Modeling of Initial Stages of Annealing for Amorphizing Arsenic Implants

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Abstract— **We have analyzed the initial stages of annealing for amorphizing arsenic implants. The comparison of TED simulations to experimental data shows results that appear inconsistent with the standard assumption of complete removal of point defects from the regrown amorphized layer. Our analysis suggests that high arsenic concentrations may stabilize retention of vacancies during solid phase epitaxial regrowth and thereby lead to the formation of a vacancy-rich layer near the surface within the regrown region. The presence of this vacancy rich layer is able to help account for both increased initial diffusion within the peak region for high temperature annealing and increased clustering in the peak region for lower temperatures.**

I. Introduction

Most modeling of Transient Enhanced Diffusion (TED) has focused on sub-amorphizing implants. However, to obtain low sheet resistance, high doses must be implanted, and the damage produced by heavy ions such as As leads to the formation of an amorphous layer. The modeling of amorphizing implants is challenging because of the lack of knowledge of the initial conditions after amorphous region regrowth. The standard approach for modeling of amorphizing implant is to assume complete removal of point defects within the amorphous layer during regrowth and "+1" [1] or net $I-V$ model for interstitials below amorphous/crystalline interface. Thus only interstitials remaining below the amorphous region enhance diffusion.

We focus our analysis on experiments by Kasnavi *et al.* [2], [3]. Both amorphizing and sub-amorphizing doses of As were implanted and the As profile was measured after various annealing times at 750 and 1050°C. We found that for amorphizing implants it was not possible to match the profile shapes at short times if the regrown region was assumed to be defect-free. While simulated profiles are very sensitive to the point defect distribution, the initial conditions for point defects after epitaxial regrowth are not well established. In this paper we suggest a correction to the frequently used method for modeling of amorphizing implants.

Ab-initio calculations [4], [5] have demonstrated that arsenic vacancy pairs and arsenic vacancy clusters are energetically more favorable than the isolated vacancies. This suggests that the high As concentration may stabilize the retention of nearby vacancies as the amorphous material regrows. We assume that after epitaxial regrowth excess vacancies remain near the surface within the limits of V-rich region, and that the vacancies are in the form of AsV pairs with concentration proportional to the arsenic concentration. The presence of this vacancy-rich region enhances diffusion at high temperature and arsenic-vacancy clustering at low temperature, leading in both cases to improved matches to experimental observations.

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II. Modeling and Simulation

A. Experimental Overview

We analyze arsenic dose loss experiments by Kasnavi *et al.* [2], [3] aimed at characterizing As dose loss kinetics. As was implanted at 32 keV through a 100Å thermally grown screen oxide and annealed at two different temperatures, 750°C and 1050°C. Implants were for two doses: 1×10^{15} cm^{-2} which is an amorphizing dose and 2×10^{13} cm^{-2} which is below the amorphization threshold. We concentrate our efforts on modeling of short time behavior, since we are interested in obtaining information on initial conditions of point defects distribution immediately following amorphous region regrowth.

B. Modeling Approach

To simulate these experiments, we use a five stream diffusion model including rapid diffusion via vacancies at high doping levels [6]. For arsenic diffusivity we use parameters from Wittel [7]. Bulk point defects diffusivity/equilibrium concentration products (e.g., $D_I C_I^*$) are from metal diffusion [8], [9], [10] with diffusivities taken from MD calculations [11], [12]. Simulations include ramp-ups with a rate of 100°C/sec. Predicting dose loss involves not only having a good model for the interface, but having the right amount of dose arriving at the interface as the anneal progress. At short times, we find dose loss is limited by the rate at which dopants arrive at the interface and not by interface processes, so we assume diffusion-limited segregation of As at the interface. The amount of TED is controlled by the dose and distribution of point defects, thus initial conditions for post implant anneal will have a large impact on dose loss dynamics.

