Hydrogen Ion-Implantation in Smart-Cut® SOI Fabrication Technique
6.774 Term Project
Joy Johnson
1. INTRODUCTION

A decade ago, the Smart-Cut® process was introduced as a technology so revolutionary and unconventional in the production of thin films that every sector of the semiconductor industry attempted to use it for one application or another. However, today the primary application of this process is that of fabricating Silicon-On-Insulator (SOI) wafers which have become the foundation for ultra-large-scale integration (ULSI) device structures as shown in Appendix A.

The Smart-Cut® process was created by Brue, Aspar, et al at LETI to obtain delamination of a thin layer in a thick substrate [1]. The process is advantageous in the production of SOI wafers, because it enables greater uniformity of the top Silicon layer while preserving its good crystal quality. Most importantly, this process is able to meet the criteria necessary for development of recent ULSI technologies which include thickness homogeneity, good crystalline quality, low cost, and excellent electrical properties while using standard equipment. In comparison with other SOI fabrication processes, it is particularly advantageous because it is relatively simple to ramp into industry and only requires one wafer to complete the SOI process. Smart-Cut® processes also provided additional evidence into the power of the use of ion beam.

2. SMART-CUT® PROCESS

Smart-Cut® process is indeed revolutionary, but what makes it so original is that it exploits the "basic physical phenomenon related to blistering, i.e. creation of microcavities, as a way of inducing in-depth splitting at the range of implanted protons over the whole wafer."[1] The process has four key steps described in detail below:

Step 1: Wafer A is capped with a thin dielectric layer of thermally grown SiO_2 which will serve as the buried oxide of the SOI structure. Then, Hydrogen ion implantation is performed on
the wafer at a dosage range from 3e16-1e17/cm² while keeping the substrate temperature in the range from 225 to ~300°C.

Step 2: Wafer A and a handle wafer B are cleaned using a modified RCA clean. Hydrophilic bonding is performed at room temperature of wafer A to wafer B (which is also oxide capped or bare). Then, the bonded wafers are checked to be void-free using infra-red spectroscopy and magic mirror observations. Wafer B plays a pivotal role in the process by serving as a stiffener and the bulk Silicon under the buried oxide of the SOI structure.

Step 3: The bonded wafers undergo a two-phase heat treatment. The first phase occurs from 400°C- 600°C and during this phase the implanted wafer A splits into two parts: a thin mono-crystalline layer of Silicon still bonded to wafer B as a SOI structure and the rest of wafer A which can be recycled and used as a handle wafer again. The split takes place because of phenomena of blistering and flaking induced by the hydrogen implantation, as shown in Appendix B. The SOI structure's upper layer is gained through this split at the hydrogen concentration depth (Rp). The second phase occurs at 1100°C to strengthen the chemical bonds.

Step 4: The new structure is touch polished using chemical mechanical polishing (CMP) since after splitting the upper layer of the SOI structure has a surface micro roughness that has to be reduced.

2.1 Explanation of Focus

Of the four primary steps in the Smart-Cut® process, "the use of ion implantation and the formation of a buried damaged layer along which splitting of a wafer occurs are the key links of the Smart-Cut® technology."[1] For the purposes of this project, I will be narrowing my focus to the hydrogen implantation done in Step 1. Particularly focusing on the role that the hydrogen ion-implantation and respective variants play in inducing the exfoliation, blistering, or creation
of microcavities and flaking which cause the in-depth splitting at the range of implanted ions over the wafer. From the literature there are two primary methods in which to produce the aforementioned physical phenomena. The first method is by performing a high-dose implantation, causing the blistering to be visible at around 2e17cm⁻² and the flaking as the dose increases. The second method, which is currently used in the Smart-Cut process, is that of medium-dose implantation and annealing. This is a two-step process in which the former performs a limited hydrogen dose implantation (from 3e16cm⁻² to 1e17cm⁻²) which allows for a layer of gaseous microbubbles to form in the lower region of the wafer and the latter performs a thermal treatment (400°C-600°C) which causes the blistering and flaking. The microbubbles grow due to Ostwald ripening and ultimately supply the internal force necessary to cause the cleavage in the hydrogen-implanted wafer[14]. It's generally accepted that the microbubbles occur at the peak in the hydrogen ion-implantation concentration profile and appear physically along the (100) plane parallel to the surface.

