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SIMULATION AND MEASUREMENT OF THE LATERAL SPREADING OF IONS IMPLANTED INTO AMORPHOUS TARGETS

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ABSTRACT

A method is presented whereby it is possible to deduce the depth dependent lateral standard deviation function from experimental depth profiles of ions implanted into amorphous target materials. These results are compared with both Boltzmann and Monte Carlo computer simulations.

INTRODUCTION

In order to validate the complex physical models and numerical algorithms which are currently being implemented in two dimensional process simulators requires the development of equally accurate measurement techniques which can yield quantitative two dimensional information. This requirement is particularly pressing in the measurement of two dimensional dopant distributions because of the difficulty in obtaining lateral information with sufficient resolution and in relating the measured quantities with actual impurity concentrations (Akasaka et al, 1972; Hill et al, 1985; Roberts et al, 1985; Lee 1986). Hence, any technique which is capable of supplying even partial information about two dimensional distributions is to be welcomed. The most promising method developed to date has been the anodic sectioning technique of Hill et al (1987, 1988) which can give quantitative two dimensional carrier concentration distributions near mask edges both before and after diffusion processing steps.

Recently Ashworth and Oven (1985, 1986), Oven and Ashworth (1987a) and Hobler et al (1987) have improved the modelling of two dimensional distributions of ions implanted into amorphous targets by the introduction of a depth dependent lateral standard deviation function $\Delta X(z)$ which models the statistical dependence between the ions depth and lateral rest co-ordinates. Hence, the measurement of such distributions without the ambiguities introduced by mask edge profiles is of interest. In this paper we present a method of obtaining information about the lateral standard deviation function using standard depth profiling techniques (Ashworth et al, 1988) and compare these results with computer simulations.

It is well known that some information about the lateral spreading of implanted ions can be obtained from the analysis of two, one dimensional depth profiles. One of these profiles, $F_\theta(z)$, is produced by implanting ions at an angle θ with respect to the target normal and the other $F_p(z)$, the projected range profile, is produced by implanting ions along the target normal.

Many authors have deduced values for the constant lateral standard deviation, ΔXo, by fitting either Gaussian (Furukawa and Matsumura, 1973a, 1973b; Okabayashi and Shinoda, 1973; Grant et al, 1975, 1976) or Pearson distributions (Wilson, 1985) to both normal and tilted depth profiles and have then used the relationship

(1) $$\Delta Xo = \left[\frac{\Delta D^2 - \Delta Rp^2 \cos^2\theta}{\sin^2\theta}\right]^{\frac{1}{2}}$$

where ΔD is the standard deviation of $F_\theta(z)$ and ΔRp is the standard deviation of $F_p(z)$. Equation (1) was first derived in this context by Furukawa and Matsumura (1973a) on the assumption of a two dimensional Gaussian distribution. In fact, the formula is more general, being independent of the assumed two dimensional function and depends only on the assumptions that the target is amorphous, uniform and infinite (as opposed to semi-infinite) in extent.

In principle more detailed information about the lateral spreading of ions is contained within these two depth profiles. However, because the experiments mentioned above were performed using crystalline targets in which channelling effects were almost certainly present it is not possible to extract extra lateral information from such published data. We have hence performed a series of experiments using amorphous targets in an attempt to validate the lateral spreading model. The interpretation of the experimental data is similar in concept to that performed by Matsumura and Stephens (1977) who deduced the depth dependent lateral spread function for proton damage in GaAs.

THEORY

Consider an ion beam incident upon an amorphous target at an angle θ with respect to the target normal as shown in Figure 1. We wish to calculate the depth profile $F_\theta(z)$ with respect to the unprimed coordinate system.

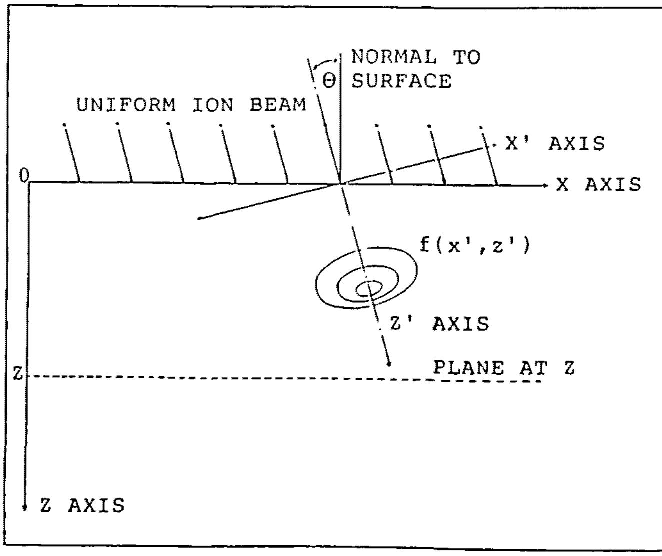

Fig. 1 Definition of co-ordinate systems.

