Appropriate Initial Damage Conditions for "Three-Stream" Point Defect Diffusion Models

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Abstract— **This paper describes progress made in modeling transient enhanced diffusion (TED) on the basis of "Three-Stream" point defect diffusion models. Such kind of models show artificially high transient diffusion at temperatures below approx. 800°C when standard initial damage conditions are used. Using appropriate conditions for the initial distribution of dopants, point defects and clusters, however, we were able to achieve surprisingly good results for TED experiments between 600°C and 1100°C and temperature ramp rates between 10°C/min (FA) and 100°C/sec (RTP) even with a "Three-Stream" diffusion model.**

I. Introduction

Accurate modeling of dopant diffusion and activation still is one of the key challenges in simulation of silicon front-end processes. Due to the extensive use of ion implantation in IC fabrication and the need to activate the implanted dopants by high temperature annealing, transient enhanced diffusion dominates the total redistribution of dopants. Moreover device dimensions of most advanced IC technologies become so small that even a few nanometers in junction location influence the device behavior. Under such extreme conditions physics-based simulation models and an accurate description of relevant process parameters are indispensable.

The most accurate models of today's standard simulation tools are those based on the coupled diffusion of dopants and point defects. We can distinguish between so called "Three Stream" and "Five Stream" models. "Three Stream" models are derived under the assumption that the reactions between point defects and pairs are in local equilibrium while "Five Stream" models include full dynamic pairing of dopants and point defects. Both kind of models not only predict high concentration and oxidation enhanced diffusion very accurately, in conjunction with appropriate clustering models they also can describe TED effects very well.

At low temperatures, however, the equilibrium approximation of point defects and pairs is not justified and we have shown earlier that "Three Stream" models totally fail to predict TED below 800°C [1].

In this paper we show how the application of "Three Stream" models can be extended down to 600°C without loosing accuracy compared to the more complex "Five Stream" models.

II. Influence of Interstitial Clusters

TED of interstitial diffusers such as phosphorus and boron strongly depends on the kinetics of interstitial cluster formation and dissolution [2], [4]. Recently, Cowern et al. [3] reported dramatic variations of interstitial cluster dissociation energies versus cluster size for clusters containing less than approximately 10 interstitials, while they reproduced the earlier extracted energies for larger clusters, also known as {311} defects. According to their work, the correct modeling of small clusters is essential to describe low temperature TED accurately.

We found that a simple extension to a first-order equation [4] and meaningful initial conditions are sufficient to give excellent results for TED over a wide range of annealing conditions. The interstitial cluster equation we use, is given in Eq. (1) [1],

$$\partial_t C_c = k_g C_c C_I + k_{g1} C_I^2 - k_r C_c \qquad (1)$$

where C_c is the concentration of interstitials in clusters and C_I the concentration of free interstitials. The second term in Eq. (1) is the correction of the originally published equation [5], dominating at the very end of the dissolution of clusters. Thus it accounts for the dissolution of small clusters into free interstitials when interstitial concentration approaches its local equilibrium value. As shown in Fig. 1 this equation is in good agreement to the experimental data of Poate [2].

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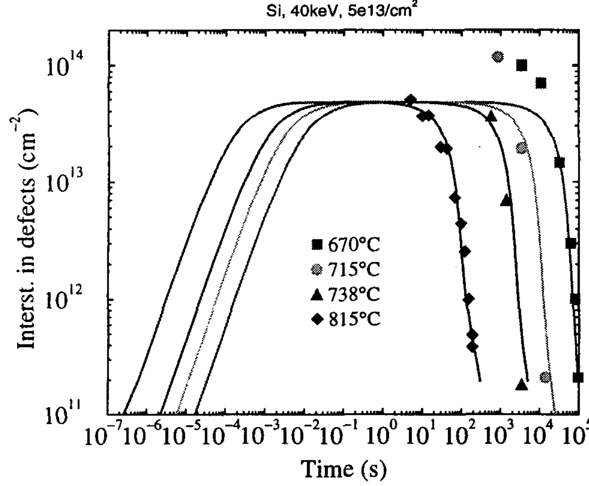

Fig. 1. Time evolution of interstitials in {311} defects. Experimental data (symbols) from Ref. [2], simulation results (solid lines) based on Eq. (1) and standard initial damage conditions.

