Invited

Dopant Diffusion in Si and SiO₂ During Rapid Thermal Annealing

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1. Introduction

A significant number of papers have been published over the past 15 years which have characterized dopant diffusion in ion implanted Si during rapid thermal annealing (RTA). Fair et al [1] first showed a definite relationship between the annealing of ion implant damage and the transient-enhanced diffusion (TED) of arsenic and boron. Since that time the vast majority of research in TED has been based upon one-dimensional dopant profile measurements. Significant success has been demonstrated recently in accounting for the TED of low-dose B implants as a result of the annealing of {113} defects [2]. However, TED of B in Si at high doses is complicated by the production of extended defects, including projected range defects at very high dose. Amorphizing implants produce the added complications of rapid dopant activation during solid-phase regrowth of the amorphous layer and the evolution of end-of-range dislocation loops which act as generation and recombination centers for excess point defects.

Rather than try to review and summarize all of the data and models on one-dimensional TED of ion-implanted B, P, and As in Si during RTA, this paper will address three important aspects of RTA that are technologically important, but have been largely ignored: 1) TED of implanted B and As in 2D; 2) optical radiation effects on implanted B and As activation in Si; and 3) TED of B in ultrathin gate oxides.

2. TED in 2D

The relationship between lateral and vertical impurity diffusion distances in silicon is mathematically well established for profiles that have been diffused at high temperatures for a long time. And this relationship is experimentally verified. However, for small thermal budget RTA diffusions of ion implanted dopants, there is a significant discrepancy between experiment and simulation regarding the lateral-to-vertical diffusion depths for (D₁)₁/² < 1x10⁻⁶ cm for B, P, and As. We have compared available Monte Carlo models and analytical models contained in process simulators with measurements from over 60 shallow 2D dopant profiles obtained by cross-section TEM. The simulation of 2D implantation profiles as well as 2D dopant diffusion compares rather poorly with experimental data in the low thermal budget regime.

For example, results for B are shown in Fig. 1 (3). Boron was implanted at 1x10¹⁵ B/cm², 10 keV at a 0⁰ tilt angle into an MOS transistor structure with a 40 nm oxide sidewall spacer. A 550 °C, 30 min anneal was followed by a 10 sec, 1050 °C anneal in nitrogen. In Fig. 1, digitized 2D profile data from the TEM micrograph are shown overlaid onto TSUPREM4 simulations. The Pearson IV implant model was used as well as default annealing models. While the vertical depth data and simulations agree in the region away from the sidewall spacer edge, the simulations underestimate the lateral extent of the B penetration under the sidewall/gate region. Results using UT Marlowe also compared poorly with 2D data.

![Digitized data from a TEM micrograph (Ref. 3) are shown overlaid onto TSUPREM4 simulations. Boron was implanted at 1x10¹⁵ B/cm², 10 keV at a 0⁰ tilt angle into an MOS transistor structure with a 40 nm oxide sidewall spacer. A 550 °C, 30 min anneal was followed by a 10 sec, 1050 °C anneal in nitrogen. The Pearson IV implant model was used as well as default annealing models. While the vertical depth data and simulations agree in the region away from the sidewall spacer edge, the simulations underestimate the lateral extent of the B penetration.](image-url)

There appear to be two significant issues with the simulation models for As and B: 1) getting the as-implanted 2D profile right, and 2) accounting for lateral TED diffusion, especially in the low-concentration range, during short anneals. A comparison between 2D ion implantation and diffusion models has been made for several low-thermal-budget annealing cases. Truly useful 2D process simulations require high accuracy of 10 nm in the location of lateral diffusion contours. However, none of the simulation cases we studied gave anything near this accuracy over multiple concentration contours, especially in the low concentration ranges where such accuracy is most critical. We find that diffusion during RTA is not isotropic, due in part to the surface boundary condition on point-defect recombination.
3. Optical Radiation Effects on Dopant Activation

We compared TED and electrical activation of ion implanted B and As wafers annealed in either an HTE-Eaton RTP vertical furnace or an AST 2800 RTP system using the same time-temperature cycles on both systems (matched ramp-up, ramp-down and soak). We find that W-halogen radiation enhances As activation and deactivation rate coefficients as shown in Fig. 2. We model the effect on the basis of non-equilibrium recombination-enhanced phonon kick effect (thermal spike) localized at the As-V defect.

![Fig. 2 Observation of optically enhanced As deactivation rates at temperatures below 850 °C.](image)

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![Fig. 3 Comparison between B activation after 800 °C, 5 min RTA and furnace anneals for high dose B implants at 30 keV.](image)

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We also show that optical absorption effects have a significant effect on B electrical activation at 800 °C, but little effect on B TED. Fig. 3 shows a comparison between 800 °C, 5 min furnace and RTA anneals of high dose B implants. Optical effects apparently enhance the supply of vacancies in the near surface region to overcome local limitations on V and I concentrations, especially where projected range dislocations exist.

4. B TED in SiO₂ During RTA

We have recently developed diffusion-defect-based models that characterize B furnace diffusion in gate oxides as a function of F and H content as well as oxide thickness [4]. However, enhanced diffusion effects of B in oxides during RTA have been observed, as shown in Fig. 4. Zhang [5] reported substantial B penetration during 1050 and 1100 °C, 10 sec RTA, whereas the furnace models only predict < 20 Å diffusion lengths. These results are either due to higher than anticipated temperatures during RTA, or a non-equilibrium concentration of peroxy linkage defects produced within the oxide bounded by polycrystalline silicon and the single-crystal substrate. We have explored several models to explain the latter effect.

![Fig. 4 Calculated vs measured B penetration lengths in oxides. B penetration through oxides: nitrided oxide (●) and SiO₂ (▲); no penetration: nitrided oxide (○) and SiO₂ (△). RTA anneals result in anomalous penetration.](image)

Fig. 4. Calculated vs measured B penetration lengths in oxides. B penetration through oxides: nitrided oxide (●) and SiO₂ (▲); no penetration: nitrided oxide (○) and SiO₂ (△). RTA anneals result in anomalous penetration.

5. Conclusions

While much effort has been expended worldwide on modeling and characterizing 1D diffusion effects during RTA, 2D effects have been given only slight attention. And 2D diffusion is most critical in controlling subthreshold conduction in short-channel MOSFETs as well as in eff. We have also observed optically enhanced activation of B and As during RTA. The use of RTA during source/drain annealing of p⁺ gate MOSFETs also aggravates B penetration through gate oxides.

References