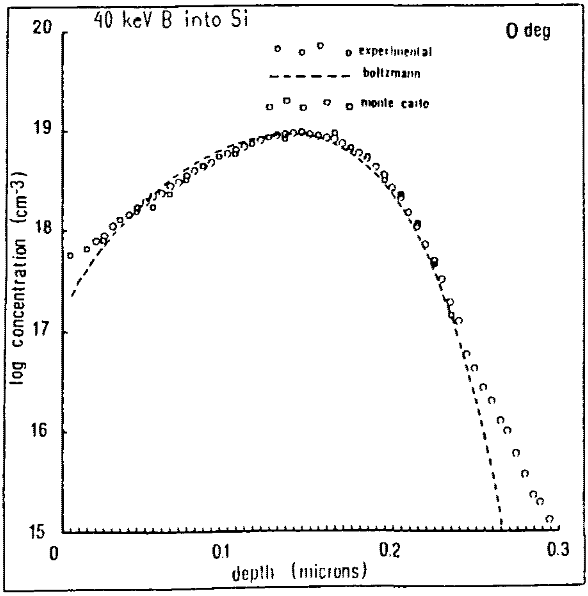

Fig. 2 A comparison of 40keV boron profiles. Normal incidence.

Let us assume that the normalized two dimensional single ion rest distribution function specified with respect to the primed coordinate system is represented by

$$f(x',z') = \frac{F_p(z')}{\sqrt{2\pi}\Delta X(z')} \exp\left\{ - \frac{x'^2}{2\Delta X^2(z')} \right\} \tag{2}$$

where $F_p(z')$ is the normalized projected range distribution function and $\Delta X(z')$ is the depth dependent lateral standard deviation. In writing down equation (2) we have made the implicit assumption that $F_p(z')$ and $\Delta X(z')$ remain unaltered if the primed coordinate system is rotated about its origin, i.e. the presence of the surface does not significantly perturb the two dimensional distribution of those ions which come to rest inside the substrate. It is assumed that the surface truncates the distribution but does not otherwise distort it. This assumption can be expected to be valid for those ions which come to rest deep inside the substrate since the vast majority of these ions would not have undergone large angle scattering events near the surface. However, it can be expected to break down for large tilt angles θ, and for those ions which come to rest near the surface. Obviously, this assumption can only be checked by comparison with computer simulations. The perturbing effect of a surface on the projected range distribution for infinite targets has been calculated by Fedder and Littmark (1981).

We further assume that we may neglect the contribution to $F_\theta(z)$ by any ions which are back-scattered beyond the (x',y') plane i.e. ions which come to rest with a negative value of z'. This is a necessary assumption since it is not possible to measure the projected range profile $F_p(z)$ for negative values of z.

Summing the contributions from all ions incident upon the surface we find that $F_\theta(z)$, the concentration of ions at depth z (unprimed coordinate system) which have been implanted at an angle θ, is given by Oven and Ashworth (1987b) as

$$F_\theta(z) = \frac{\Phi}{\sqrt{2\pi}\tan\theta} \int_0^\infty \frac{F_p(z')}{\Delta X(z')} \exp\left\{ - \frac{(z'\cos\theta - z)^2}{2\sin^2\theta\,\Delta X^2(z')} \right\} dz' \tag{3}$$

where Φ is the normal incident dose.

Equation (3) is a first order non-linear integral equation which can be used to determine $\Delta X(z)$ given the experimentally measured profiles $F_\theta(z)$ and $F_p(z)$ for amorphous target materials. A simple numerical method has been developed to solve equation (3) (Oven and Ashworth, 1987b) to yield $\Delta X(z)$.

Figures 2 and 3 show ion implantation profiles calculated from both a Boltzmann simulation code (Oven and Ashworth, 1987a) and a Monte Carlo code (Oven and Ashworth, 1988) for 40keV boron ions (Dose 10^{14} cm^{-2})implanted into amorphous silicon at implantation angles of 0° and 45° with respect to the target normal. Also shown are the experimental profiles obtained from SIMS measurements (Ashworth et al, 1988).

