Laboratory Report
Department of Microelectronics & VLSI Technology
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Main Campus: Haringhata, Nadia, PIN:741249

LAB REPORT

DOPANT DIFFUSION (TCAD)

Work objectives

The objective of this laboratory work is to use *Athena* semicon-ductor process simulator to study the *thermal dopant diffusion* in the Si wafer.

Amit Sarkar

Date:20-06-2021 **Signature of the Student**

Signature of the Lab Instructor

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Date	Topic discussed	Remarks	Signature of supervisor
20/06/2021	EXPERIMENT 1.		
20/06/2021	EXPERIMENT 2		
20/06/2021	EXPERIMENT 3		
20/06/2021	EXPERIMENT4		

EXPERIMENT 1: This experiment is of implantation and annealing. Boron is implanted and the profile diffused. For this anneal of a medium dose implant in an inert ambient the default fermi diffusion model is used. Tempreture is varied from 800 to 1200 C , Energy is varied from 50Kev to200Kev and time is varied from 50 to 300 seconds , dose is varied from 1e12 to 1e15.

SOFTWARE USED: Silvaco S.EDA tools

THEORY:

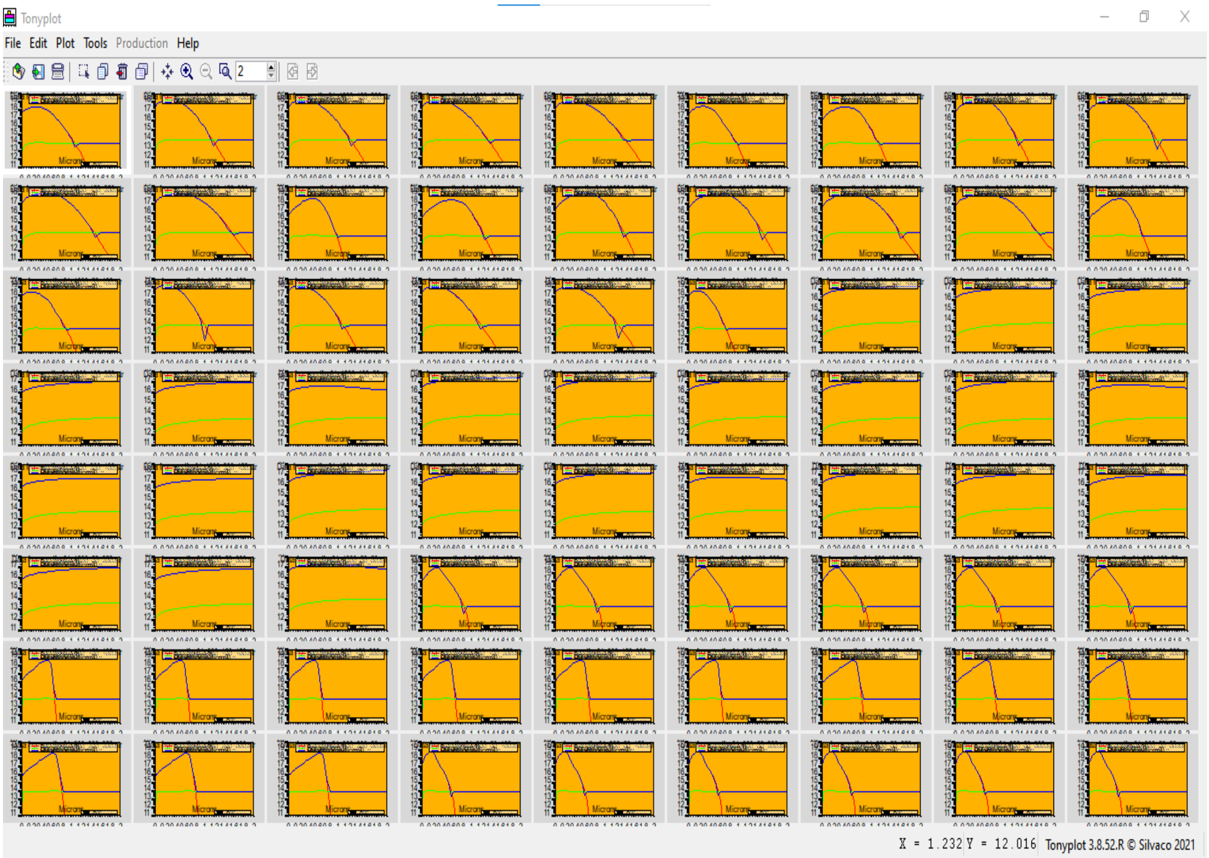
The Fermi Model

The Fermi Model assumes that point defect populations are in thermodynamical equilibrium and thus need no direct representation. All effects of the point defects on dopant diffusion are built into the pair diffusivities. The main advantage for using the Fermi Diffusion model is it will greatly improve the simulation speed, since it does not directly represent point defects and only needs to simulate the diffusion of dopants. Also, the Fermi Model usually results in an easier numerical problem due to the avoidance of “numerical stiffness”. But since point defects are not directly simulated, the Fermi model cannot deal with certain process conditions in which the defect populations are not in equilibrium, such as in wet oxidation (where Oxidation Enhanced Diffusion (OED) is important), emitter-base diffusions and wherever implantation results in an initial high level of implant damage.

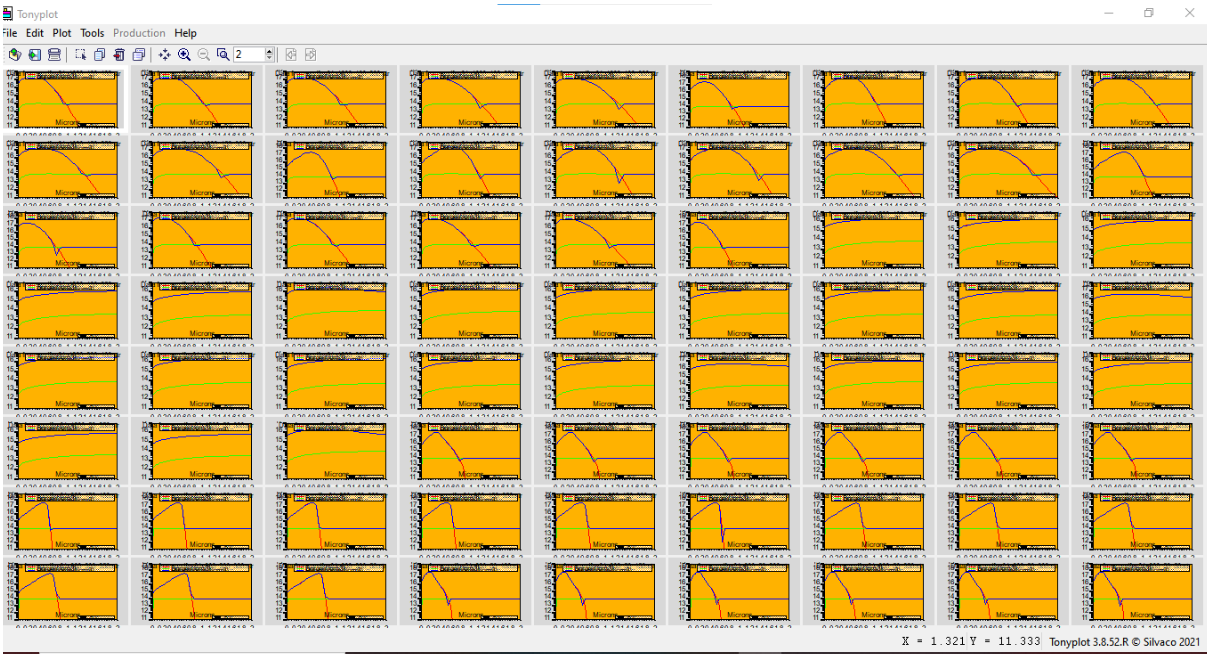
To use the Fermi Model, specify FERMI parameter in the METHOD statement.