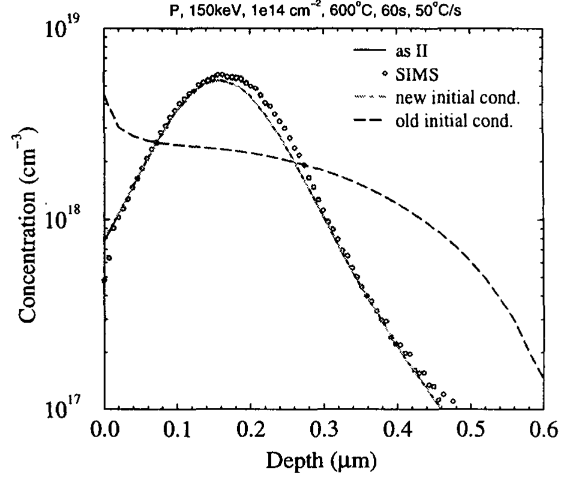

Fig. 2. Simulation results with standard (dashed line) and improved (dashed-dotted line, matches solid line) initial damage conditions compared to phosphorus SIMS profile after 60 seconds at 600°C RTP process.

III. Initial Conditions and Diffusion Models

Besides the model for interstitial clusters, the amount and configuration of crystal damage after ion implantation is a critical factor in modeling TED. In our simulations, the amount of damage is proportional to the implanted dopant concentration. This approximation is known as the "+n" model [6].

TABLE I

Generally used (TSUPREM4 default) and modified initial damage conditions

initial condition	default	new
dopant	substitutional	substitutional
interstitials (C_I)	$C_d - C^*_{pairs}$	$C_d - C^*_{pairs} - C^*_c$
vacancies (C_V)	C^*_V	C^*_V
I-clusters (C_c)	$\ll C^*_I$	C^*_c

As far as the damage configuration is concerned, we distinguish between generally used initial conditions [7], [8], labeled 'default' in TABLE I, and our new conditions.

Generally, the implantation damage is assumed to consist entirely of free interstitials C_I minus the equilibrium concentration of dopant interstitial pairs C^*_{pairs}.

When simulation starts with the default initial damage conditions, interstitial clusters need roughly 0.1 seconds at 670°C (and of course even longer at lower temperatures) to absorb the maximum concentration of interstitials (see Fig. 1). Since "Three-Stream" models start with the equilibrium concentration of dopant-point defect pairs, diffusion starts with extremely high concentrations of mobile pairs resulting in very fast diffusion even at low temperatures. The dashed line in Fig. 2 shows an example of a 60 seconds RTP anneal at 600°C, simulated with `pd.full` of TSUPREM4 [7] and default initial damage conditions.

Changing the initial conditions according to TABLE I, where besides pairs also clusters are assumed to be in local equilibrium, eliminates the artificially high diffusion at low temperatures. As also shown in Fig. 2, diffusion after 60 seconds at 600°C is completely suppressed, when the new initial conditions are used (dashed-dotted line lies on top of solid line). Under the auxiliary condition of an effective "+n" model ($C_I + C_c = nC_d$, where C_d is the implanted doping concentration), we can estimate the equilibrium concentration of interstitials bound in clusters as:

$$C^*_c = (2(1-r))^{-1}\left(C_r + (2-r)nC_d \right. \quad (2)$$
$$\left. -\sqrt{C_r^2 + 2(2-r)C_r nC_d + (rnC_d)^2}\right), \quad (3)$$

where $C_r := k_r/k_{g1}$ and $r := k_g/k_{g1}$. At low temperatures the concentration C^*_c is very close to nC_d so that

most of the damage is clustered from the very beginning of the diffusion process. The dissolution of clusters starting with the modified initial conditions is shown in Fig. 3 and it is worth noting that absolutely no parameter change is necessary when the initial conditions are changed.

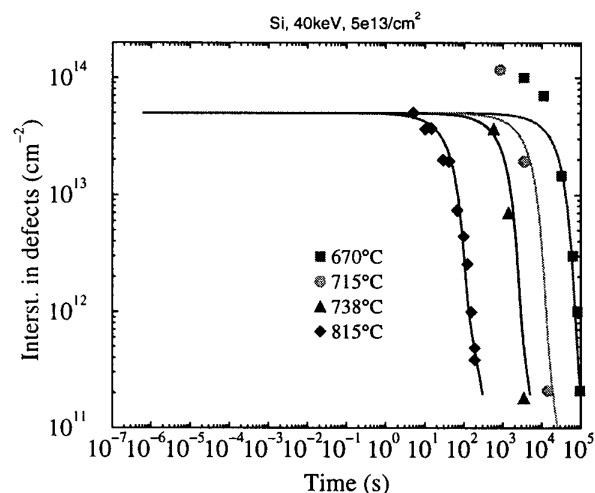

Fig. 3. Same as Fig. 1 but with modified initial damage conditions: {311} defects are assumed to be in local equilibrium with free interstitials at the beginning of the ramp up. Ramp up has been started at 500°C.

IV. Experimental Results and Discussion

Figs. 4-6 show simulation results with old (dashed lines) and new (dashed-dotted lines) initial conditions in comparison to experimental data. All simulations ramp up from 500°C. The lower the annealing temperature is, the larger is the difference between default and new initial conditions. But even at higher temperatures, where the difference in diffusion depth between both initial conditions is low, the new conditions give much better results near the surface. In Fig. 5, the surface profile is much better reproduced with our modified approach for a RTP anneal of 9 min at 800°C.