2.2 Previous Findings on Hydrogen Implant to Damage Relationship

According to Choyke et al, high dosage proton implants cause extreme ion bombardments which in turn cause the macroscopic physical effects mentioned. Using this knowledge, much of the literature notes that the use of damage energy calculations, primarily from backscattering and channeling (in addition to recoiling atoms, cascades, etc) can be used in analysis of the hydrogen ion implantation step and its role in inducing splitting at the projected range. The use of a seemingly problematic physical phenomenon is what makes the Smart-Cut® process so unconventional, but it is also the source of many of the complaints of the process as we will examine in section 3.
There have been a few previous studies on the general damage of hydrogen implantation which extract damage profiles on the assumptions that scattering and dechanneling can be thought to originate from random displaced silicon atoms at a given depth and that the defect distribution is the same as the damage energy distribution. Chu et al found that as the implant energy was decreased, the backscattering yield is slightly decreased [9]. Additionally, as expected for most ion implantation profiles, as the implant energy increased they saw an indirect relationship with projected range (Rp), or depth. Using Ziegler's method, they also find a relatively direct relationship between defect concentration and the implant energy. I will test this with a comparison of the percentage of the silicon atoms randomly displaced from the lattice site, which the relative scale is cited in the article, with added complexity of dosage and tilt variation. In all of the papers I have reviewed on this topic there have been very narrow range and damage distributions which can be attributed to many overshot predictions of stopping power. As well the depth distributions have been deeper than normal B or As profiles, but this can be easily explained by the fact that H is a light ion which will cause it to travel farther and have a broader distribution. In conclusion, the general consensus of the literature confirmed by Höchbauer et al is that the generation of the gaseous microbubbles and subsequent cleavage is contingent upon lattice damage resulting from the hydrogen ion-implantation [10].

3. PRIOR RESEARCH AND PROBLEMS

The Smart-Cut® process solves many problems that other methods of fabricating SOI wafers create, however it presents its own problems as well. Smart-Cut leaves a final thickness of the device layer "not easily controlled due to polishing to remove the surface roughness"[8], thus there has to be an abbreviated Smart-Cut® process that addresses this by accurately
controlling the thickness variations, possibly without a polishing operation. Additionally, there needs to be a process of SOI wafer fabrication where uniformity and thickness of the SOI device layer are independently controlled and selected. There has been such a process proposed, with an etch stop layer beneath the device layer, avoiding CMP and controlling the uniformity and thickness of the device layer [8]. The need for uniformity and control of the final thickness of the device layer is the primary problem found in the literature, showing as one of few, the lack of research into the fundamental mechanisms and relationships of this process. As of 2004, there has been lack of in-depth studies on this technology and thus a lack in the “fundamental understanding of the Smart-Cut® Process’ basic mechanisms” and any knowledge gained at this level will be “significantly beneficial for further production process development and large-scale implementation of this novel technique.” [7] So, my simulations will seek to be a comprehensive overview of all of the existing relationships between the key variants in Step 1; those being implant energy, dosage, depth (Rp), damage energy, tilt and their subsequent effect on the splitting and/or cleavage mechanism.

4. SIMULATIONS & RESULTS

At a range of different implant energies (85-200keV) I will examine changes in the projected range (in some cases depth), the 3 other moments of the ion distribution, defect distribution, and ion spatial arrangement as I vary the implant energy, tilt and dosage. Primarily these simulations will serve as a verification of relationships that exist between the variants that can be enhanced in the Smart-Cut® process, since the projected range and defect distribution determine where and how effective the physical phenomena of splitting occurs in the SOI structure.
4.1 SIMULATION SETUP