OBSERVATION:

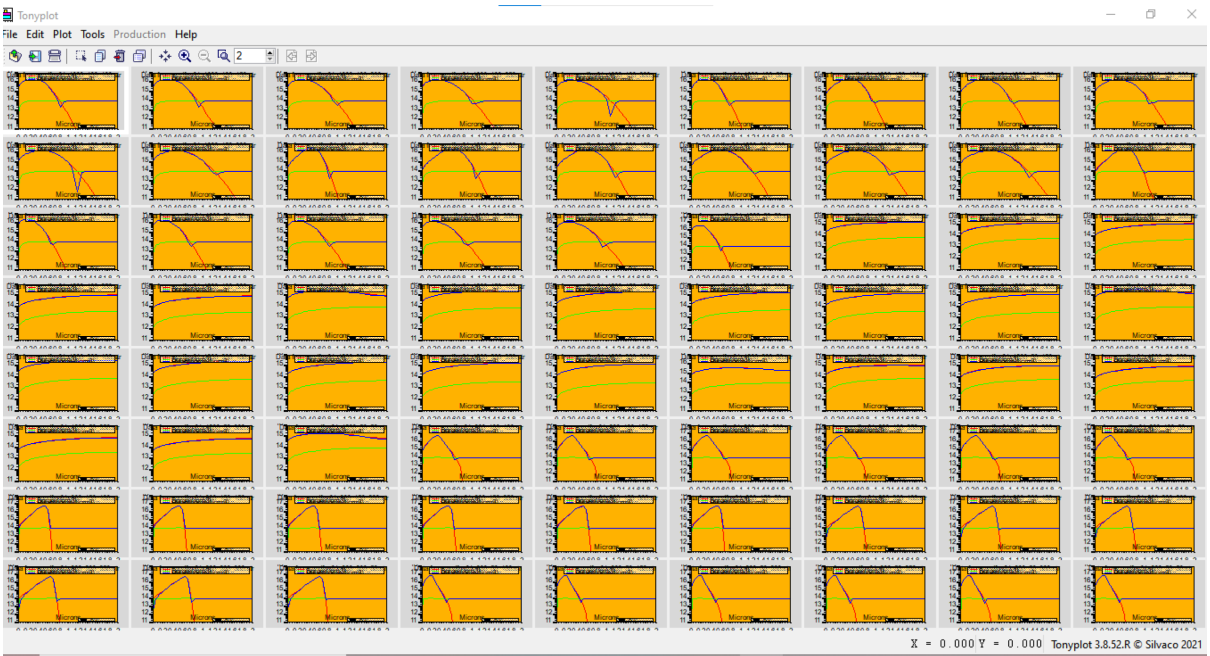
Dose-1e14, Tempreture is varied from 800 to 1200 C , Energy is varied from 50Kev to200Kev and time is varied from 50 to 300 seconds



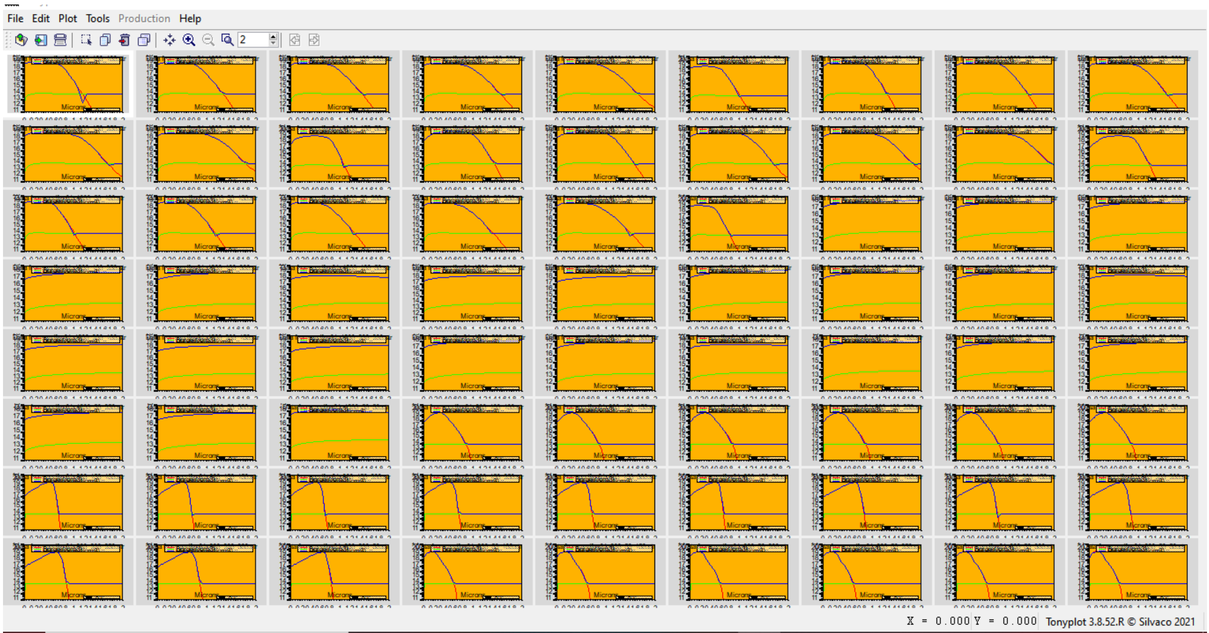
Dose-1e13 ,Tempreture is varied from 800 to 1200 C , Energy is varied from 50Kev to200Kev and time is varied from 50 to 300 seconds



Dose-1e12, Tempreture is varied from 800 to 1200 C , Energy is varied from 50Kev to200Kev and time is varied from 50 to 300 seconds



Dose-1e15 Tempreture is varied from 800 to 1200 C , Energy is varied from 50Kev to200Kev and time is varied from 50 to 300 seconds



Conclusion: As we increase tempreture doping penetrates deeper into silicon substrate but the peak decreases.As we increase time doping penetrates deeper into silicon substrate also the peak decreases.As we increase dose the peak increases as well as dopant penetrates deeper into substrate.As we increase energy the peak increases as well as dopant penetrates deeper into substrate.

