UCRL-JC-132379
PREPRINT

The Effect of Ramp Rate and Annealing Temperature on Boron Transient Diffusion in Implanted Silicon: Kinetic Monte Carlo Simulations

M.J. Caturla
M. Foad
T. Diaz de la Rubia

This paper was prepared for submittal to the
Ion Implantation Conference
Kyoto, Japan
June 21-24, 1998

June 17, 1998

Lawrence Livermore National Laboratory

The effect of ramp rate and annealing temperature on Boron transient Diffusion in Implanted Silicon: kinetic Monte Carlo simulations

M.J. Caturla[1], M. Foad[2] and T. Diaz de la Rubia[1]

1. Lawrence Livermore National Laboratory, Livermore CA 94550
2. Applied Materials, Santa Clara, CA 95050

Abstract- We present results of recent kinetic Monte Carlo simulations of the effect of annealing time and ramp rate on boron transient enhanced diffusion (BTED) in low energy ion implanted silicon. The simulations use a database of defect and dopant energetics derived from first principle calculations. We discuss the complete atomistic details of defect and dopant clustering during the anneals, and the dependence of boron TED on ramp rate. The simulations proviede a complete time history of the evolution of the active boron fraction during the anneal for a wide variety of conditions. We also studied the lateral spreading of the boron during the annealing for two different conditions, furnace anneal and ramp anneal.

I. Introduction

As the device size shrinks it becomes more and more important to understand and quantify phenomena such as transient enhanced diffusion of dopants such as boron. Models that predict the behavior of boron during different annealing conditions are necessary to reduce the cost in the development of future devices. For these models to be predictive they must include all the physical phenomena underlying the macroscopic effect of enhanced Boron diffusivity. In particular, ultra shallow profiles [1] present many challenges for the construction of predictive models. Several issues must be investigated in order to understand all the processes occuring during the implantation and annealing of these very low energy implanted dopants, such as the interaction of the dopants with the surface. Moreover, in order to reduce the thermal budget for the production of such devices, new high temperature processes are being used [2]. These anneals consist, mostly, on the rapid increase of the temperature, with ramp rates from 75 C per second, to as fast as 150 C/s, to temperatures as high as 1050 C. This differs from the conventional furnace anneal during several minutes at medium temperatures, 800 C . In this paper we present a first approach to the understanding of the ramp rate on the activation of boron atoms. We use kinetic Monte Carlo simulations, following the approach by Heinisch to study radiation damage problems in metals [3]. This kinetic Monte Carlo simulation, uses as input parameters the migration energies of vacancies, interstitials and boron atoms, the binding energies of clusters of defects, both vacancies and interstitials and mixed clusters, such as those formed by boron atoms and silicon self-interstitials. The values for these energies have been extracted from a variety of simulations. The energetics for boron migration and for the binding energies of B-I clusters calculated by Zhu [4, 5] have been used in this simulation. The diffusivities and binding energies of small clusters used in the model were calculated by G. Gilmer [6] using molecular dynamics simulations with the Stillinger-Weber interatomic potential. The different energies for migration and binding set the rate for migration and dissociation of defects and clusters. Jump distances are set to first nearest neighbors. For more details on the simulation model see ref. [7, 8]. We simulate the implantation of 1 keV Boron to a dose of 10^{14} ions/cm^2 into silicon using this model. The damage produced by the energetic particles were obtained using a binary collision model, UT-Marlowe [9], proved to give accurate distribution profiles for energies as low as 1 keV in the case of boron. Individual ions are included in the simulation box at a rate given by the dose rate, in this case 10^{12} ions/cm^2/s.

Following the inplantation we have studied the evolution of the boron for different annealing conditions, the conventional furnace anneal at 800 C for 30 minutes, and ramp anneals to a final temperature of 1050 C, with different ramp rates.

