EVOLUTION OF DEFECTS IN AMORPHIZED SILICON

By

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A THESIS PRESENTED TO THE GRADUATE SCHOOL
OF THE UNIVERSITY OF FLORIDA IN PARTIAL FULFILLMENT
OF THE REQUIREMENTS FOR THE DEGREE OF
MASTER OF SCIENCE

UNIVERSITY OF FLORIDA

2006
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By

Adrian Ewan Cameron
To Mom, Dad, Evins, and Bill.
ACKNOWLEDGMENTS

The author would like to thank his parents for their unwavering support throughout his academic career. He would also like to thank his advisor, Dr. Mark Law, for his direction and guidance as well as Dr. Kevin Jones for his work on TEM and his insight and knowledge of this area. The author would also like to thank the SWAMP group for their help, especially Renata, Ljubo, Russ, Danny, Michelle, Diane, Erik, Serge, and everyone else who has helped prepare samples, answer questions, take TEM pictures, and teach the author how to use lab equipment. Thanks are also extended to Dr. Scott Thompson for serving on the thesis defense committee. The author would like to thank Zoe for her help and for proofreading. A huge thank you goes to Teresa for keeping the SWAMP group moving and organized so well.
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Abstract of Thesis Presented to the Graduate School of the University of Florida in Partial Fulfillment of the Requirements for the Degree of Master of Science

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By

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August 2006

Chair: Mark E. Law
Major Department: Electrical and Computer Engineering

In order to maintain the current trend of laterally scaling CMOS transistors for better performance and higher transistor density, vertical dimensions must also be scaled to minimize short channel effects. One way to achieve shallow vertical junctions is through pre-amorphizing implants (PAI) at low energy to reduce ion channeling during implantation of the dopant species. These PAI steps create end-of-range (EOR) damage just below the amorphous/crystalline interface. Understanding how this EOR damage evolves is important to process modeling and to future technologies. As the PAI energy is reduced, the damage region is placed closer to the surface. The objective of this study is to explore how several aspects of the surface affect the evolution of the EOR damage. These aspects include proximity to the surface through lowered implant energy, reaction rates of interstitials at the surface, and an electrical field set up at the surface.

The first experiment in this thesis investigates the EOR damage evolution for several low-energy Ge⁺ PAIs. Silicon wafers were implanted with Ge⁺ with doses of
5e14 cm\(^2\) at 10keV, 2e15 cm\(^2\) at 5 and 10keV, and 5e15 cm\(^2\) at 5 and 10keV. Anneals were performed at 750°C for 5, 15, 30, 45 and 60 minutes. Plan-view transmission electron microscopy (PTEM) was used to determine that at all conditions, small, unstable dislocation loops were formed in the EOR region. Implant dose and energy seemed to have no effect on trends regarding the dissolution time of the defects. The results were in general agreement with previous work. From the PTEM analysis, decay time constants were extracted for modeling purposes.

In the second experiment in this thesis, a model of \{311\} evolution was used for FLOOPS simulations. The recombination rate of interstitials at the surface was controlled using the variable “ksurf” for implant energies of 40, 80, and 160keV at a dose of 1e15 cm\(^{-2}\). Changing the “ksurf” variable had little effect on the dissolution of \{311\}’s, with a sharp drop around “ksurf” = 1e-6 cm/s which then levels off for increasing values.

An additional part of the second experiment involved adding modifications to the above model. This model uses an electrical field set up by the silicon/oxide interface to explain both pile-up and junction broadening of boron. The key variable for these simulations is the “pin” value, which controls the magnitude of the field at the surface. The effect of this field on \{311\} dissolution was investigated for the 40keV implant condition. The results show that the effect does not show a trend, but rather no real effect on the decay rate. This is not surprising since the modifications were developed to influence dopant ions and not silicon interstitials.
CHAPTER 1
INTRODUCTION

1.1 Background and Motivation

The integrated circuit (IC) has been a part of the growing worldwide technology industry since its invention in 1959. The invention is credited to Jack Kilby of Texas Instruments and Robert Noyce of Fairchild Semiconductor [1]. Since its inception, the integrated circuit has grown in complexity from several parts to several hundred million. The reason for this growth is the evolution of the complementary metal-oxide semiconductor transistor, or CMOS. The trend in complexity has followed Moore’s Law, which predicts that the number of transistors on an integrated circuit will double approximately every year [2]. Through technological innovation, that law has been anticipated and hurdles overcome so that the prediction has been surprisingly accurate.