EXPERIMENT 2: This experiment shows how boron diffusion profile in Si with dry O2 and without dry O2 used.

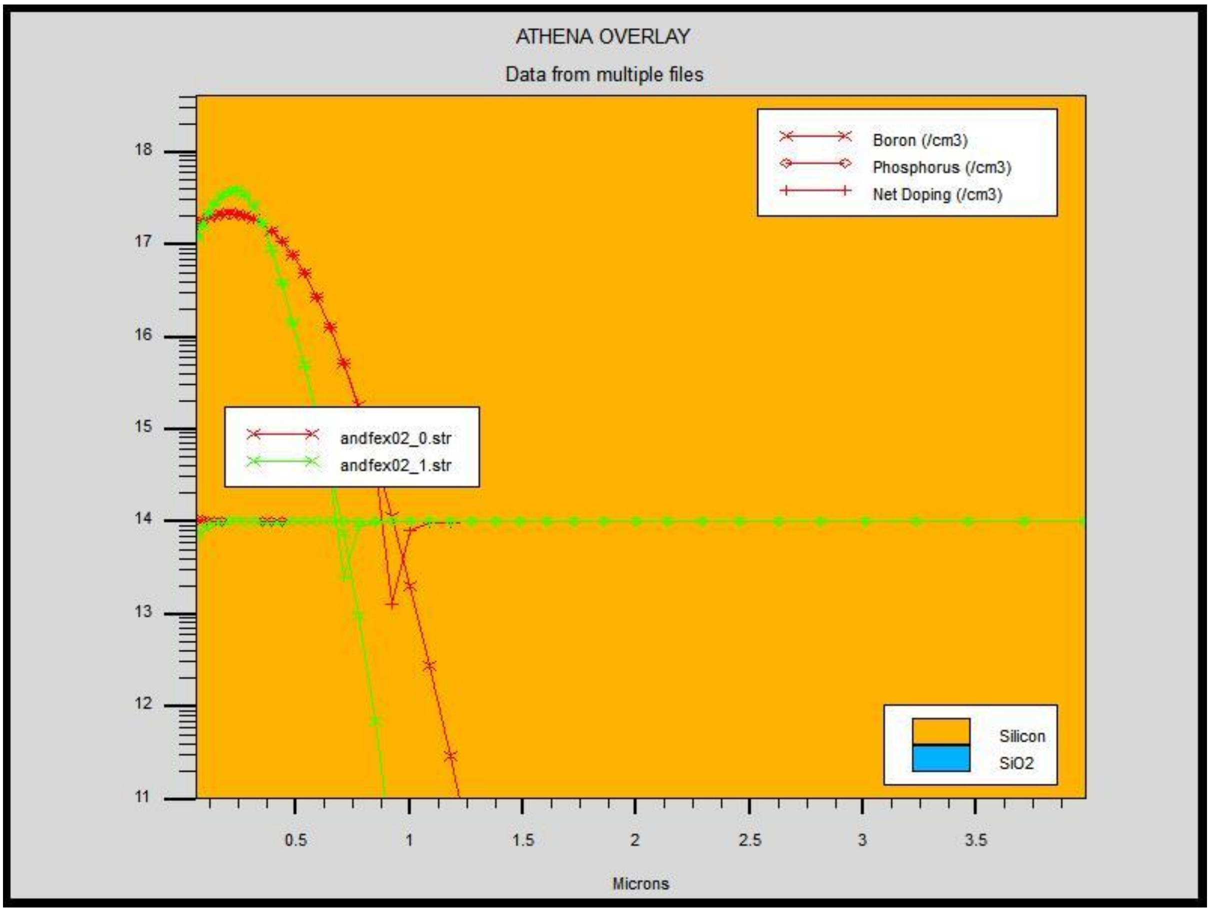
SOFTWARE USED: Silvaco S.EDA tools

THEORY: To model oxygen enhanced diffusion the TWO.DIM diffusion model must specified on the METHOD statement. When this model is specified, the interstitial and vacancy concentration will be calculated along with the impurities. This model loosely couples the point defects, generated by the oxidizing Si-SiO2 interface, with the diffusing boron. After this it reruns the simulation without dry O2.

The Two Dimensional Model

In this model, the point defect populations are directly represented and evolved in time. If there is a super/supra saturation of point defects, it will affect the dopant diffusivity through a simple scale factor, which goes to unity as the actual defect concentration approaches the equilibrium defect concentration. Therefore with equilibrium defect profiles, the Two Dimensional Model merely reduces to the Fermi Model, although in a more computational inefficient manner, since solving for point defects is not required. The pair coupling between defects and dopants in this model is assumed to be one-way. The diffusion of dopants is highly influenced by the diffusion of point defects, while the diffusion of the point defects,however, is regarded as totally independent of dopant diffusion. Stated in physical terms, this corresponds to a pairing between defects and dopants with zero binding energy. To turn on the Two Dimensional Model, specify parameter TWO.DIM in the METHOD statement. The Two Dimensional Model is based on the Fermi Model, so read the Fermi Model description before continuing. The major difference between the Fermi Model and the Two Dimensional Model is the direct representation and evolution of non-equilibrium point defect populations. Therefore, there are three different sets of governing diffusion equations: one for dopants, one for point defect interstitials and one of point defect vacancies. In addition, you also need to take into account the {311} cluster formation and dissolution, bulk and interface recombination, and the generation of point defects through oxidation.

OBSERVATION:



Conclusion : Its observed that boron diffuses more in Si than in SiO2

EXPERIMENT 3: This experiment demonstrates the diffusion models for Oxidation Enhanced Diffusion (OED). To model OED the TWO.DIM diffusion model must specified on the METHOD statement. When this model is specified, the interstitial and vacancy concentration will be calculated along with the impurities. This model loosely couples the point defects, generated by the oxidizing Si-SiO2 interface, with the diffusing boron.This example re-runs the simulation using the fermi model to compare results. The temp is varied from 800C to 1200 C.The time is varied from 30s to 300s.

