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Editors: Thomas O. Sedgwick, Thomas E. Seidel and Bor-Yeu Tsaur

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Implanted Dopant Activation and Diffusion in Silicon



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DIFFUSION MODELING OF THE REDISTRIBUTION OF ION IMPLANTED IMPURITIES

ALWIN E. MICHEL

IBM Research Center, Yorktown Heights, New York 10598

ABSTRACT

Transient enhanced diffusion during rapid thermal processing has been reported for most of the common dopants employed for silicon device fabrication. For arsenic a large amount of the available data is fit by a computational model based on accepted diffusion mechanisms. Ion implanted boron on the other hand exhibits anomalous tails and transient motion. A time dependence of this displacement is demonstrated at lower temperatures. High temperature rapid anneals are shown to reduce some of the anomalous motion observed for low temperature furnace anneals. A model is described that links the electrical activation with the diffusion and describes both the transient diffusion of rapid thermal processing and the large anomalous diffusion reported many years ago for furnace anneals.

INTRODUCTION

Rapid thermal processing (RTP) provides a promising technique to minimize the displacement of ion implanted impurities while activating the impurities and annealing the implantation damage. It also provides a source of experimental data in a previously inaccessible time region. Some of the studies have reported the occurrence of anomalously high transient diffusion during the short time anneals. Since the minimization of dopant motion is a major technological concern, an understanding of the phenomena involved is highly desirable.

Computational diffusion models have been used for many years to describe the impurity redistribution during the heat treatment with furnaces. These models can also be applied to RTP and are useful in determining the magnitude of any anomalous diffusion. They also can be modified and serve as a touchstone in evaluating proposed physical phenomena.

Transient enhanced diffusion has been reported for most of the common dopants employed for silicon device fabrication.²⁻⁵ However, there is a lack of agreement among various experiments and there is considerable controversy concerning the explanation. One of the major experimental problems in RTP is accurate measurement of the temperature of the sample. In some cases the temperature reported was in error by 50 to 100 °C. In a round robin experiment conducted by T. Seidel differences in reduction of the unannealed peak concentration for a 10 sec. 1100 °C anneal had a total spread of nearly 50 percent. Much of the experimental discrepancy is attributable to this problem.

The present paper will address only the species of arsenic and boron since they are the most likely candidates for shallow junction applications. They also represent extremes in terms of implantation effects and diffusion characteristics.

ARSENIC

For arsenic, much of the experimental data are successfully fit with the previously developed model employing conventionally accepted diffusion mechanisms.^{7,3} Some of the effects that measurement techniques and sample preparation have on the resulting profiles and how they are treated are discussed.

In comparing the results between computed and experimental profiles the resolution of the measurements must be considered. The concentration enhanced diffusion of

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arsenic generates very abrupt impurity profiles which are smeared by the resolution of the measurement equipment. In the case of SIMS arsenic profiles are frequently obtained using a cesium sputtering beam or an oxygen "bleed" to provide high sensitivity. Both of these techniques result in an increase the exponential tail of the SIMS profile. Fig. 1 shows an example of a calculated profile with and with out the adjustment for the resolution factor and the corresponding SIMS data.

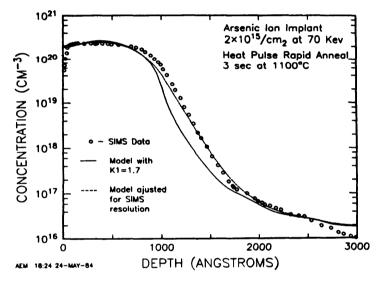


Fig. 1 Comparison of calculated with SIMS profile showing the effect of adjustment of the calculated profile for SIMS resolution.

In addition to the temperature determination another experimental problem occurs in the case of arsenic and that is the possibility of evaporative loss of dopant from the surface in samples that do not have an oxide cap. If the profile measurements are made using the SIMS technique they are frequently normalized to the implanted dose. Fig. 2 shows the concentration profiles from the data of Sedgwick⁸ for various anneal times at 1100°C during which surface evaporation took place. The evaporation is accommodated in the model by fixing the surface concentration at a low value and discarding all of the arsenic diffusing to the surface. The solid curves show the fit obtained by using an established diffusion model and have been corrected for SIMS resolution. The same model has been employed to fit some data obtained from the "round robin" experiment conducted by T. Seidel shown in Fig. 3. Here the calculated profiles were convoluted with a 20 nm Gaussian resolution function to correct for the RBS dispersion.

Since arsenic amorphizes the lattice at concentrations of $2x10^{14}$ /cm² one would expect a significant difference in the behavior of the point defects and hence the anomalous diffusion for fluences below and above this threshold value. A study of the profile motion during RTP for a wide range of implant fluence is presented in reference 6. Fig. 4 shows the comparison of the calculated and measured displacements for a 10 sec. 1100° C anneal.