II Results

After the final dose has been reached most of the Boron is forming cluster of the type BI (one boron and one silicon self-interstitial) or BI2 (one boron and two self-interstitials). Vacancies are forming small clusters (size 2 or 3) and interstitials are mostly single. Only 25% of the total implanted dose is active after the implantation. Fig 1 shows the evolution of the boron clusters for the annealing of the sample up to a temperature of 1050 C, with a temperature increase of 150 C every second. On the right axis we present the concentration of boron in clusters as a function of time. As we mentioned earlier, after implantation most of the boron clusters are of the type BI and BI2. As the temperature increases bigger boron clusters grow, such as B3I. In the right axis of fig 1 we show the percentage of boron active during the annealing (solid line).

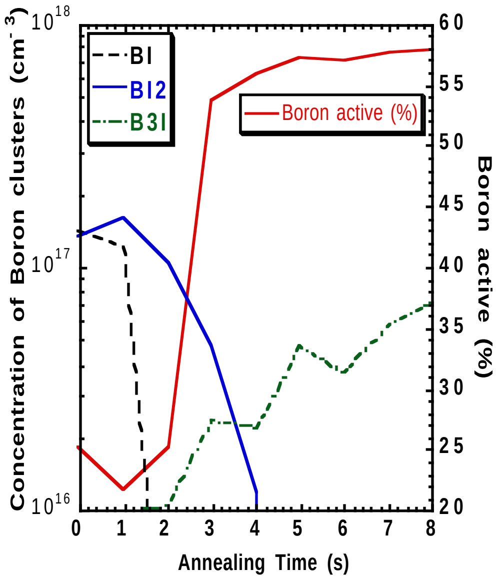

Fig 1. Evolution of the boron clusters during annealing from 27 C to 1050 C with temperature increase of 150 C every second. The left axis shows the concentration of different boron clusters, BI, BI2 and B3I. The right axis shows the percentage of Boron active in the sample during annealing.

After the implantation only ~25% of the total implanted dose is active. After 2 seconds the amount of boron active increases rapidly until it reaches maximum value of 58% of the total implanted dose. We should point out that ~30% of the implanted boron atoms accumulate at the surface. The interaction of the dopants with the surfaces needs to be investigated in more detail.

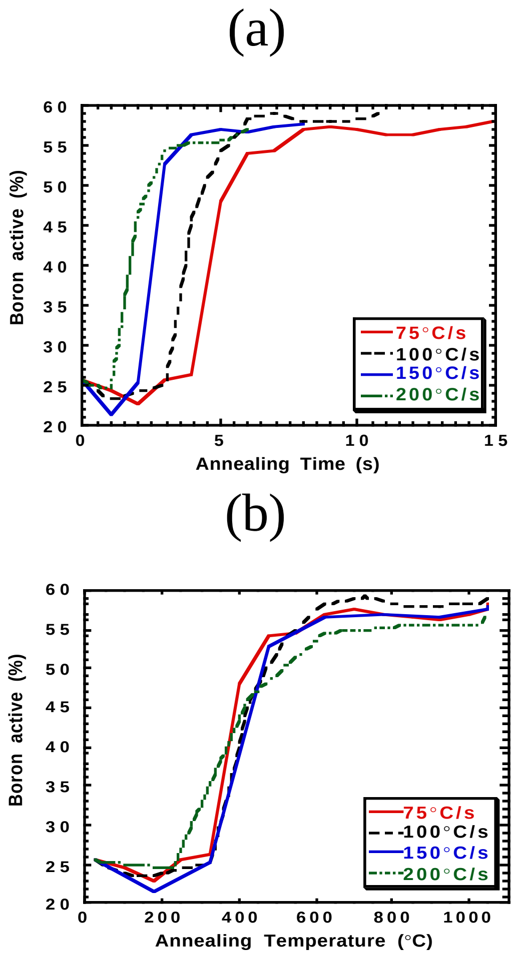

Fig 2. Percentage of boron active during annealing from 27 C to 1050 C of a 1 keV B profile, 10^{14} ions/cm^2 and for different ramp rates as a function of (a) annealing time and (b) annealing temperature.