SOFTWARE USED: Silvaco S.EDA tools

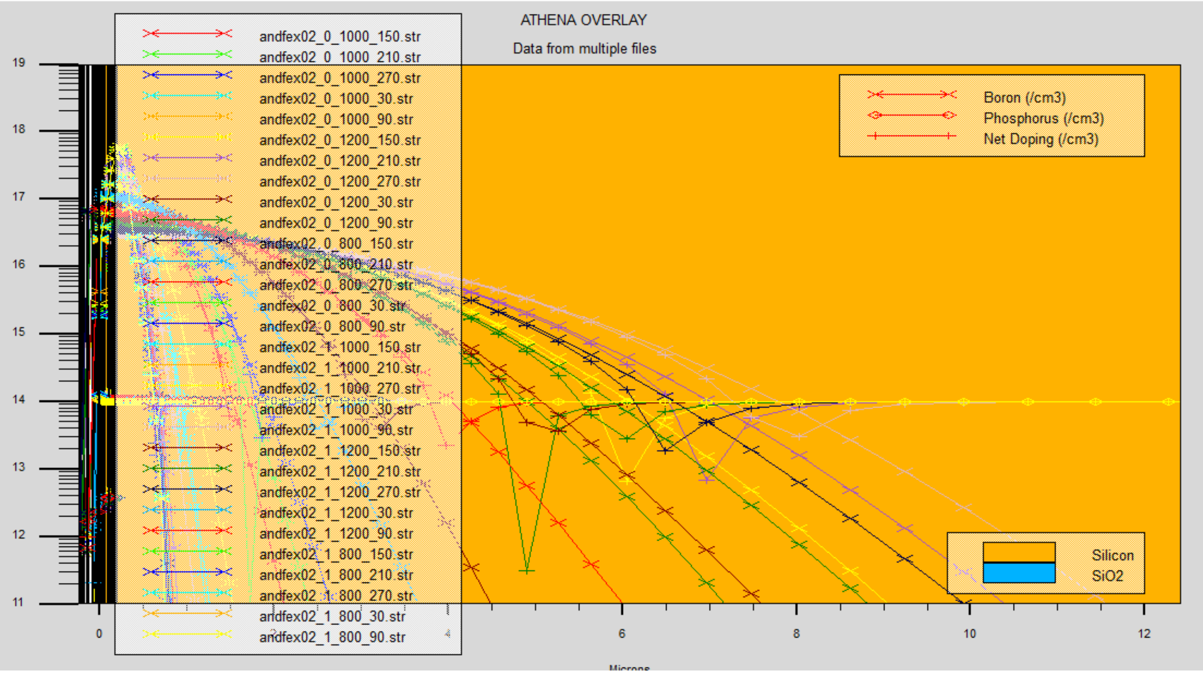
THEORY: ***The Two Dimensional Model***

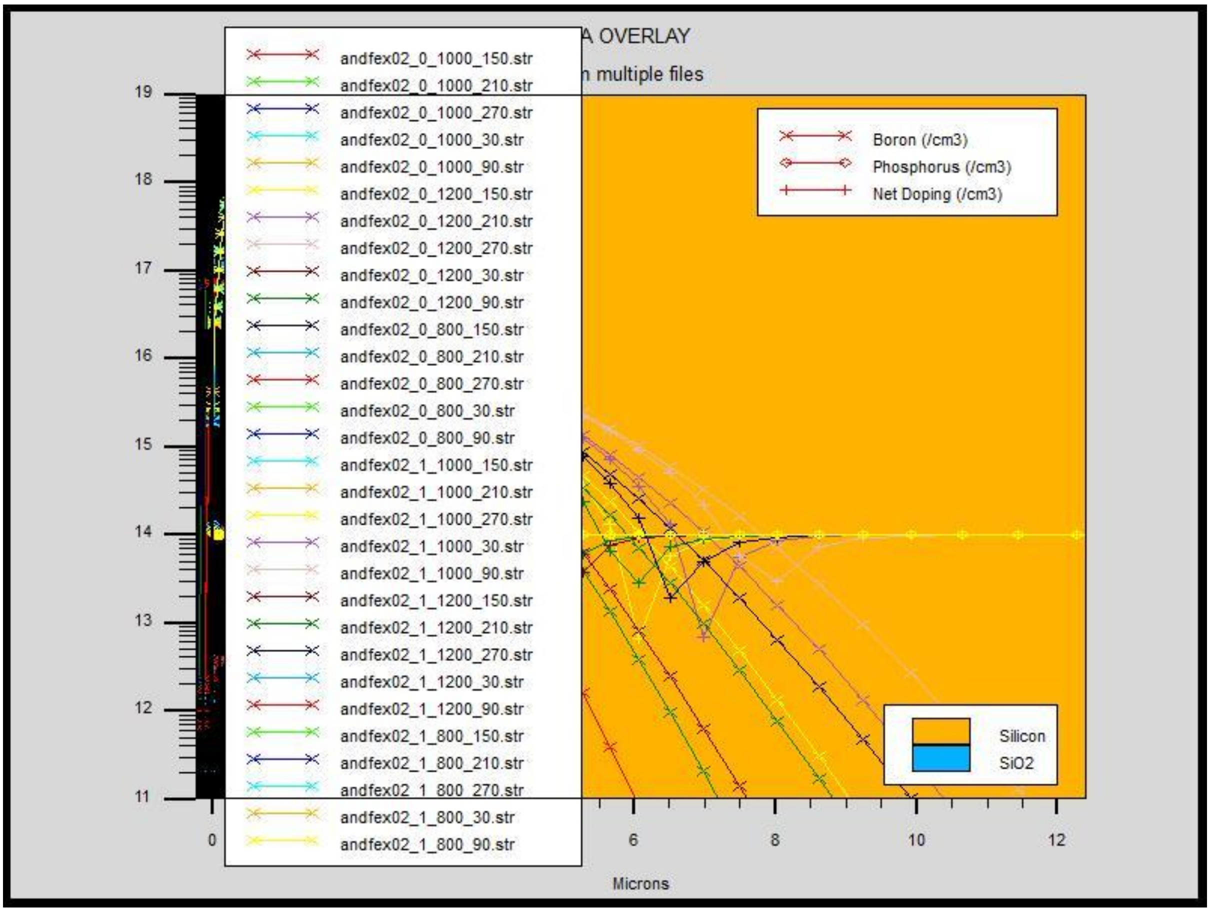
In this model, the point defect populations are directly represented and evolved in time. If there is a super/supra saturation of point defects, it will affect the dopant diffusivity through a simple scale factor, which goes to unity as the actual defect concentration approaches the equilibrium defect concentration. Therefore with equilibrium defect profiles, the Two Dimensional Model merely reduces to the Fermi Model, although in a more computational inefficient manner, since solving for point defects is not required. The pair coupling between defects and dopants in this model is assumed to be one-way. The diffusion of dopants is highly influenced by the diffusion of point defects, while the diffusion of the point defects,however, is regarded as totally independent of dopant diffusion. Stated in physical terms, this corresponds to a pairing between defects and dopants with zero binding energy. To turn on the Two Dimensional Model, specify parameter TWO.DIM in the METHOD statement. The Two Dimensional Model is based on the Fermi Model, so read the Fermi Model description before continuing. The major difference between the Fermi Model and the Two Dimensional Model is the direct representation and evolution of non-equilibrium point defect populations. Therefore, there are three different sets of governing diffusion equations: one for dopants, one for point defect interstitials and one of point defect vacancies. In addition, you also need to take into account the {311} cluster formation and dissolution, bulk and interface recombination, and the generation of point defects through oxidation.