4.1.1 TSUPREM-4 Simulations

Initially, I decided to perform simulations in TSUPREM-4, however this program does not have a direct method for modeling hydrogen ion implantation thus, I used the “New Impurity” functionality to create a hydrogen impurity using its atomic weight and number, as well as its diffusion impurity coefficients on oxide from other readings (DIX.0=0.5, DIX.E=3.4). I modeled two other well-known elements that are normal to TSUPREM-4, those being Boron and Arsenic as shown in the code in Appendix H and then implemented the new Hydrogen impurity. In TSUPREM-4, initially I gave the implant model the dosage and ideal energy commonly found in the literature \[8\], 3.5e16/cm² and 95keV and the Monte Carlo parameter an input of N.ION=100000 in order to more accurately compare it with my TRIM output. I also assumed that the SiO₂ capped layer was 150nm, because that is the accepted capping thickness for SiO₂ layers and no papers actually specified a thickness. (Fitted values for Lattice Binding Energy (2), Surface Binding Energy (4.7), Displacement Energy (15)). My input code includes the thermal growth of the SiO₂ in addition to the Hydrogen ion implantation as shown in Appendix G. I decided to use the Monte Carlo ion implant model in TSUPREM4 which models the crystal to amorphous transition that occurs during ion implantation including the effects primarily of reflected ions and damage from vacancies and interstitials. I plan to use it to find the dependency of dose, depth, and energy on the effectiveness of creating the cavities for the Smart-Cut process by looking at the effects of the afore mentioned variants on the implantation profile/distribution. This form of Monte Carlo calculations are limited in functionality in that they are a superset of Monte Carlo ion implantation functionality of the process simulator PEPPER. The calculations used in TSUPREM-4 are under the primary assumption that the ions
involved in implantation lose energy through two processes: nuclear scattering and interactions with the electrons of the target atoms. Nuclear scattering is the process based on binary collision theory, in which the nucleus of an ion elastically scatters off the nucleus of a target atom. The latter is the interaction of the ion with the electrons of the target atoms; this is an inelastic process which does not alter the ion’s direction of motion.

4.1.2 TRIM Simulations

In the literature there was also modeling done using TRIM92 so I decided to also investigate using this software. SRIM is the umbrella of the programs, of which TRIM is a part of. TRIM calculates the stopping and range of ions into a substrate through the use of quantum mechanical handling of ion-target atom collisions. The calculation is much more accurate and efficient than that of TSUPREM-4, because any material can be set up for calculation and the calculation is efficiently done through the use of statistical algorithms which allow the ions to jump between collisions be calculated and then averaged over gaps. Long range interactions are described by including the target's “collective electronic structure and interatomic bond structure” [9] when the calculation is setup (tables of nominal values are supplied). More specifically, Monte Carlo Transport Calculation of ion interactions with multi-layer complex targets, is done under the TRIM program. TRIM is one of the most comprehensive software programs of its kind, in that it can accept complex targets with up to eight different layers and will calculate the 3D final distribution of the ions as well as the kinetic phenomena of ion energy loss, including target damage, ionization, etc.

I set up the TRIM program on the GUI much like I did the TSUPREM-4 code I wrote.; I Setup the ion to be Hydrogen on a SiO₂ capped layer that was 150nm. I specified tilt and implant energy since those are the only inputs allowed by TRIM (Temperature and dose cannot be
specification or adjustment). After running the simulation, I pulled plots of the Ion Range, Ion Track, Damage Events, and Collision Events as shown in Appendices C-F.

### 4.2 Simulation Outcomes

I used the following matrix of variants for the TRIM Monte Carlo Calculations using the *Detailed Calculation with full Damage Cascades Option* which follows every recoil above the lowest displacement energy of the target atom, carefully calculated at 100,000 ions. Tables 1 & 2 below give a summary of the Ion Range Distributions and Profiles shown in Appendix C.

Table 1. TRIM Monte Carlo Simulation Outputs at 0° Tilt

<table>
<thead>
<tr>
<th>Implant Energy (keV)</th>
<th>Ion Range (Rp) (Å)</th>
<th>Straggle (Å) (σ)</th>
<th>Skewness (γ)</th>
<th>Kurtosis (β)</th>
<th>Backscattered Ions</th>
</tr>
</thead>
<tbody>
<tr>
<td>85</td>
<td>7253</td>
<td>784</td>
<td>-1.877</td>
<td>11.3247</td>
<td>50</td>
</tr>
<tr>
<td>95</td>
<td>8062</td>
<td>805</td>
<td>-1.9140</td>
<td>11.8051</td>
<td>59</td>
</tr>
<tr>
<td>125</td>
<td>14000</td>
<td>847</td>
<td>-3.1153</td>
<td>21.5443</td>
<td>30</td>
</tr>
<tr>
<td>175*</td>
<td>8601</td>
<td>2363</td>
<td>-1.2036</td>
<td>3.9377</td>
<td>25</td>
</tr>
<tr>
<td>200*</td>
<td>7783</td>
<td>2827</td>
<td>-0.7421</td>
<td>2.5302</td>
<td>21</td>
</tr>
</tbody>
</table>