Arsenic vacancy clusters have been included to account for immobilization of As during low temperature anneal. *Ab-*

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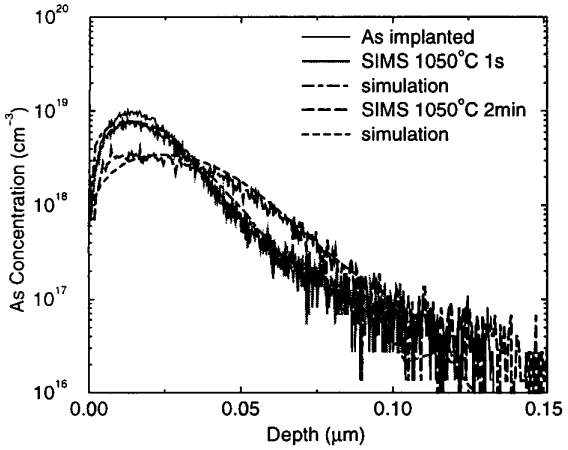

Fig. 1. Simulation of 2×10^{13} cm^{-2} 32 keV arsenic implant (non amorphizing) annealed at 1050°C for 1 s and 2 min compared to the data from Kasnavi. "+1" model for interstitial works well.

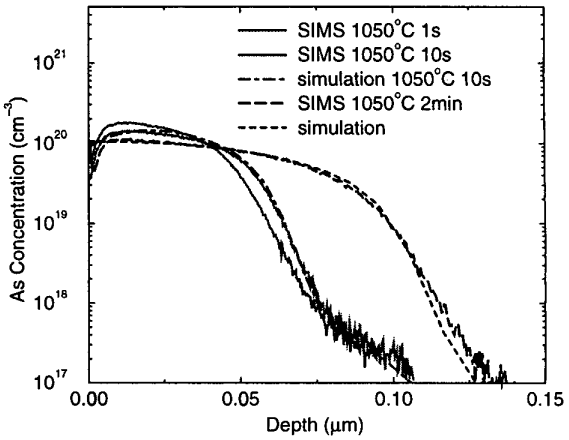

Fig. 2. Simulation of 1×10^{15} cm^{-2} 32 keV arsenic implant annealed at 1050°C for 10s and 2 min compared to the data from Kasnavi. As the starting conditions for simulator, SIMS profile for 1 s anneal has been used. TED is over in first 1 s at 1050°C

initio calculations [5] suggested that As_4V cluster is the most energetically favorable configuration. We assumed diffusion limited accumulation of arsenic into As_4V via As_2V and As_3V. Formation energies of the clusters were calibrated to fit electrical activation data [13], [14].

Fig. 1 shows a comparison of our simulation for non-amorphizing implants to annealing results from Kasnavi *et al.* [2]. "+1" model for interstitials was used. Simulation match experimental results quite well for short times as well as at longer times. Fig. 2 shows simulation of long time anneal of amorphizing arsenic implant. For initial conditions the SIMS profile at 1 s has been used. TED is over in first 1 s of anneal.

Figs. 3 and 4 show a comparison of simulations to short-time annealing results from Kasnavi *et al.* [2], [3]. As can be seen, the simulations do not match the SIMS measurements. At 1050°C (Fig. 3), the widely accepted modeling assumption (no point defects after epitaxial regrowth) shows insufficient diffusion in the peak region and/or excessive diffusion in the tail region. The depth of amorphous/crystalline interface is sensitive to implant conditions, and varying the assumed amorphous/crystalline interface positions makes it possible to match either the peak or the tail of the SIMS profile, but not both.

At 750°C (Fig. 4), the deviation is more subtle, but the SIMS data show a noticeable shift of the peak towards the surface along with narrowing, while the simulation predicts just a broadening. We find that the clustering process in the peak is limited by the availability of vacancies and a good match can be found if the vacancy diffusivity is increased by several orders of magnitude. We attribute the difficulty with fitting the amorphizing implant data to lack of knowledge regarding initial conditions for point defect in epitaxially regrown regions. Longer time simulations which are less sensitive to the initial conditions fit the experimental data quite well.