The good results indicate that interstitials indeed are clustered very rapidly during temperature ramp up and that the size distribution of clusters plays a minor role, at least as long as a significant amount of {311} defects is formed.

Of course, our very simple approach has its limits. For low implantation doses only small clusters are formed, since the damage concentration is too low to form the

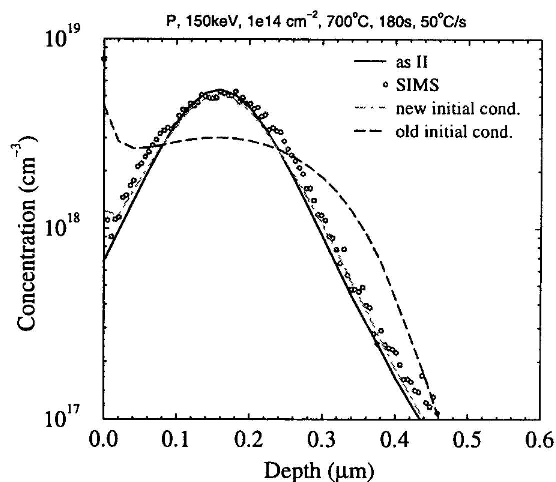

Fig. 4. Simulation results with standard (dashed line) and improved (dashed-dotted line) initial damage conditions compared to phosphorus SIMS profile after 180 seconds at 700°C RTP process.

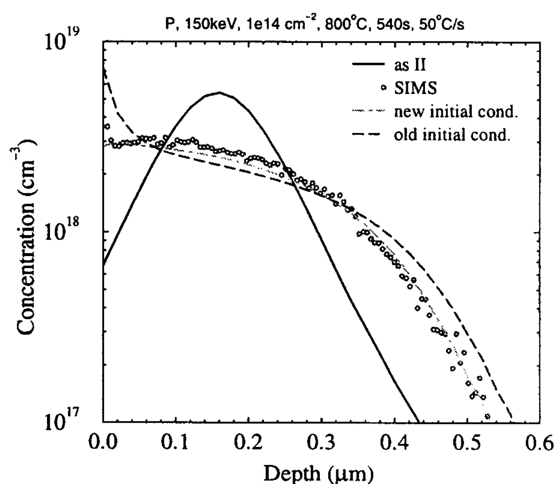

Fig. 5. Similar to Fig. 4 but after 540 seconds at 800°C RTP process. At temperatures above 800°C diffusion depth becomes less sensitive to the initial damage condition. However, surface pile up is largely overestimated with standard initial conditions.

larger {311} clusters. Under such conditions our method overestimates the duration of TED. Nevertheless, our initial conditions are much more reasonable than assuming dopant defect pairs in local equilibrium, while starting the diffusion simulation with an extremely high supersat-

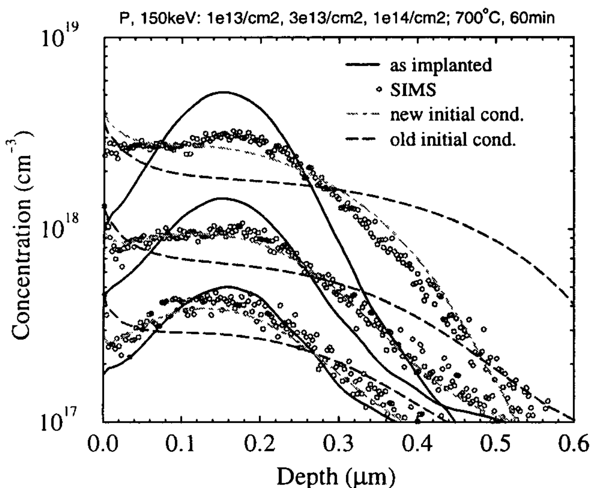

Fig. 6. Simulation results with standard (dashed line) and improved (dashed-dotted line) initial damage conditions compared to phosphorus SIMS profiles after 60 minutes at 700°C furnace annealing process.

uration of free interstitials. Therefore, even for low implantation doses, our initial conditions are better than the default conditions.

So far, we verified our initial damage conditions for phosphorus implantations only. In case of boron, the initial conditions become more complex because interstitial clusters compete with boron-interstitial clusters. If the binding energies of boron-interstitial clusters are known, the distribution between different types of clusters in equilibrium can be calculated and our method should be applicable for boron as well.

V. Summary

In conclusion, the combination of a "Three-Stream" diffusion model, an extended first-order interstitial cluster model and modified initial damage conditions, where clusters start at their equilibrium concentration, gives surprisingly good results for TED experiments. Unphysical diffusion at low temperatures is fully suppressed and the effect of temperature ramp rates on diffusion is well reproduced for furnace and rapid thermal processes.

Acknowledgments

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