MINIMIZATION SOLUTION METHOD

Due to the fact that the two experimental functions $F_\theta(z)$ and $F_p(z)$ are known only at discrete values of their arguments it is, in general, not possible to solve equation (3) for the unknown function $\Delta X(z)$. Further, because the values of the two known functions are obtained from experimental measurements, these quantities will contain various instrumentation errors and noise and will thus only be known to a finite accuracy. Taking into consideration the above factors we redefine the problem of solving equation (3) as a *minimization problem.* We hence seek the function $\Delta X(z)$ which minimizes the following quantity

$$\sigma[\Delta X(z)] = \int_0^\infty w(z) \left[\ln\{F_\theta(z)\} - \ln \left\{ \frac{\phi}{\sqrt{2\pi}\tan\theta} \int_0^\infty \frac{F_p(z')}{\Delta X(z')} \exp\left\{ - \frac{(z'\cos\theta - z)^2}{2\sin^2\theta\, \Delta X^2(z')} \right\} dz' \right\} \right]^2 dz \qquad (4)$$

where $w(z)$ is a weighting function. We are essentially finding the function $\Delta X(z)$ which minimizes σ in the least squares sense. However, since the functions $F_\theta(z)$ and $F_p(z)$ vary over many orders of magnitude we minimize the square of the difference of the logarithms of the functions.

There remains to be assigned a representation for the unknown function $\Delta X(z)$. In order that $\Delta X(z)$ should be able to form any shape forced upon it by the minimization routine it was decided to represent it by means of a series of piecewise linear segments. Hence, no preconceived idea about its shape, e.g. a polynomial, was forced upon it.

In principle, it is now possible to find the function $\Delta X(z)$ which minimizes equation (4) by using any number of standard direct search techniques. If $\Delta X(z)$ is represented by a series of line segments with N nodes then the search is directed in an N dimensional space. It was found, however, that such an approach was slow to converge and resulted in a representation of $\Delta X(z)$ which oscillated wildly. Hence, the following technique was adopted which resulted in rapid convergence with no oscillations on test data : The function $\Delta X(z)$ was first represented by one linear segment and a

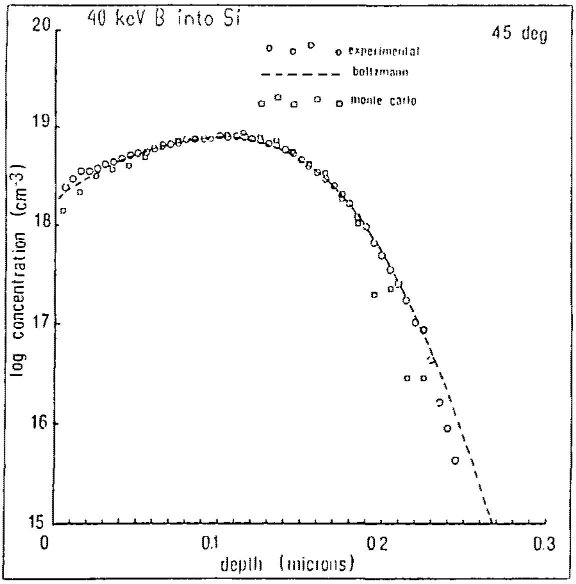

Fig. 3 A comparison of 40keV boron profiles .45 degree incidence.

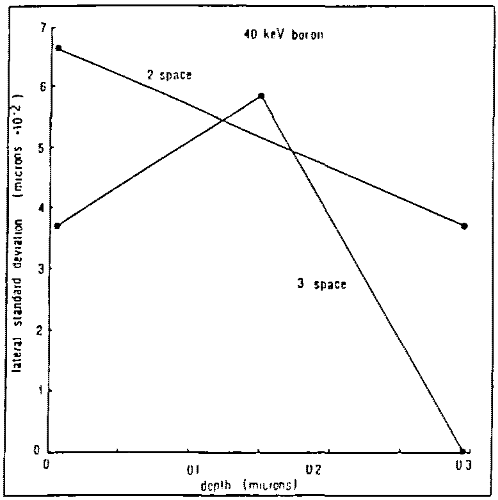

Fig. 4 Linear segment representations of $\Delta X(z)$ for 40keV boron ions.

minimization in a two dimensional space was performed. After convergence to a small value of σ an extra node was inserted, mid-way in z between the existing nodes, and a further minimization was performed in 3 space. This procedure was then repeated. In general, after a minimization in N space the space was increased to (2N-1) dimensions. This procedure preserves the continuity in σ in changing from N to (2N-1) dimensions. Figure 4 shows a sequence of linear segment representations of ΔX(z), referred to as $\Delta X_N(z)$, after the search in N space using the experimental data shown in figures 2 and 3. The quality of the final fit can be assessed by comparing the experimental profile $F_\theta(z)$ with the profile obtained by re-computing $F_\theta(z)$ using the right hand side of equation (3) with the linear segment representation $\Delta X_N(z)$ used in the integrand. Figure 5 shows this comparison after the minimization in 2 space and 33 space.