Table 2. TRIM Monte Carlo Simulation Outputs at 5° Tilt

<table>
<thead>
<tr>
<th>Implant Energy (keV)</th>
<th>Ion Range (Rp) (Å)</th>
<th>Straggle (Å) (σ)</th>
<th>Skewness (γ)</th>
<th>Kurtosis (β)</th>
<th>Backscattered Ions</th>
</tr>
</thead>
<tbody>
<tr>
<td>85</td>
<td>7228</td>
<td>784</td>
<td>-1.7928</td>
<td>10.550</td>
<td>70</td>
</tr>
<tr>
<td>95</td>
<td>8033</td>
<td>810</td>
<td>-1.9482</td>
<td>12.1755</td>
<td>45</td>
</tr>
<tr>
<td>125</td>
<td>14000</td>
<td>849</td>
<td>-3.0365</td>
<td>20.9276</td>
<td>42</td>
</tr>
<tr>
<td>175*</td>
<td>8518</td>
<td>2557</td>
<td>-.9019</td>
<td>4.1033</td>
<td>21</td>
</tr>
</tbody>
</table>
Hydrogen Ion-Implantation in Smart-Cut SOI Fabrication Technique

6.774 Term Project
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<p>| | | | | | |</p>
<table>
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</tr>
</thead>
<tbody>
<tr>
<td>200*</td>
<td>7844</td>
<td>2767</td>
<td>-1.2267</td>
<td>2.8995</td>
<td>23</td>
</tr>
</tbody>
</table>

*These values may be slightly inaccurate b/c of such high dosage in a light ion implantation;
Must be repeated by *Surface Sputtering/Monolayer Collisions* calculations instead of the
*Detailed Calculation with full Damage Cascades* however these calculations can take >10hours
to complete, causing my machine to timeout.

Each of the four moments in Tables 1 & 2 can be calculated using the following formulas.

\[
R_p = \int_{-\infty}^{\infty} u f(u) \, du
\]

\[
\sigma = \sqrt{\int_{-\infty}^{\infty} (u - R_p)^2 f(u) \, du}
\]

\[
\gamma = \frac{\int_{-\infty}^{\infty} (u - R_p)^3 f(u) \, du}{\sigma^3}
\]

\[
\beta = \frac{\int_{-\infty}^{\infty} (u - R_p)^4 f(u) \, du}{\sigma^4}
\]

(1)

As shown in the tables, the Ion Range and Straggle both increase as a function of implant energy
which verifies Bruel et al’s assumptions [3].

From the Ion Range plots, I took the Ion Ranges in (atoms/cm³/atoms/cm²) to predict
impurity concentration at a specific implant dose, using the simple formula:

\[
IONRanges \left( \frac{atoms}{cm^3} \right) \times IMPLANTATIONDose \left( \frac{ions}{cm^2} \right) = IMPURITYConcentration \left( \frac{atoms}{cm^3} \right)
\]

(2)
to examine the change in the ion distribution with the variation in implantation energies as well as tilt angle from the Table 1 of Variants.

Table 3 gives a summary of plots from TSUPREM-4 simulations in Appendix G.

Table 3. TSUPREM-4 Monte Carlo Simulation Outputs of Ion Range (um)

<table>
<thead>
<tr>
<th>Ion Implant Energy (keV)</th>
<th>Dosage of 2e17 cm(^{-2})</th>
<th>Dosage of 3.5e16 cm(^{-2})</th>
</tr>
</thead>
<tbody>
<tr>
<td>85</td>
<td>.76</td>
<td>.8</td>
</tr>
<tr>
<td>95</td>
<td>.85</td>
<td>.85</td>
</tr>
<tr>
<td>125</td>
<td>1.03</td>
<td>1.25</td>
</tr>
<tr>
<td>175</td>
<td>1.26</td>
<td>1.26</td>
</tr>
<tr>
<td>200</td>
<td>1.38</td>
<td>1.40</td>
</tr>
</tbody>
</table>

For the TSUPREM-4 simulations at a dose of 2e17 cm\(^{-2}\), the ion range in Table 4 at with an impurity concentration \(\sim 10^{22}\) cm\(^{-3}\) and the simulations at a dose of 3.5e16 cm\(^{-3}\) show an impurity concentration \(\sim 10^{21}\) cm\(^{-3}\) proving that I was able to replicate the original graphs of M.Bruel, et al [3]. Additionally, it verifies that irregardless of dosage ion implant energy has a direct relationship with ion range or depth.