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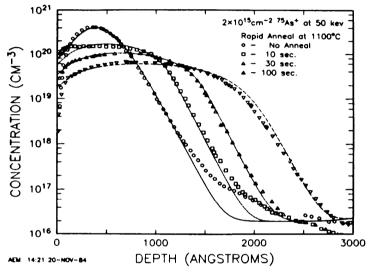


Fig. 2 Comparison of the modeled arsenic profiles for various RTP times with the data from Ref. 8.

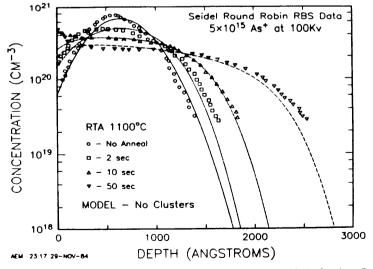


Fig. 3 Comparison of the modeled arsenic profiles for various times with the data from Ref. 6.



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Quite good agreement with this model has also been obtained for anneals at higher temperatures, up to 1200°C, for times ranging between 10 and 240 sec. Sheet resistance calculations for these measurements also compare satisfactorily. Since the clustering is reduced substantially at these high temperatures, very high concentrations are needed. While there is some indication that the clustering mechanism is operative for these higher temperature anneals, the time constants for the arsenic cluster formation are uncertain. For very short anneals it is possible that the clusters have not formed which results in more displacement than predicted by the equilibrium model. An example for a 5 sec. anneal is shown in Fig. 5 where the data is taken from the work of Pennycook. While the agreement is better without the clustering the displacement difference is only 15 nm which is of the order of the experimental uncertainty for a single measurement.

BORON

Ion implanted boron, unlike arsenic, appears to have a genuine transient enhanced diffusion. Hodgson¹⁰ reported a transient motion for pulse anneals using the Nova arc lamp in the temperature range between 900 and 1200 °C. The displacement was attributed to boron in the channeling tail being largely in interstitial positions and diffusing rapidly until it combines with a silicon vacancy. This work has generated much interest and experimentation, however, there is still a lack of agreement concerning the mechanisms and hence also absent is a comprehensive model to predict the boron redistribution

The rapid anneal experiments on boron suffer from the same problem of temperature measurement as discussed above and hence it is difficult to evaluate the published experimental data. In addition in the case of boron it is clear that the redistribution is intimately connected with the defect structure and the presence of other impurities. 11,12 In the following discussion some experimental data is presented pertinent to the transient enhanced diffusion of boron. Also data illustrating the use of RTP anneal to eliminate the substantial anomalous diffusion obtained during low temperature furnace anneals. Then

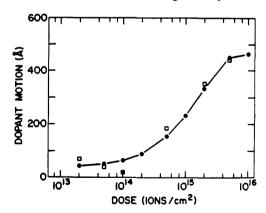


Fig. 4 Arsenic displacement at 0.1 times the peak concentration as a function of implant dose at 70 Kev. The RTP is 10 sec, at 1100°C. The solid points connected by the line are taken from the calculated profiles and the open squares are the experimental data from Ref. 8.



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a simple model that links the transient and anomalous diffusion effects to the same cause is described. Although the model is incomplete, it is able to fit much of the data.

Recently Sedgwick¹³ reported a temperature independent displacement of about 40 nm for 10 sec. anneals in the temperature range between 900 and 1150 °C but no significant motion at 800 °C. See Fig. 6. Note that the displacement is nearly constant at 50 nm between 900 and 1100 °C and is negligible at 800 °C.

The time dependence of the transient effect is investigated for boron implants of $2x10^{14}/\text{cm}^2$ The maximum boron concentration for these conditions is less than the boron solubility limit¹⁵ and less than a factor of 2 above the intrinsic concentration at 900°C and thus one expects nearly intrinsic diffusion. The SIMS profiles for 900, 950, and 1000°C are shown in Fig. 7. Since the intrinsic diffusion length at the highest temperature of 1000°C is only 4 nm there is clearly an anomalous diffusion. It is evident that the anomalous displacement is complete by 5 sec. at 1000°C and it requires nearly 60 sec. to saturate at 900°C. It is also apparent that the rate of the displacement diminishes with time. There is a similar variation observed in the sheet resistance, i.e., the boron activation is complete once the anomalous displacement is saturated.