There are other more tangible benefits to transistor scaling as well. As the minimum feature size decreases, the cost per transistor shrinks as does the cost per function for a given area. In addition, smaller components require less power to operate and produce less heat, which improves reliability. There are physical limitations which work to counteract these benefits, such as the escalating cost of research and development to overcome obstacles like junction leakage, lithographic limitations, and short-channel effects.

The benchmark for overcoming technological hurdles and establishing new technologies as cutting edge is the International Technology Roadmap for Semiconductors (ITRS). The latest version of this map was completed in 2005, and
predicts the needs of the industry for the near and long-term future in all aspects of production, from doping and size requirements to lithography, packaging, metrology, and factory integration for both logic devices and memories, both volatile and non-volatile. The ITRS also predicts when new technologies should be ready for production and if manufacturing solutions are known or unknown for future requirements. Several of the key features for the next several years can be found in Table 1.1.

The convention for labeling a technology node is usually to refer to the minimum feature size, which is normally the gate length of a transistor. Some conventions refer to the physical gate length while others refer to the printed gate length. Regardless of which convention is used, the junction depth for the source and drain areas are on the same order of magnitude. This work focuses on issues pertaining to ultra-shallow junctions, one of the front-end processes (FEP) in semiconductor production. The need for ultra-shallow junctions arises from several issues. First, the ITRS maintains a sheet resistance requirement for the contact area of the source and drain. As the junction depth decreases, scaled with gate length, the resistivity increases since a deeper junction can incorporate more active carriers and hence lower resistivity. Therefore it is necessary to find ways of implanting more carriers into the shallow junctions and activate them during the annealing process, which is described later. Second, shallower junctions improve the short-channel effects of small gate length transistors. Figure 1.1 illustrates two transistors with equal gate lengths, but one has shallow junctions. The depletion region of the shallow junction has less effect on the channel, thereby reducing the effective channel length and the short-channel effects.
Table 1.1 ITRS values for the next several technology nodes for key parameters of interest. MPU is a logic, high-performance, high-production chip.

<table>
<thead>
<tr>
<th>Year</th>
<th>2006</th>
<th>2007</th>
<th>2009</th>
<th>2011</th>
<th>2013</th>
</tr>
</thead>
<tbody>
<tr>
<td>DRAM ½ pitch (nm)</td>
<td>70</td>
<td>65</td>
<td>50</td>
<td>40</td>
<td>32</td>
</tr>
<tr>
<td>MPU physical gate length (nm)</td>
<td>28</td>
<td>25</td>
<td>20</td>
<td>16</td>
<td>13</td>
</tr>
<tr>
<td>Junction depth $X_j$ (nm)</td>
<td>30.8</td>
<td>27.5</td>
<td>22</td>
<td>17.6</td>
<td>n/a</td>
</tr>
<tr>
<td>S/D extension (nm)</td>
<td>9</td>
<td>7.5</td>
<td>7</td>
<td>5.8</td>
<td>n/a</td>
</tr>
<tr>
<td>Extension lateral abruptness (nm/decade)</td>
<td>3.5</td>
<td>2.8</td>
<td>2.2</td>
<td>1.8</td>
<td>n/a</td>
</tr>
<tr>
<td>MPU Functions per chip (Mtransistors)</td>
<td>193</td>
<td>286</td>
<td>386</td>
<td>773</td>
<td>1546</td>
</tr>
<tr>
<td>Transistor density, logic (Mtransistors/cm²)</td>
<td>122</td>
<td>154</td>
<td>245</td>
<td>389</td>
<td>617</td>
</tr>
<tr>
<td>Transistor density, SRAM (Mtransistors/cm²)</td>
<td>646</td>
<td>827</td>
<td>1348</td>
<td>2187</td>
<td>3532</td>
</tr>
<tr>
<td>Equivalent Oxide Thickness (EOT) (nm)</td>
<td>1.84</td>
<td>1.84</td>
<td>1.03</td>
<td>0.75</td>
<td>n/a</td>
</tr>
<tr>
<td>Vdd (V)</td>
<td>1.1</td>
<td>1.1</td>
<td>1.0</td>
<td>1.0</td>
<td>0.9</td>
</tr>
<tr>
<td>Number of mask levels, MPU</td>
<td>33</td>
<td>33</td>
<td>35</td>
<td>35</td>
<td>37</td>
</tr>
</tbody>
</table>