The Fermi Model

The Fermi Model assumes that point defect populations are in thermodynamical equilibrium and thus need no direct representation. All effects of the point defects on dopant diffusion are built into the pair diffusivities. The main advantage for using the Fermi Diffusion model is it will greatly improve the simulation speed, since it does not directly represent point defects and only needs to simulate the diffusion of dopants. Also, the Fermi Model usually results in an easier numerical problem due to the avoidance of “numerical stiffness”. But since point defects are not directly simulated, the Fermi model cannot deal with certain process conditions in which the defect populations are not in equilibrium, such as in wet oxidation (where Oxidation Enhanced Diffusion (OED) is important), emitter-base diffusions and wherever implantation results in an initial high level of implant damage. To use the Fermi Model, specify FERMI parameter in the METHOD statement.

OBSERVATION:

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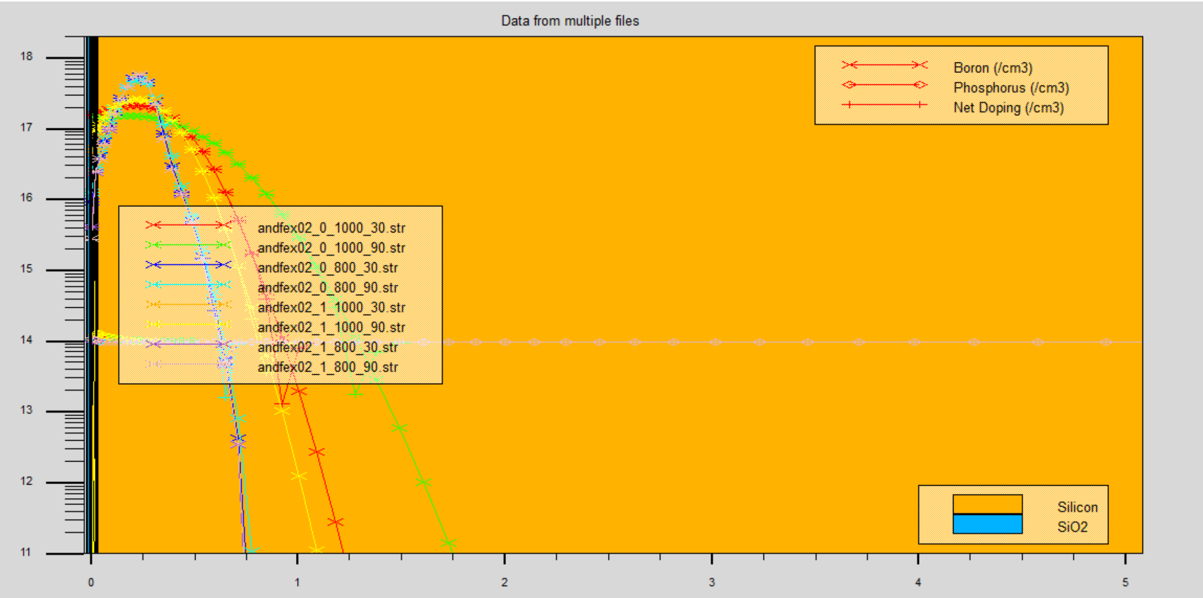
Net Doping (/cm3)
Silicon
SiO2
Microns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andfex02_1_800_30.str
andfex02_1_800_90.str
Silicon
SiO2

Conclusion: If we increase tempreture the diffusion of dopant increases but peak decreases, and if we increase time the diffusion increases but the peak decreases. In method fermi diffusion of dopant is more but in method TWO.DIM diffusion is less but it has higher peak. The overlay plot at the end of the simulation demonstrates the extra oxidation enhancement to the diffusion depth.

EXPERIMENT 4: This experiment demonstrates the damage enhanced diffusion effect in a heavy arsenic implant here dam factor is varied as 0.05,0.2 and 0.05 ,dose is varied from 1.0e13 to 1.0e15 .Energy varied from 40Kev to 220Kev .Tilt angle varied from 6 degree to 10 degree.

SOFTWARE USED: Silvaco S.EDA tools

THEORY: Diffusion enhancement due to defects introduced during heavy implants are responsible for the Transient Enhanced Diffusion (TED) or Rapid Thermal Annealing (RTA) effect.One of the key parameters in TED modeling using the full.cpl model is the amount of implant damage generated by the implant. This is controlled using the UNIT.DAMAGE model. The parameter DAM.FACT scales the interstitial concentration relative to the doping profile.

The Fully Coupled Model

The Fully Coupled Diffusion Model is identical to the Two Dimensional Model. Be familiar with that model before reading any further. The one important difference is that the diffusion of the defects is now influenced by the diffusion of the dopants by the addition of the joint pair fluxes to the flux terms in the governing equation of the defects. Therefore, there is a true two-way interaction between the diffusion of dopants and the diffusion of point defects, which gives this model its name. The fully coupled model is slightly more CPU-intensive than the two dimensional model, but encompasses the capability of reproducing certain important aspects of semiconductor processing such as the Emitter Push Effect in the case of phosphorus diffusion.From a physical viewpoint, however, this original fully coupled model suffers from the shortcoming of not explicitly representing pairs, and the consequential lack of a subdivision of defects and dopants into paired and non-paired fractions. Therefore, this model cannot

reproduce the saturation of the dopant diffusivity that is believed to occur at very high damage concentration due to a total pairing of dopants. In other words, the model relies on the dilute approximation (i.e., the assumption that the concentration of pairs is much smaller than both the dopant and the defect concentrations). To use the Fully Coupled Model, specify parameter FULL.CPL in the METHOD statement .