We have done simulations for different ramp rates and the same final temperature, 1050 C. Ramp rates between 75 C/s and 200 C/s were considered in these simulations. In fig 2(a) we show the result values of the percentage of boron active during annealing for these ramp rates as a function of annealing time. Observe that, as expected, the maximum activation is observed at earlier times as the ramp rate increases. Fig 2(b) shows the percentage of active boron for the different ramp rates as a function of annealing temperature. Observe that for all cases the activation of boron occurs in a narrow temperature gap, between 350 C and 600 C, independently of the different ramp rates. We can not extract any conclusions about the different total activations at the end of the anneal, since the differences observed are in the error of the calculation. As for the final boron concentration profile, no significant differences were observed in the simulations for all the different ramp rates studied.

We have simulated the furnace anneal of the 1keV B profile for a temperature of 800C and a total time of 60 minutes. Fig 3 shows the concentration of the boron as a function of depth for the as-implanted profile, furnace anneal and anneal at a ramp of 150C/s up to 1050 C. The larger broadening is observed for the case of furnace anneal. For a concentration of 1017 cm-3, the profile broadens to a depth of 110nm for the case of furnace anneal while only to 80nm for the case of a ramp anneal. We also studied the lateral spreading of the implanted profile. For the case of furnace anneal 2.3% of the implanted boron diffused under the gate while only 0.9% of the implanted boron diffused in the ramp case.

We can conclude that ramp anneals provide of a larger activation of the boron than in the case of furnace anneals, with smaller boron enhanced diffusion. More simulations are on the way in order to study the effect of the ramp anneal on the final amount of boron active.

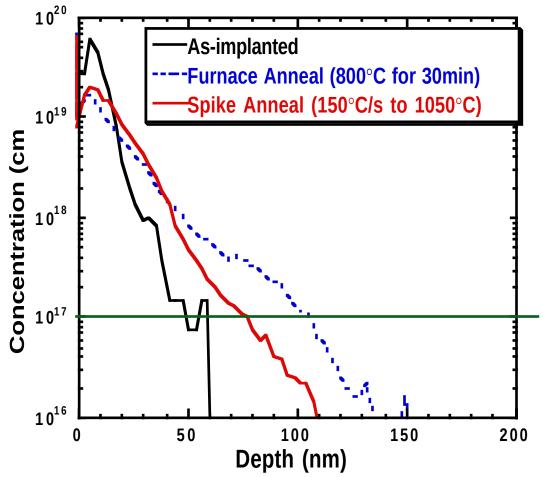

Fig 3. Boron concentration as a function of depth for as-implanted, 1 keV B, 10^{14} ions/cm^2, furnace anneal at 800C for 30 minutes, and a ramp anneal to a temperature of 1050 C, with temperature increase of 150 C per second.

References

[1] M. Foad, J. England, S. Moffatt, D. Armour, Ion Implantation Tech. Austin, Tx, June 96

[2] P. Singer, Semicond. Internat. June 96, 72-80

[3] H. L. Heinisch, Nucl. Instrum. and Methods, **B102**, 47 (1995)

[4] J. Zhu, T. Diaz de la Rubia, C. Maihot, Phys. Rev. **B54**, 4741 (1996)

[5] J. Zhu, Mater. Res. Soc. Symp. Proc. **469**. 151 (1997)

[6] G. Gilmer, T. Diaz de la Rubia, M. Jaraiz, Nucl. Instrum. and Methods **B102**, 257 (1995)

[7] M. D. Johnson., M. J. Caturla, T. Diaz de la Rubia., J. Appl. Phys. (in press)

[8] M. J. Caturla, M. D. Johnson, T. Diaz de la Rubia, Appl. Phys. Lett. (in press)

[9]. S. Tian, S. J. Morris, B. Obradovic, M. F. Morris, G. Wang, G. Balamurugan., A. F. Tasch, C. Snell, U.T, Marl;owe, Version 4.0 (1996)

Acknowledgment

This work was performed in part under the auspices of the US Department of Energy by Lawrence Livermore National Laboratory under contract W-7405-Eng-48