4.3 Comparison of Simulations (TSUPREM-4 & TRIM)

Table 4. Comparison of achieved Ion Range(um) in TSUPREM-4 and TRIM simulations at ideal dosage, 3.5e16 cm\(^{-2}\).

<table>
<thead>
<tr>
<th>Ion Implant Energy (keV)</th>
<th>TSUPREM-4 Ion Range</th>
<th>TRIM Ion Range</th>
</tr>
</thead>
</table>
From Table 4, we can also deduce using the “back of the envelope” formula (2) that the impurity concentration at which these values were achieved in TRIM was one order of magnitude different than that of TSUPREM-4 (~10^{21} vs. ~10^{22}, respectively).

5. CONCLUSION

Through the use of my Monte Carlo simulations in both TRIM and TSUPREM-4, I was able to characterize many of the relationships present in the Hydrogen ion-implantation in Step 1 of the Smart-Cut process.

Through the TRIM simulations of the Ion Ranges, I was able to generate the ion profiles/distributions which show the direct relationship between implant energy and depth. As shown in Appendix C and Table 1, one can see as the energy is increased from 85keV to 200keV the depth is increased (The 175keV and 200 keV graphs had to be regenerated using Surface Sputtering/Monolayer Collision Steps” due to TRIM’s use of the concept of free flight paths for the ions causing “anomalous peaks and dips in our graph.”) One can also see that the profiles are slightly skewed toward the surface similar to the simulated profiles for Boron, since both are relatively light ions and more likely to backscatter off the silicon atoms. This relationship is only slightly shifted due to the change in tilt from 0° to 5° [Appendix C], the tilt can affect the number
of ions channeled in certain crystalline orientations as well as cause the implanted profiles to have a reduced number of incident ions and be foreshortened. The depth is only decreased on average by approx. 30 Å, causing me to assume that there is very little change actually caused by a change in tilt with the exception of foreshortening, and the direct relationship between implant energy and depth is maintained. Specifically, at the ideal energy of 95keV, the range at 0° tilt is 8062 Å and the range at 5° tilt is 8033 Å.

Additionally from the TRIM simulations in Appendix D which generated the damage events, namely target displacements, which from the Chu papers [9] can be used to examine the defect distribution. Defect concentration can be expressed as the amount of Silicon atoms displaced from the lattice site. So as we examine the target displacements we are looking at a relative estimate of defect concentration and since we know that the defects are what cause the physical phenomena at the Smart-cut layer to be split we can determine best fit parameters for that occurrence. In Appendix D, I recreate similar defect distributions to those in Chu’s paper, showing that in effect the defect concentration occurs at a greater depth for higher energy implants, so the physical phenomena and splitting will take place at a greater depth as well. At the ideal energy of 95keV, the defect concentration peaks around 0.75um according to both my simulation and Chu’s paper.

An additional observation that can be made from the TRIM simulations in Table 1 and Table 2 is that when there is no tilt, the number of backscattered ions is at a maximum at the ideal 95keV. From the literature we know that the damage energy includes backscattering in its calculations and this damage energy is directly related to predictability of the physical phenomena that enable the Smart-cut splitting mechanism. Regardless of the tilt, Tables 1 and 2 verify that straggle and projected range increase as a function of implant energy. In Appendices
D and E, I also observed the movement in the number of displacements and vacancies to greater depths with greater ion implant energy which proves the assumption that damage energy components help to determine the depth at which the physical phenomena of the Smart-Cut® process occurs.

It should also be noted that from Appendix F, the Ion Track in TRIM shows that regardless of the tilt, the ions behave radially and spatially in the same fashion, the only change is the actual shift in depth at which they are implanted.

I also repeated parallel simulations in TSUPREM-4 to generate the ion profiles and verify the relationships that I observed in TRIM. I was able to verify that as in TRIM, implant energy and ion range/depth have a strong direct relationship. I was also able to show (Table 4) that this relationship is irregardless of dose. Dosage only affected the projected range of implanted H ions, and not as drastically as has been previously assumed. Also I was able to show that the ideal 3.5e16 cm\(^{-3}\) dosage gave a better profile than that of the high dosage version, proving the greater efficiency of the two step process versus one as noted in the literature. Both simulators show the steep skewed profile expected for the light Hydrogen ions and the abnormal depth of Hydrogen ion-implantation, though at different concentrations.