Source: [3]
1.2 Ion Implantation

Ion implantation is the current dominant technology in control of forming source/drain areas as well as threshold shift implants and source/drain extensions. The dopant ion is accelerated and focused on the wafer using electric fields. The dose of atoms is controlled by longer implant times or a higher beam current. The energy and
mass of the atoms control the projected range, $R_P$, which is the peak of the dopant profile after implantation. The dopant profile follows a Gaussian statistical distribution [1] described by the equation:

$$C(x) = C_P \exp\left( \frac{-(x-R_P)^2}{2\Delta R_P^2} \right)$$

where $C_P$ is the peak concentration predicted by the dose and the straggle, or $\Delta R_P$. $X$ is measured into the substrate with $x=0$ the surface of the wafer. Often, implantation is done through a masking oxide for better control of the projected range and the concentration peak, which is usually desired to be very near the surface.

### 1.2.1 Ion Stopping

As the ion is implanted into the lattice, it must have a force act on it to stop. The two mechanisms for ion stoppage are nuclear stopping and electronic stopping. If the ion is not stopped sufficiently near the surface, it can tunnel deep into the substrate, deepening the junction depth. Figure 1.2 shows examples of tunneling, nuclear stopping, and electronic stopping.

For nuclear stopping, the ion must collide with an atom in the lattice. The resulting collision can displace the lattice atom and usually will if it is a primary collision. The collision can result in a secondary damage cascade from both the dopant ion and displaced lattice atom. Both atoms can travel deeper into the bulk, or the implanted ion can actually backscatter toward the surface. Nuclear stopping causes damage to the lattice, which will be discussed in the next section.

There are two types of electronic stopping: local and non-local. Non-local electronic stopping refers to the drag an ion experiences in a dielectric medium. The illustration for this can be seen in Figure 1.2 (C). An analogy is a particle moving through a viscous medium [1]. Local electronic stopping involves collisions of electrons
when the implanted ion is close enough to a lattice atom such that the electron wavefunctions overlap [1], causing a momentum transfer. This event is illustrated in Figure 1.2 (D). The dominant mechanism for ion stoppage is nuclear stopping for low-energy implants, and this also has the greatest effect on trajectory.

![Figure 1.2 Examples of behavior on implanted ions. A) Tunneling when the ion is not stopped. B) Nuclear stopping, which displaces a lattice atom and can cause secondary damage. C) Non-local electronic stopping of electrical drag on an ion in a dielectric medium. D) Local electronic stopping involving collisions of electrons. All figures from Plummer et al. [1].](image)

### 1.2.2 Amorphization and Implant Damage

One way to limit the depth of the implant profile is through a pre-amorphizing implant, or PAI, which eliminates the possibility of ion channeling. This implant is performed with a non-dopant atom, usually Si$^+$ or Ge$^+$ such that the electrical characteristics are unchanged, or a co-implanted species such as BF$_2^+$ where fluorine is
the amorphizing ion and boron is the dopant. If the dose and energy are sufficiently high enough, the implant will destroy the lattice structure and an amorphous layer will now be the top layer of the substrate. Beneath the amorphous layer a highly damaged layer with a supersaturation of interstitials will exist. The damage in this area is classified as Type-II damage by Jones and is referred to as end-of-range, or EOR damage [4, 5]. In contrast, Type-I damage occurs for non-amorphizing implants close to the concentration peak at the projected range.