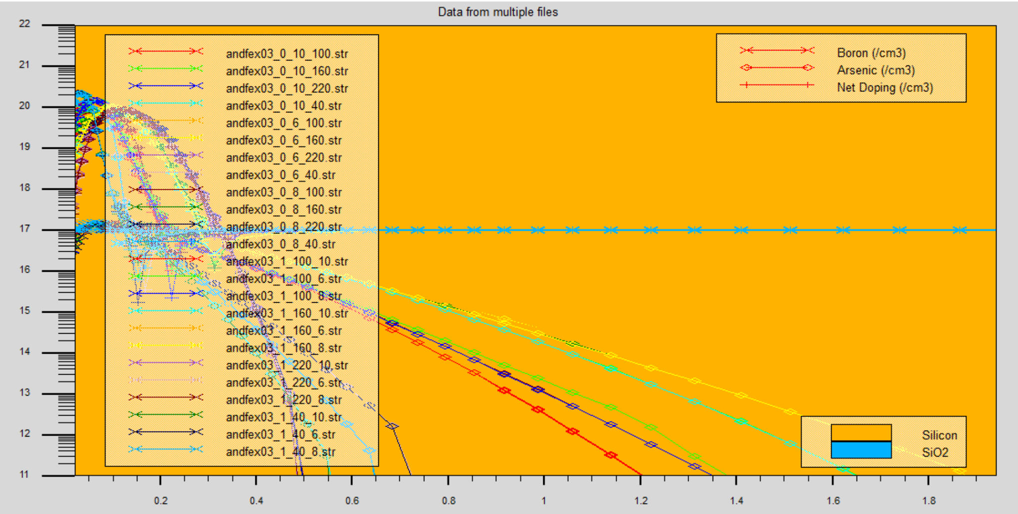
OBSERVATION:

Dam factor -0.05

Dose-`1.0e15`

`Energy varied from 40Kev to 220Kev`

`Tilt angle varied from 6 degree to 10 degree.`

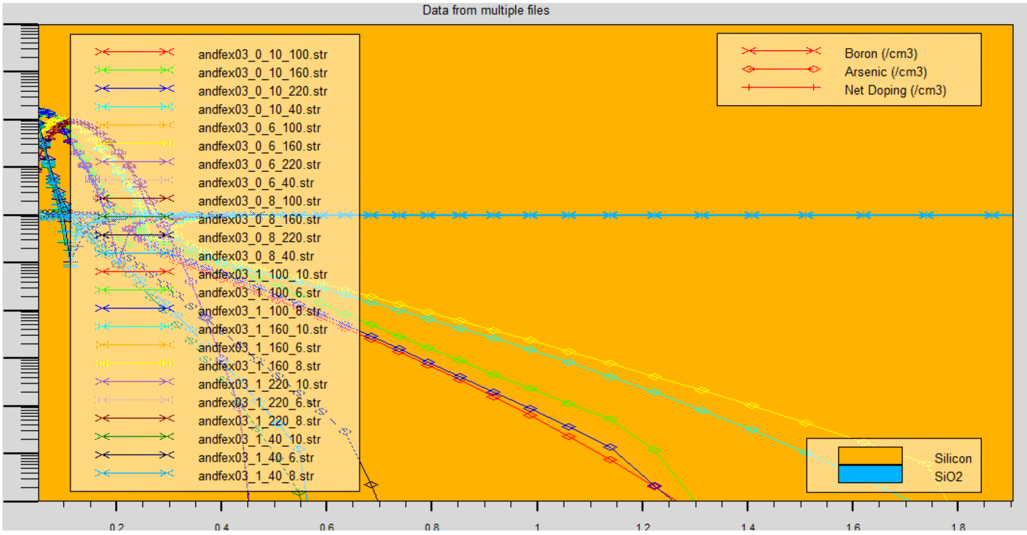


Dam factor -0.05

Dose-`1.0e14`

`Energy varied from 40Kev to 220Kev`

`Tilt angle varied from 6 degree to 10 degree.`



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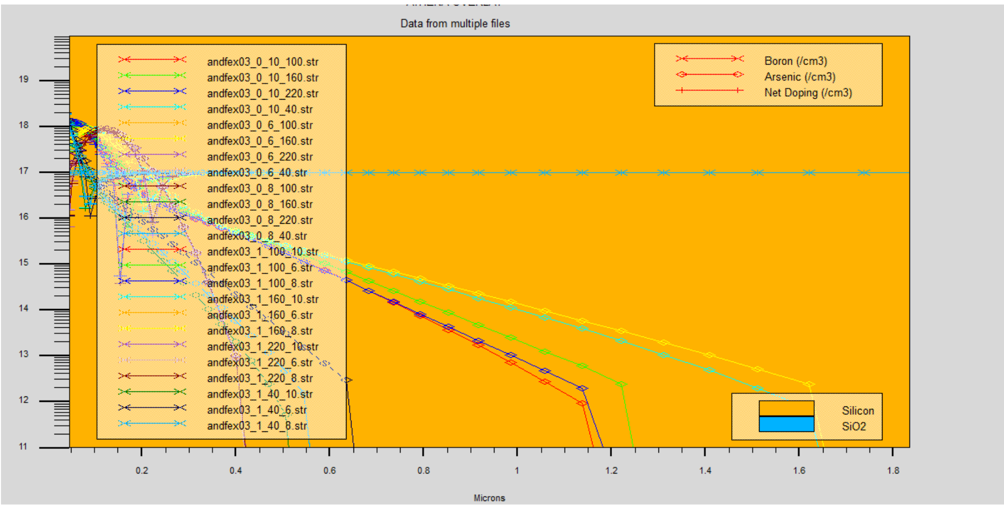
Dam factor -0.05

Dose-1.0e13

Energy varied from 40Kev to 220Kev

Tilt angle varied from 6 degree to 10 degree.

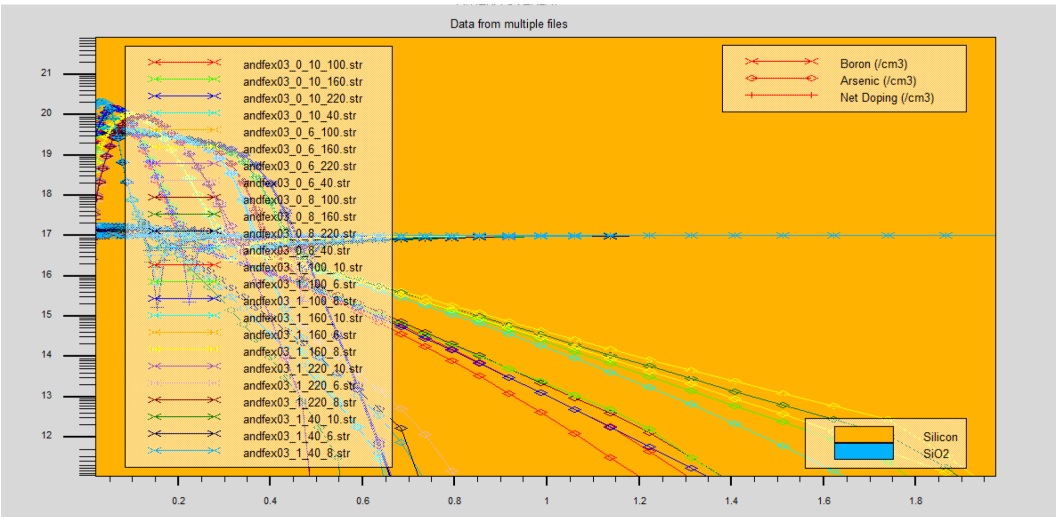


Dam factor -0.5

Dose-1.0e15

Energy varied from 40Kev to 220Kev

Tilt angle varied from 6 degree to 10 degree.