As a concluding statement, I do feel that TRIM is more robust and accurate than TSUPREM-4, however both yield similar results to support the correlations of the variants in this process.
References


Appendices

Appendix A: Diagram of Smart-Cut Process

Appendix B: High Resolution TEM image of Smart-Cut region before splitting

Appendix C: TRIM Simulations: Ion Ranges

Appendix D: TRIM Simulations: Damage Events- Target Displacements

Appendix E: TRIM Simulations: Damage Events- Vacancies

Appendix F: TRIM Simulations: Damage Events- Ion Track of Depth vs. Y-Axis

Appendix G: TSUPREM-4: H Ion Implant Simulations

Appendix H: TSUPREM-4: H Ion Implant Code

Appendix I: TSUPREM-4: “New Impurity” Test Code for Arsenic and Boron
Appendix A.

Diagram of Smart-Cut Process
Appendix B.

**Fig. 5** High resolution TEM of the smart Cut region just before splitting.
Appendix C.

TRIM Simulations: Ion Ranges

Hydrogen Ion-implantation at 85keV at 0°

Hydrogen Ion-implantation at 95keV at 0°

Hydrogen Ion-implantation at 125keV at 0°

Hydrogen Ion-implantation at 175keV at 0°

Hydrogen Ion-implantation at 200keV at 0°
Hydrogen Ion-implantation at 85keV at 5°

Hydrogen Ion-implantation at 95keV at 5°

Hydrogen Ion-implantation at 125keV at 5°

Hydrogen Ion-implantation at 175keV at 5°

Hydrogen Ion-implantation at 200keV at 5°
Appendix D.

TRIM Simulations: Damage Events - Target Displacements

Hydrogen Ion-implantation at 85keV at 0°

Hydrogen Ion-implantation at 95keV at 0°

Hydrogen Ion-implantation at 125keV at 0°

Hydrogen Ion-implantation at 175keV at 0°

Hydrogen Ion-implantation at 200keV at 0°
Hydrogen Ion-implantation at 85keV at 5°

Hydrogen Ion-implantation at 95keV at 5°

Hydrogen Ion-implantation at 125keV at 5°

Hydrogen Ion-implantation at 175keV at 5°

Hydrogen Ion-implantation at 200keV at 5°
Appendix E.

TRIM Simulations: Damage Events- Vacancies

Hydrogen Ion-implantation at 85keV at 0°

Hydrogen Ion-implantation at 95keV at 0°

Hydrogen Ion-implantation at 125keV at 0°

Hydrogen Ion-implantation at 175keV at 0°

Hydrogen Ion-implantation at 200keV at 0°
Hydrogen Ion-implantation in Smart-Cut SOI Fabrication Technique
6.774 Term Project
Joy Johnson

Hydrogen Ion-implantation at 85keV at 5°

Hydrogen Ion-implantation at 95keV at 5°

Hydrogen Ion-implantation at 125keV at 5°

Hydrogen Ion-implantation at 175keV at 5°

Hydrogen Ion-implantation at 200keV at 5°
Appendix F.

TRIM Simulations: Ion Track of Depth vs. Y-Axis

Hydrogen Ion-implantation at 85keV at 0°

Hydrogen Ion-implantation at 95keV at 0°

Hydrogen Ion-implantation at 125keV at 0°

Hydrogen Ion-implantation at 175keV at 0°

Hydrogen Ion-implantation at 200keV at 0°
Hydrogen Ion-implantation at 85keV at 5°

Hydrogen Ion-implantation at 95keV at 5°

Hydrogen Ion-implantation at 125keV at 5°

Hydrogen Ion-implantation at 175keV at 5°

Hydrogen Ion-implantation at 200keV at 5°
Appendix G.
TSUPREM-4 Simulations
Hydrogen Ion-Implantation in Smart-Cut SOI Fabrication Technique
6.774 Term Project
Joy Johnson
Appendix H.

