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Establishing the physical basis of advanced diffusion models

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The simulation of P and B diffusion under perturbed point defect conditions presents problems for standard process modeling programs. Well-known issues are the kink-tail and emitter-push effects that occur during high-concentration P diffusion, as well as similar effects in the case of B diffusion. Transient diffusion after ion implantation of P and B also shows complex behaviour associated with point defects. These troublesome issues have become especially important now that advanced technologies using highly-doped, very shallow junctions are becoming widespread.

Recently, Morehead and Lever proposed a specific mechanism which might account for the anomalous high-concentration diffusion effects. In their model [1], the impurity X (e.g. B, P, Au) is assumed to diffuse via an intermediate migrating species X_m of interstitial type. The formation reaction for such a species in its simplest form is just

$$X_s + I \rightleftharpoons X_m \qquad (1)$$

where X_s is the substitutional impurity and I is the silicon interstitial. Generation, diffusion and recombination of the migrating species relocates Si interstitials from under the peak of the impurity profile, to regions of low impurity concentration. Hence for a shallow doping profile, a diffusion enhancement occurs in the tail of the profile, due to the interstitial concentration enhancement. Morehead and Lever used a steady-state model in which the fluxes of the impurity and the point defects were balanced. More recently this model has been extended by Mulvaney [2], Crandle [3] and others, to include transient effects in which the migrating impurity species is considered explicitly. Such effects are relevant to diffusion after ion implantation [3].

The central assumption in such models is that B and P diffusion occurs via an intermediate migrating species. However, the validity of this assumption has never been proved. As a result the model has not gained universal acceptance. This paper presents the necessary evidence to resolve this central issue for the case of B. We are able to show *directly, for the first time* that B does diffuse via an intermediate species of interstitial type. Furthermore the reaction rate associated with equation (1), important for the transient diffusion problem, can be estimated.

We first discuss the statistics of diffusion via an intermediate species. For low impurity concentrations, the diffusion exhibits exponential behaviour at short times, in contrast with Fick's Law which predicts Gaussian profiles. This contrasting behaviour arises because the impurity migrates some distance in its intermediate form, before recombining to become substitutional again. The effect is not considered in the simplified model of Morehead and Lever, although it can be observed in numerical simulations using multi-stream models. An analytical formulation is possible in the case of low impurity concentrations. Exponential diffusion behaviour at short times is a tell-tale signature of an intermediate species. It can in principle be observed experimentally, provided that sufficiently narrow impurity profiles can be obtained. The clearest signature is expected at low temperatures, where the migration length is expected to be larger.

Fig. 1(a) compares the above model with experimental results on the diffusion of narrow 'δ-doping' profiles [4]. Symbols represent data for low-concentration B diffusion at 600°C in O_2 ambient, showing the signature of exponential diffusion. The solid line represents the excellent fit obtained with the model. The only free parameters are the migration length (10 nm) and the generation frequency for the migrating species ($1.26 \times 10^{-6} s^{-1}$ in this case). This frequency seems remarkably low at first sight. However it is in fact consistent with expectations based on the kickout rate by silicon interstitials at this temperature. In contrast, Fig. 1(b) shows the poor fit obtained with a Gaussian distribution.

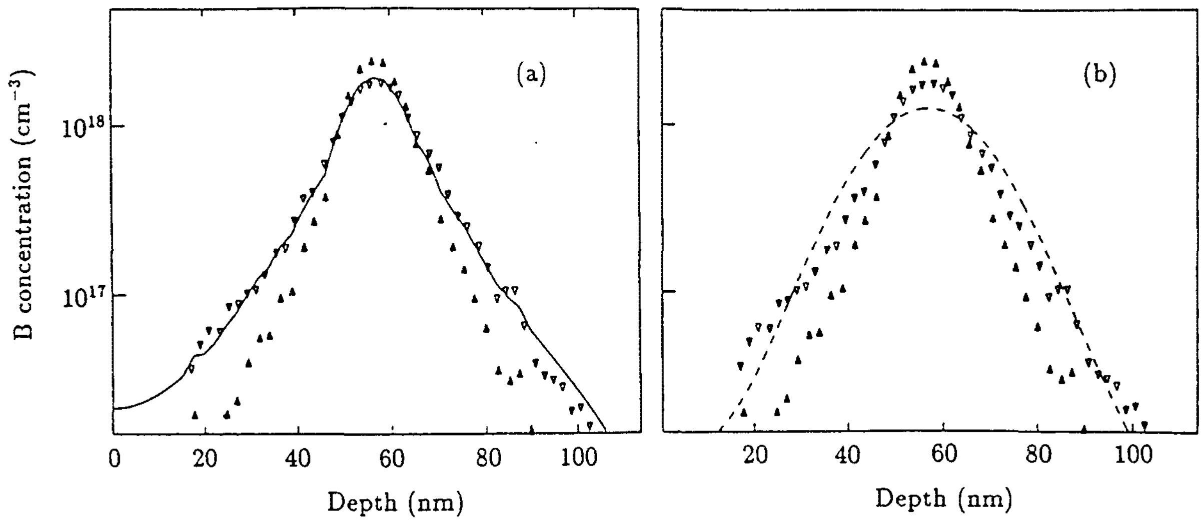

FIG. 1. Diffusion of a B δ-doping profile at 600°C in O_2 ambient. Solid symbols - as-grown profile; open symbols - diffused profile. (a) Present model - solid line; (b) Fick's Law - dashed line.

In summary, results on the statistics of B diffusion at low concentrations provide the first direct evidence of diffusion via an intermediate species. The physical effects proposed by Morehead and Lever for the case of high-concentration diffusion, are a direct consequence. With this knowledge, advanced models coupling the dopant and the point defects, can be applied with confidence to the case of B diffusion.

References

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