Dam factor -0.5

Dose-`1.0e14`

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Energy varied from 40Kev to 220Kev

Tilt angle varied from 6 degree to 10 degree.
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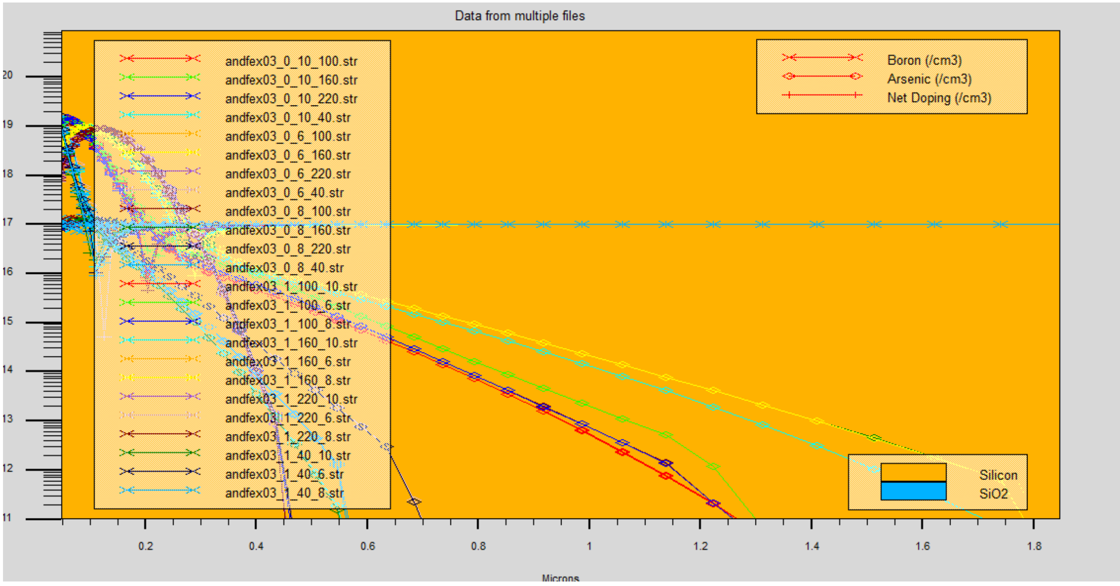
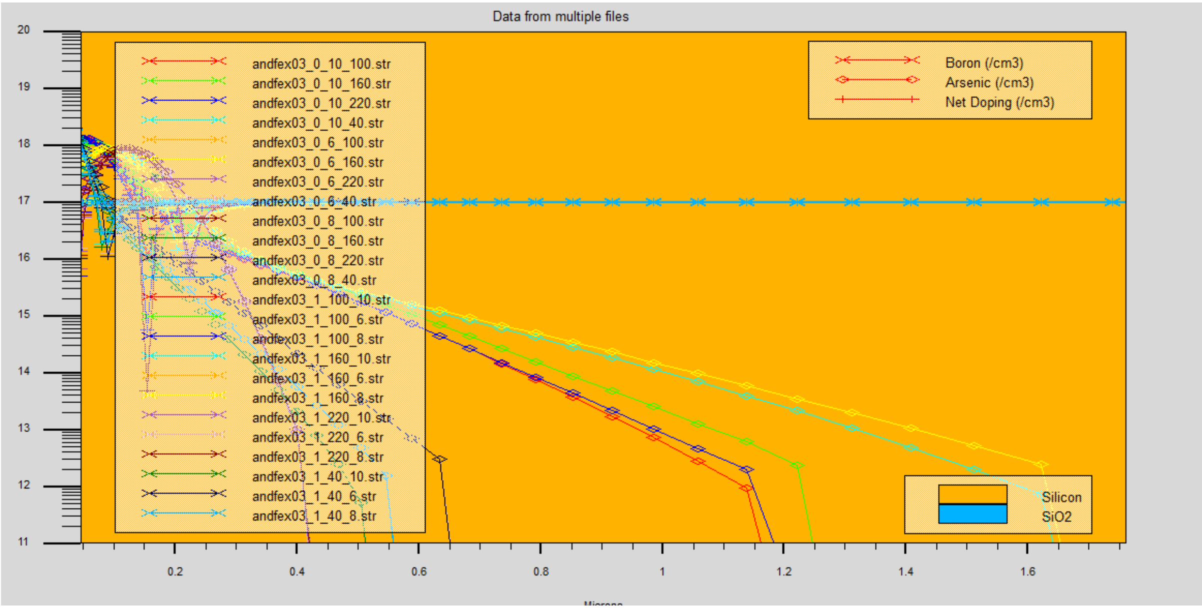


Dam factor -0.5

Dose-`1.0e13`

Energy varied from 40Kev to 220Kev

Tilt angle varied from 6 degree to 10 degree.