As a result of the nuclear stopping described above, lattice atoms are displaced from their sites in the crystal structure. This creates an interstitial and a vacancy in the lattice, described as a Frenkel pair [1, 6]. New interstitials can also have secondary collisions with lattice atoms, creating more Frenkel pairs. Most of the Frenkel pairs will recombine very quickly during the annealing process after implantation. Interstitials, however, remain in excess in proportion to the implanted dose. This is referred to as the “+1” model [7]. These interstitials have no corresponding vacancy and can form clusters and nucleate into larger, more stable defects, since they must either diffuse to the surface or deeper into the bulk.

If the implant conditions are of sufficient energy and dose, amorphization occurs. This event can be considered as a critical-point phenomenon where the onset of amorphization leads to cooperative behavior of the defects which greatly accelerates the transition away from a crystalline lattice [8]. When this is the case, the “+1” model is no longer very accurate, since the amorphous region consists totally of interstitials with no long-range order and the EOR damage consists of a supersaturation of interstitial point defects created from implanted ions and recoiled atoms from the amorphous region. This
“recoil” model by Jones [9] predicts a reduction in EOR density with increasing dose. Robertson et al. [5] found that the total number of interstitials in the EOR region was constant with a changing dose rate for an amorphizing Si⁺ implant with dose of 1e15cm⁻². Other research [9, 10, 11] has shown that the number of interstitials in the EOR region is a function of implant beam energy. Other conditions such as implant temperature and species also have an impact on EOR formation, but no single condition has shown a one-to-one correspondence to EOR density [11].

1.3 Damage Annealing

After the implantation process, the wafer is heated to high temperatures, to repair damage done to the substrate. During this time, the crystal lattice is regrown, a process referred to as solid-phase epitaxy, or SPE. Frenkel pairs will begin to be annihilated at relatively low temperatures around 400°C [1]. After they recombine, an excess of interstitials still remain, in accordance with the “+1” model. These interstitials are not reincorporated into the lattice because the dopant ions take their place and are then electrically active.

1.3.1 Solid-Phase Epitaxy

The process of recrystalizing the amorphized silicon substrate during annealing is called solid-phase epitaxy (SPE). It is a process of layer-by-layer regrowth from the amorphous/crystalline interface back to the surface. The rate of regrowth is fast, and can be up to 50 nm/min for <100> oriented silicon at 600°C [1]. As recrystallization occurs, the introduced dopant atoms are incorporated into substitutional lattice sites and become electrically active. The rest of the regrown crystal is mostly defect free, however, a region of large damage just beneath the original amorphous/crystalline interface can exist. This is the EOR damage region.
1.3.2 End-Of-Range Defect Evolution

The interstitials in the EOR damage can evolve into several defect types depending on the implant and the annealing conditions. One such type is the \{311\} defect, a rod-like structure that inhabits the \{311\} plane and grows in the \langle110\rangle direction. As Frenkel pairs are annihilated very quickly, the remaining interstitials will bond to form small clusters. These clusters can form \{311\} defects if the implant energy is high enough, or small dislocation loops. King et al. [12], King [13], and Gutierrez [14] have shown that 5keV implant energy is not high enough to nucleate \{311\}’s with Ge\(^+\) and that in many cases 10keV may not be enough. If \{311\}’s do form, they can eventually dissolve into Frank loops and eventually perfect dislocation loops. Eaglesham et al. [15] have proposed that the dissolution of the \{311\} defects correlated the anomaly of transient-enhanced diffusion which depends on interstitials to drastically increase dopant diffusivity for those species which exhibit an interstitialcy-driven diffusion process such as boron. Additionally, Li and Jones [16] have shown that \{311\} defects are the source of interstitials for dislocation loops.