C. Point Defect Distribution

In order to estimate damage distributions after ion implantation we run TRIM simulation for As implantation into Si. The resulting point defect distribution for a 32 keV 10^{15}cm^{-2} implant are plotted in Fig. 5. The vertical line shows the approximate location of the amorphous/crystalline interface. The vacancy rich region formed near the surface (down to 100Å) is inside the amorphous layer.

We assume that after epitaxial regrowth excess vacancies remain within the limits of V-rich region. The vacancies are assumed to be in the form of AsV pairs with a concentration linearly proportional to the As concentration. This proportionality constant is one of the fitting parameters of our simulations, with an extracted value of 0.4. The other parameter is critical damage level for amorphization (10% was used), which determines the depth of the amorphous crystalline interface. In both cases, the same values are used for both the 750 and 1050°C simulations. As can be seen in Figs. 6 and 7, including excess vacancies in this manner makes it possible to account for observed behavior at both high and low T. In conjunction with high concentration diffusion effects [6], the initial vacancy excess increases diffusion and dose loss in the peak region at 1050°C, while reducing tail diffusion as the interstitial excess is annihilated more rapidly. At 750°C, As clusters are able to form readily due to the initial vacancies present. Clustering is most favored near the surface V-rich region, while interstitials from the EOR damage dissolve the right side of the clustered peak. Thus the profile both sharp-

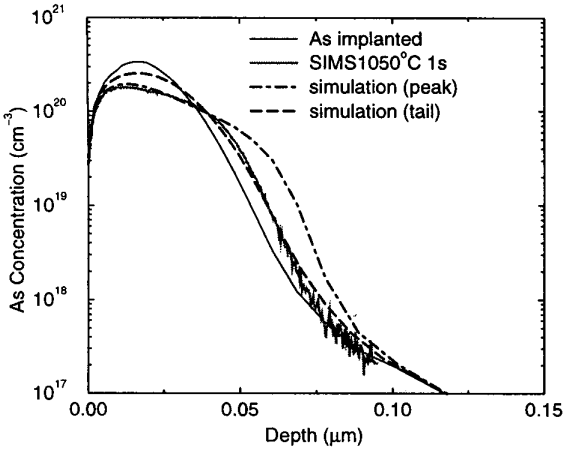

Fig. 3. Simulation of 1×10^{15} cm^{-2} 32 keV arsenic implant annealed at 1050°C for 1 s compared to the data from Kasnavi. "+1" model for interstitial and complete removal of point defects within the amorphous layer during regrowth is assumed. Two simulations, corresponding to different position of amorphous crystalline interface, match either peak or tail of As profile, but not both.

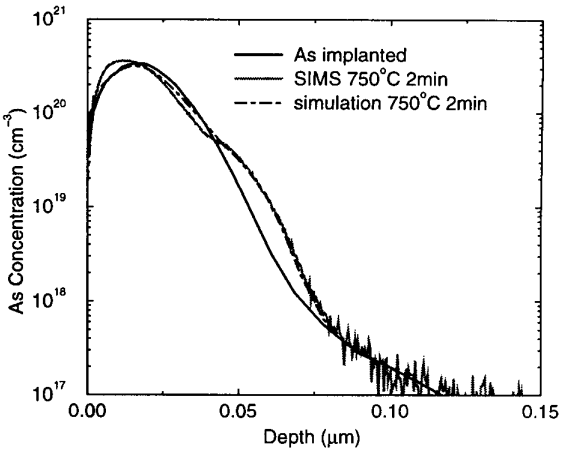

Fig. 4. Simulation of 1×10^{15} cm^{-2} 32 keV arsenic implant annealed at 750°C for 2 minutes compared to the data from Kasnavi. "+1" model for interstitial and complete removal of point defects within the amorphous layer during regrowth is assumed. The simulation shows significantly less clustering at the peak than indicated by the experimental profile.

ens and shift towards the surface.