COMPARISON WITH COMPUTER SIMULATIONS

Figure 6 shows the depth dependent lateral standard deviation function ΔX(z) calculated at the end of the minimization procedure in 33 space. For comparison, the depth dependent lateral standard deviation function calculated from Boltzmann transport equation simulations (Oven and Ashworth, 1987a) and Monte Carlo simulations (Hobler et al, 1987) are shown. It can be seen that there is a very pleasing agreement between the two simulations and the experimental curve for depths greater than 0.1 μm. However, the curves diverge considerably in the near surface region. An explanation of this divergence of the experimental curves in the near surface region is possible on the basis of the breakdown of one of the assumptions made in the derivation of equation (3). In the derivation it was assumed that the rest distribution of ions in the primed co-ordinate system was given by equation (2), simply truncated by the surface. Hence, the rest distribution of an ion in x' at a constant z' was assumed to be Gaussian, with standard deviation ΔX(z'), truncated on one side at x' = z' tan θ = $x_\dagger$. It can be expected that the true rest distribution will be lower than this assumed distribution since ions cannot, in practice, be returned from beyond a lateral distance $x_\dagger$ and then come to rest with x' < $x_\dagger$. Hence, the number and spread of the ions which come to rest at depth z' is reduced.

Figure 7 shows ΔX(z) calculated from experimental profiles for 30 keV boron ions implanted into pre-amorphised silicon. The angle of incidence for the tilted profile was again nominally 45°. For comparison, the simulated curves are also shown. It can be seen that there is good agreement between the curves for depths greater than 0.08μm. A comparison between figures 6 and 7 shows that the predicted variation in lateral spread with incident ion energy has been experimentally observed. Using the experimentally determined

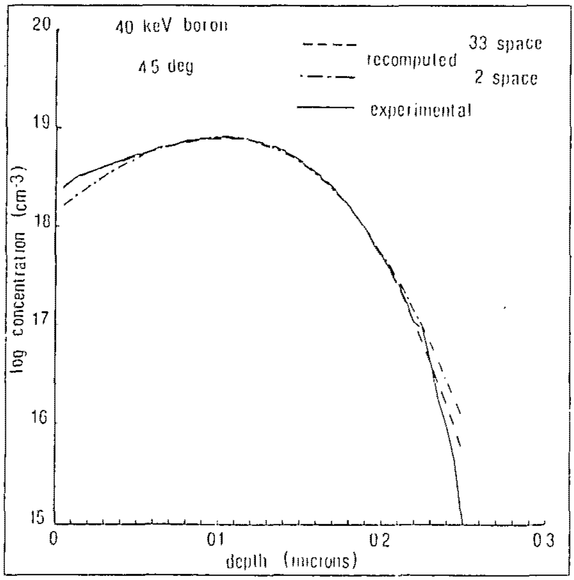

Fig. 5 Recomputed and experimental $F_{\theta}(z)$.

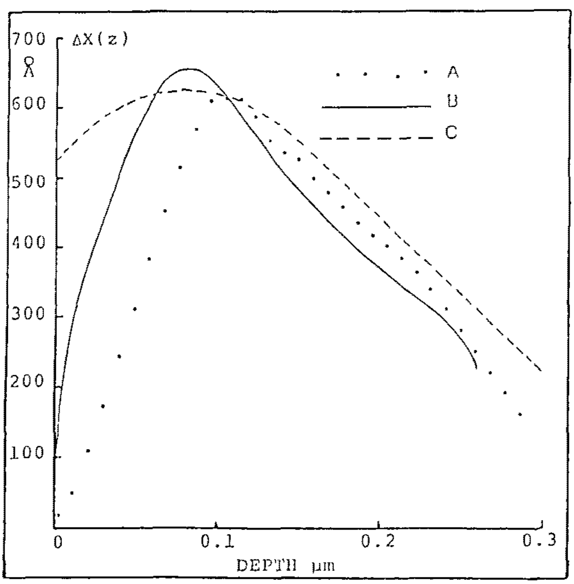

Fig. 6 Depth dependent lateral standard deviation function $\Delta X(z)$, (A) experimentally derived, (B) Boltzmann, (C) Monte Carlo. 40keV boron in pre-amorphised silicon.

