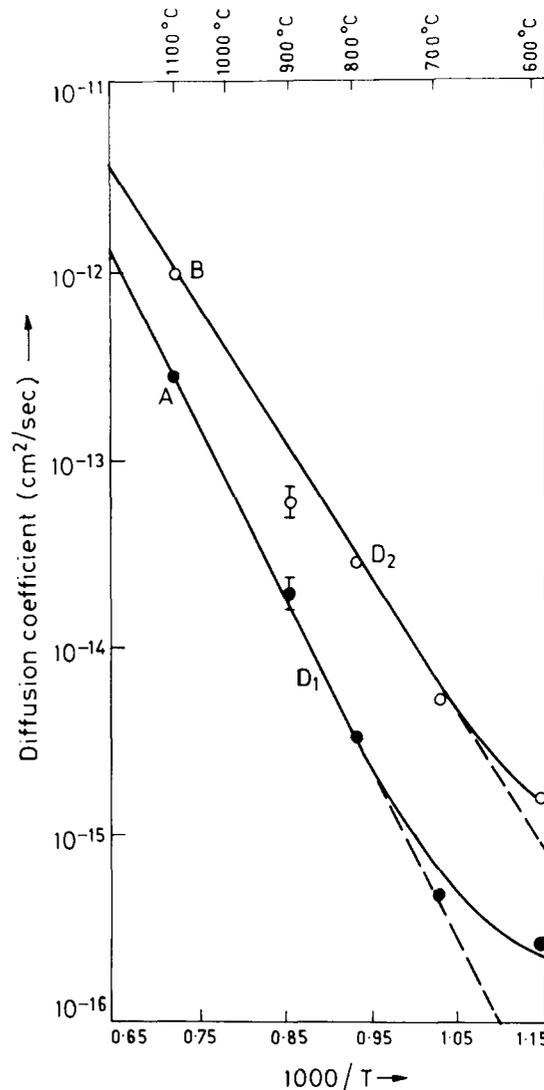


FIG. 2. Diffusion constants measured at different temperatures as calculated from the diffusion profiles obtained by Schewettmann and Kendall.³ D_1 and D_2 correspond to the slow and fast diffusants discussed in the text. The points A and B are obtained by the authors.

The model presented by Fair and Tsai¹⁴ for the diffusive migration of phosphorus predicts, with reasonable accuracy, the phosphorus kink formation as well as the base push effect. According to this model, the physical explanation of these anomalous effects lies in the enhancement of vacancy concentration in silicon caused by the dissociation of the phosphorus-doubly ionized vacancy pairs that flow from the surface into the silicon bulk. The free electron concentration in this region will be less than the actual phosphorus concentration. The total phosphorus concentration can be obtained from the relationship

$$C = n + 2.04 \times 10^{-41} n^3. \quad (4)$$

The triangles represent the actual concentration in Fig. 1, as calculated from the above equation. The end of the surface region is assumed to lie at the point where the Fermi level drops below 0.11 eV from the conduction band which is identified as the state level for doubly ionized vacancies. This occurs at a characteristic electron concentration n_e given by¹⁵

$$n_e(T) = 4.65 \times 10^{21} \exp\left(-\frac{0.39 \text{ eV}}{kT}\right). \quad (5)$$

The value corresponds to 1100 °C is marked over the profile obtained in Fig. 1. But in the present profile obtained, the kink formation is in the region 10^{18} – 10^{17} cm^{-3} .

In the impurity concentration less than $1.0 \times 10^{17} \text{ cm}^{-3}$, it is difficult to observe appreciable current in the four-point probe resistivity measurements for an accurate value of impurity concentration. In addition to that in the Eq. (1) one has to subtract substantial values to get the conductivity of removed layer, which will cause appreciable error in impurity estimation. To overcome this difficulty both forward and reverse current directions were tried and average values are given.

Similar types of profiles were obtained by Schwettmann and Kendall³ at different annealing times. We analyzed their data to obtain the two diffusion coefficients, as in our case, and plotted them with our results as a function of tempera-

tures, as shown in Fig. 2. The existence of two diffusion coefficients is seen to emerge clearly from Fig. 2. The curves of the figure can be fitted to the following two empirical relations:

$$D_1 = 1.365 \times 10^{-6} \exp(-1.829/kT) \text{ cm}^2/\text{S (slow)},$$

$$D_2 = 1.907 \times 10^{-7} \exp(-1.431/kT) \text{ cm}^2/\text{S (fast)}. \quad (6)$$

The experimental results obtained are plotted with the calculated curve, using the above empirical relationships for D_1 and D_2 . It can be seen that the initial profile (broken line in Fig. 1) with a slow diffusivity coefficient is a Gaussian profile. Below $1.0 \times 10^{18} \text{ cm}^{-3}$, the fast diffusivity coefficient dominates. The second profile can be represented as Gaussian with a surface concentration of $2.2 \times 10^{18} \text{ cm}^{-3}$ which leads to the apparent kink and tail structure of the profile.

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