The lack of a transient effect for short anneals at 800°C reported by Sedgwick¹³ has been confirmed by the author for a fluence as high as 1x10¹⁵/cm² Although at 800°C there is no significant displacement during RTP for times of the order of 10 sec., substantial anomalous diffusion at low temperatures for furnace anneals was reported many years ago by Hofker.¹⁶ Fig. 8 illustrates the magnitude of the effect at 800°C for a boron implants of 2x10¹⁴/cm² ¹⁴ The two curves represent the extremes of the sample to sample variation for ostensibly identical treatment. The displacement is much greater than that obtained with the RTP treatments at higher temperature and the electrical activation is still incomplete.

If the wafers are given an RTP treatment and subsequently a furnace anneal the amount of displacement obtained during the latter depends on the completeness of the activation during the RTP. Fig. 9 shows the results obtained for various 900°C RTP cycles followed by the furnace anneal of Fig. 8. The sample with the 30 sec. RTP exhibited an additional displacement of 80 nm during the furnace anneal while the sample with the 120 900°C RTP showed no additional motion. Since the difference in displacement obtained between the 30 and 120 sec. RTP is only 40nm, a net decrease in depth of 40 nm is obtained for the combined process. Similar reduced motion is obtained with RTP preanneal at 950 and 1000°C. Also no additional motion is obtained during the 800°C furnace cycle if the wafer is first given a 5 sec. 1000°C RTP as shown in Fig. 10.

One of the features of the above profiles, both for the short time lower temperature RTP cycles and the furnace anneals, is that there is greater displacement at lower concentration than near the peak and the as implanted profiles develop "wings". These, of course, are one of the main features that must be fit by a computational model.

There are two methods that have been thus far applied. One is due to Fair, 11 in which the diffusion coefficient has a spatial variation related to the concentration of point defects. In the region of high damage the the formation of extended defects acts as a sink and the diffusion is assumed to be normal. Outside of the region of high damage the diffusion coefficient is enhanced by the excess point defects which decay with a time constant of 4.4 sec. The magnitude of the enhancement is temperature sensitive with an activation energy of 2 ev.

Another approach, taken by Morehead, ¹⁷ assumes that only a fraction of the impurity is mobile. The mobile fraction diffuses with an enhanced diffusion coefficient due to a supersaturation of point defects created by the implant. The enhancement is also exponentially increased with temperature.



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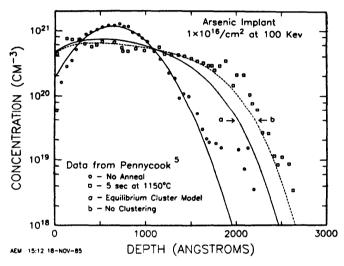


Fig. 5 Comparison of the calculated arsenic profile with and without the arsenic clustering effect included with the experimental data of Ref. 5.

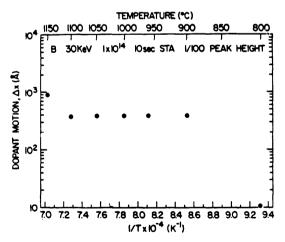


Fig. 6 Experimental measurements of the boron displacement for a 10 sec. RTP cycle as a function of reciprocal temperature illustrating the the nearly constant motion at high temperature and none at 800°C.



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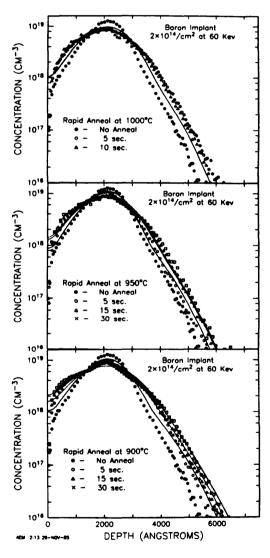


Fig. 7 SIMS profiles illustrating the time dependence of the transient displacement during RTP at a) 900°C, b) 950°C, and c) 1000°C. Lines are calculated profiles.



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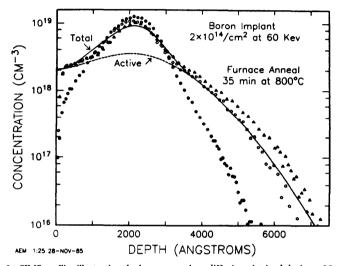


Fig. 8 SIMS profiles illustrating the large anomalous diffusion obtained during a 35 min., 800°C furnace anneal. Lines are calculated profiles.

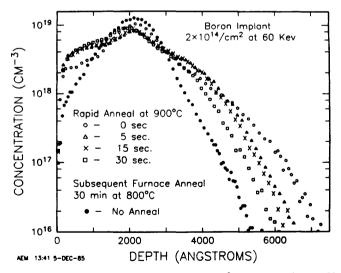


Fig. 9 SIMS profiles showing the effect of adding a 900°C RTP step prior to a 30 min., 800°C furnace anneal. The curves illustrate the increasing reduction in the displacement obtained by increased RTP pre-anneal time.