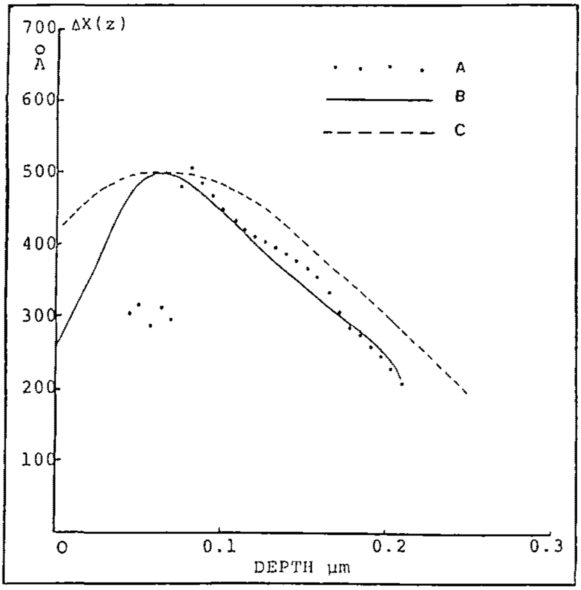

Fig. 7 Depth dependent lateral standard deviation function ΔX(z), (A) experimentally derived, (B) Boltzmann, (C) Monte Carlo. 30keV boron in pre-amorphised silicon.

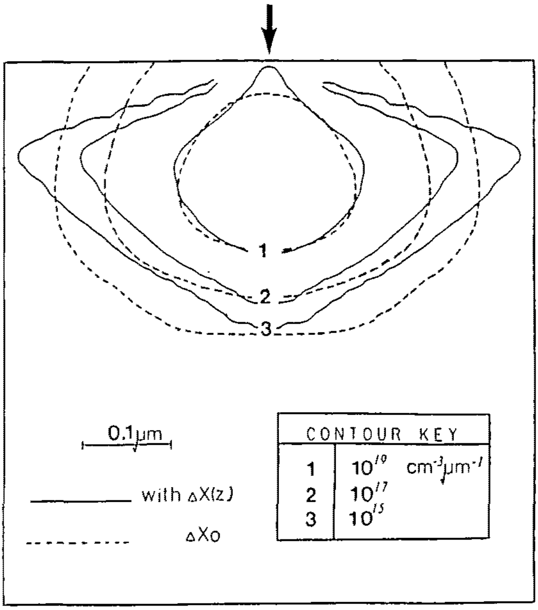

Fig. 8 Reconstruction of two dimensional distribution functions for 40keV boron implanted into amorphous silicon. Dose $10^{14}cm^{-2}$.

functions $F_p(z')$ and $\Delta X(z')$ a two dimensional single ion rest distribution function can be reconstructed from equation (2). Figure 8 shows the experimentally derived two dimensional single ion rest distribution function for 40 keV boron ions. However, bearing in mind the above discussion, the near surface distribution should be treated with caution. For comparison, figure 8 also shows the two dimensional single ion rest distribution function reconstructed using a constant lateral standard deviation ΔXo which was found to be of the order of 550Å. The difference between these two models is clear.

Monte Carlo simulations (Hobler et al, 1987) have recently shown that the lateral distribution at each depth is not strictly Gaussian i.e. does not have a kurtosis of 3. This is a higher order effect which would require the simultaneous analyses of three one dimensional profiles. Such an experiment and analysis would be difficult to perform, but the possibility is being investigated.

It is interesting to note that, theoretically, a unique deduction of the two dimensional single ion rest distribution function (for an infinite target) requires an infinite number of one dimensional implantation profiles obtained at all angles from 0° to 90° (Berger 1959).

The method described is capable of supplying quantitative fundamental information about the two dimensional distribution of ions implanted into amorphous targets without the introduction of uncertainties due to mask edge functions. In principle, the method can be applied to other technologically important materials like SiO_2 and Si_3N_4 provided good experimental profiles are available. However, like the technique of Hill et al (1987, 1988) it does rely on the reconstruction of a two dimensional distribution from one dimensional distributions and hence requires an assumed two dimensional function.

CONCLUSIONS

A method has been presented whereby it is possible to deduce the depth dependent lateral standard deviation function from experimental depth profiles of ions implanted into amorphous target materials. Although the method does rely on an assumed analytical equation (2), it has been shown that the method is capable of yielding quantitative two dimensional information which is in reasonably good agreement with two dimensional ion implantation simulations.

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