III. Conclusion

The comparison of simulation of amorphizing arsenic implant annealing to experimental data shows that results are inconsistent with "+1" model and assumption of complete removal of point defects from amorphous layer. Our analysis suggests that high arsenic concentrations may stabilize retention of vacancies during solid phase epitaxial regrowth. Thus high concentrations of arsenic lead to the retention of a V-rich layer near the surface within the regrown region. This vacancy-rich layer enhances peak diffusion at high temperatures and increases clustering at low temperatures, allowing simulations to match experimental results in both cases.

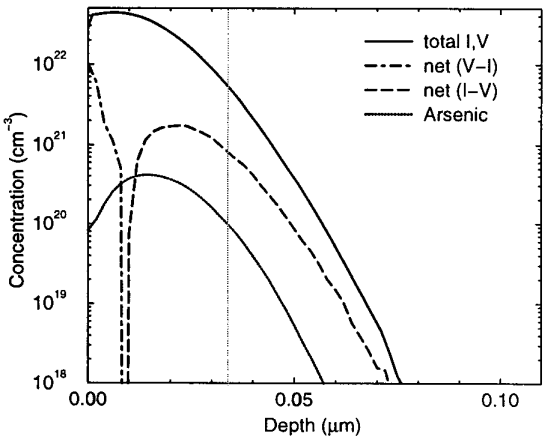

Fig. 5. TRIM simulation of 32 keV 10^{15} cm^{-2} As implant into silicon. Vertical line shows approximate location of amorphous crystalline interface. Note V-rich region near the surface is inside amorphous layer.

Acknowledgments

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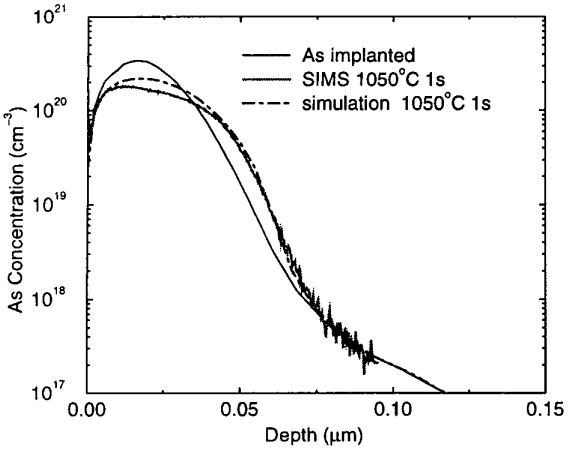

Fig. 6. Simulation of 1×10^{15} cm^{-2} 32 keV arsenic implant annealed at 1050°C compared to the data from Kasnavi. For simulation, vacancy excess is assumed to remain near the surface after epitaxial regrowth.

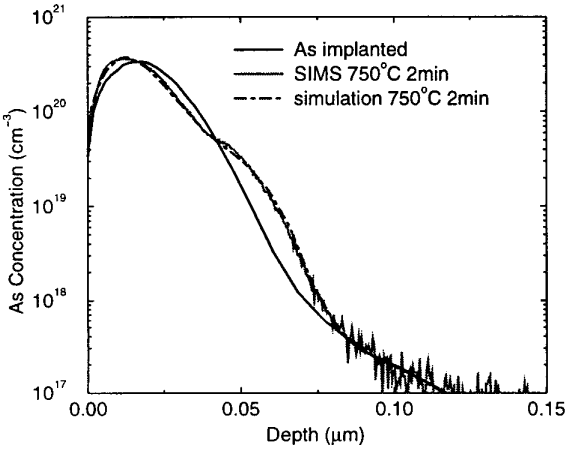

Fig. 7. Simulation of 1×10^{15} cm^{-2} 32 keV arsenic implant annealed at 750°C compared to the data from Kasnavi. For simulation, vacancy excess is assumed to remain near the surface after epitaxial regrowth.

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