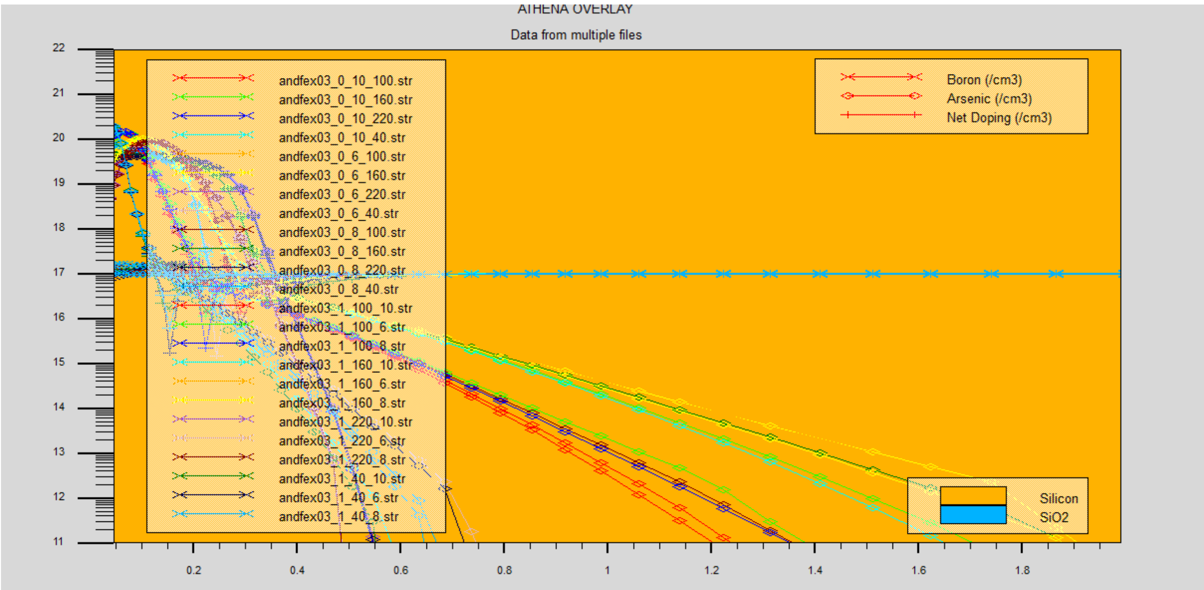


Dam factor -0.2

Dose-1.0e15

Energy varied from 40Kev to 220Kev

Tilt angle varied from 6 degree to 10 degree.

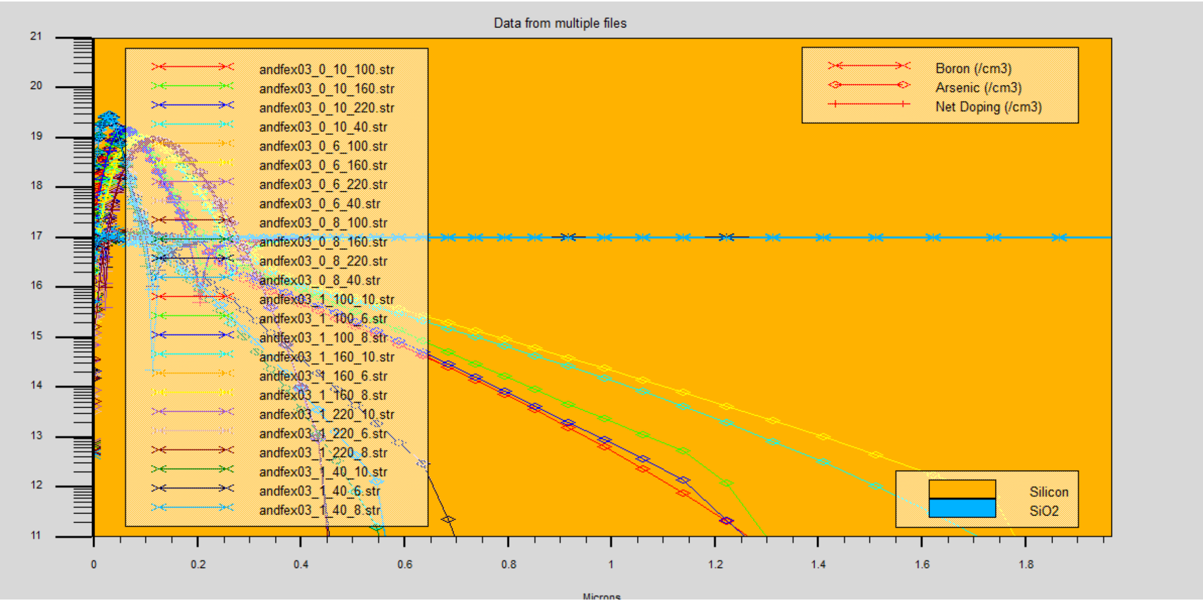


Dam factor -0.2

Dose-1.0e14

Energy varied from 40Kev to 220Kev

Tilt angle varied from 6 degree to 10 degree.

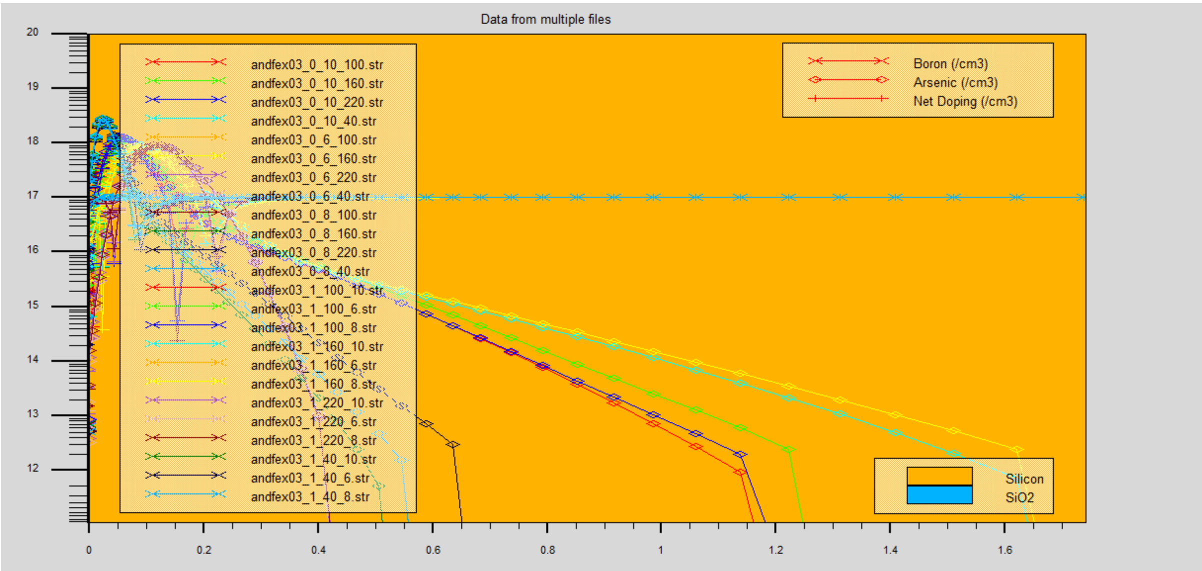


Dam factor -0.2

Dose-1.0e13

Energy varied from 40Kev to 220Kev

Tilt angle varied from 6 degree to 10 degree.



CONCLUSION: The overlay plot of the simulation demonstrates the extra implant damage enhancement to the diffusion depth when fermi model is used instead of fully coupled model.For a increase in tilt diffusion is reduced also as we increase time doping penetrates deeper into silicon substrate also the peak decreases.As we increase dose the peak increases as well as dopant penetrates deeper into substrate.As we increase energy the peak increases as well as dopant penetrates deeper into substrate.

Amit Sarkar

DATE:20-06-2021 **SIGNATURE OF STUDENT**