Code for H Ion-Implantation

$Title: 6.774 Term Project
$Function: Affects of Hydrogen Implantation in Step 1 of Smart Cut
$Author: Joy Johnson

$DEFINE A MESH
MESH GRID.FAC=0.1

$CREATE A SILICON SUBSTRATE (1e15-1e18)
INITIALIZE <100> BORON=1.0e17

$CREATE NEW HYDROGEN IMPURITY  (try with #s for Boron 1st)
$introduce with atomic # and weight
IMPURITY NEW IMPURITY = HYDROGEN AT.NUM=1 AT.WT=1.00794
$specify the activation energy & diff. coefficient
IMPURITY IMP=HYDROGEN MAT=SILICON DIX.0=0.5 DIX.E=3.4

$THERMAL OXIDATION OF SiO2 (2000A to 1um)
$0.4115
$specify the mesh spacing of growing oxide
method dy.oxide=0.00001
$specify initial native oxide thickness
ambient wetO2 initial=0.1
$specify the oxidation conditions
diffusion temperat=1000 time=6 steam
$select z= 1.0
print layers x.v=0

$HYDROGEN IMPLANTATION
$Dual Pearson
$IMPLANT HYDROGEN DOSE=3.5E16 ENERGY=95 IMPL.TAB=BORON
$Gaussian
$IMPLANT HYDROGEN DOSE=3.5E16 ENERGY=95 GAUSSIAN
$MONTECAR
IMPLANT IMP=HYDROGEN DOSE=3.5E16 ENERGY=85 MONTECAR N.ION=100000

$PLOT H IMPLANT
SELECT Z=log10(HYDROGEN) TITLE='H Ion Implant: 85 keV at 3.5E16'
LABEL=log10(H concentration)
PLOT.1D RIGHT=1.5 TOP=22 BOTTOM=17 LINE.TYPE=1

SELECT Z=log10(HYDROGEN)
PLOT.1D 'clear 'axe line.type=0 SYMBOL=2 COLOR=2
LABEL x=0.05 Y=20.2 line.type=1 LABEL= 'simulation'
Appendix I.

Code for Actual Boron Profile

$ Comparison of As as-implanted profile and simulation using dual Pearson model

$define mesh
MESH GRID.FAC=0.1

$create silicon
INITIALIZE <100> BORON=1.0e17

$Implant Boron with MonteCarlo
IMPLANT BORON DOSE=4.27e14 ENERGY=32 MONTECAR

$plot As implant
SELECT Z=log10(ARSENIC) TITLE='Plot 1.1'+
LABEL=log10(B concentration)
PLOT.1D RIGHT=0.2 TOP=21 BOTTOM=17 LINE.TYPE=1

SELECT Z=log10(BORON)
PLOT.1D clear axe line.type=0 SYMBOL=2 COLOR=2
LABEL x=0.05 Y=20.2 line.type=1 LABEL='simulation'

Test Program for “new impurity” Boron Profile

>Title: 6.774 Term Project
$Function: Affects of Hydrogen Implantation in Step 1 of Smart Cut
$Author: Joy Johnson

$DEFINE A MESH
MESH GRID.FAC=0.1

$CREATE A SILICON SUBSTRATE (1e15-1e18)
INITIALIZE <100> BORON=1.0e17

$CREATE NEW HYDROGEN IMPURITY (try with #s for Boron 1st)
$introduce with atomic # and weight
IMPURITY NEW IMPURITY = HYDROGEN AT.NUM=5.0 AT.WT=10.8
    $specify the activation energy & diff. coefficient
IMPURITY IMP=HYDROGEN MAT=SILICON DIX.0=2.11e8 DIX.E=3.46

$THERMAL OXIDATION OF SiO2 (2000A to 1um)
$0.4115
    $specify the mesh spacing of growing oxide
$method dy.oxide=0.00001
    $specify initial native oxide thickness
$ambient wetO2 initial=0.1
    $specify the oxidation conditions
$diffusion temperat=1000 time=20 steam
    $print layer start and end & total thickness on command window
$select = 1.0
$print layers x.v=0

$HYDROGEN IMPLANTATION
  $Dual Pearson
  $IMPLANT HYDROGEN DOSE=3.5E16 ENERGY=95 IMPL.TAB=BORON
  $Gaussian
  $IMPLANT HYDROGEN DOSE=3.5E16 ENERGY=95 GAUSSIAN
  $MONTECAR
  IMPLANT IMP=HYDROGEN DOSE=4.27e14 ENERGY=32 MONTECAR N.ION=1000

$PLOT H IMPLANT
SELECT Z=log10(HYDROGEN) TITLE='Plot 1' LABEL=log10(H concentration)
PLOT.1D RIGHT=0.2 TOP=21 BOTTOM=17 LINE.TYPE=1

SELECT Z=log10(HYDROGEN)
PLOT.1D ^clear ^axe line.type=0 SYMBOL=2 COLOR=2
LABEL x=0.05 Y=20.2 line.type=1 LABEL= 'simulation'