During annealing the dislocation loop behavior can be described by the Ostwald ripening theory. This theory states that the large dislocation loops grow at the expense of the smaller ones, which is a more stable configuration [17]. Similar behavior for \{311\}’s has been observed by Stolk et al. [18]. An evolution tree for the case of Si\(^+\) implantation can be seen in Figure 1.3. This figure shows the observations from several experiments [15, 16, 18, 19] that the defects undergo four stages of evolution: nucleation, growth, coarsening, and dissolution.
### 1.3.3 Transient Enhanced Diffusion

Transient enhanced diffusion (TED) is an anomalous process by which the excess of interstitials created during ion implantation greatly enhanced dopant diffusivity for very short time scales. It is important to understand this process so that simulation tools such as FLOOPS (FLorida Object Oriented Process Simulator) [21] can be accurate in their predictions of dopant diffusion.
The source of the interstitials in TED is thought to come from dissolution of the \{311\} defects for the non-amorphous implant case [15, 18, 22]. For the amorphous case, dislocation loops are also thought to play a role in TED [4, 19]. The effect of species, dose, implant energy, and annealing temperature on TED has been studied extensively. Saleh et al. [23] found that TED was dependent on implant energy for \(1 \times 10^{14} \text{ cm}^{-2} \) Si+ implants; Eaglesham et al. [24] came to the same conclusion. This supports findings by Lim et al. [25] that surface etching results in TED reduction, which demonstrates that the surface plays a role in annealing implant damage. However, during an anneal after an amorphous implant, the surface is less important since the amorphous layer acts as a diffusion barrier to interstitials in the EOR layer [26].

**1.4 Scope and Approach of this Study**

The work in this study is divided into two major parts. The first part deals with expanding the experiment first started by Gutierrez [14] in exploring the interstitial evolution for low-energy Ge+ amorphizing implants in Chapter 3. Implants of Ge+ at conditions of \(5 \times 10^{14} \text{ cm}^{-2} \) at 10keV, \(2 \times 10^{15} \text{ cm}^{-2} \) at 5 and 10keV, and \(5 \times 10^{15} \text{ cm}^{-2} \) at 5 and 10keV were made into Si wafers. Plan-view TEM is used to observe the defect evolution through a series of anneals at 750°C for 5-60 minutes. The results will be helpful in understanding the EOR kinetic behavior which will lead to improved modeling in process simulators.

The second part deals with simulations using FLOOPS and the effect of the surface on \{311\} dissolution in Chapter 4. Two sets of simulations were performed for this work. The first set deals with increasing the surface recombination rate for interstitials to observe how the surface affects the dissolution rate of \{311\}'s. A model by Law and Jones [27] is the basis for these simulations. The second set of simulations uses
modifications to that model by Seebauer et al. [28, 29, 30, 31, 32] which induces an electrical field at the silicon surface. The effect of the magnitude of this field is investigated on the \( \{311\} \) dissolution rate. Finally, further possibilities for experimentation are discussed in Chapter 5.
CHAPTER 2
EXPERIMENTAL AND DATA EXTRACTION PROCEDURES

This chapter contains an overview of the methods for sample preparation and data extraction techniques for the dose and energy dependence experiment.

2.1 Overview

Implants were performed by Core Systems, Inc. into Czochralski-grown (100) wafers. Ge+ was implanted at room temperature at a 7° tilt to reduce channeling. Samples were annealed in a nitrogen ambient at 750° C for 5-60 minutes using a quartz tube furnace. A 30-second push-pull technique was used to minimize thermal stresses. Implant damage was viewed using a JEOL 200CX transmission electron microscope (TEM). Defect counts were performed using scans of negatives created by the TEM using Adobe Photoshop 7.

2.2 TEM and Sample Preparation

Transmission electron microscopy is the primary way of directly viewing damage from an implant for this experiment. For viewing the damaged specimens from the top-down, plan-view (PTEM) is used. PTEM images allows for defects to be visible in the g\textsubscript{220} weak-beam dark-field (WBDF) condition with a g\textsubscript{*3g} diffraction pattern if the dot product of the reciprocal lattice vector and the cross product of the Burgers vector and dislocation line direction are not equal to zero [13].

PTEM samples must be made in order for the microscope to image effectively. They are prepared in the following fashion:
1. A 3mm disc is cut from the annealed sample using an ultrasonic disc cutter from Gatan, Inc. The cutter uses a silicon carbide (SiC) abrasive powder and water. The sample is held in place by mounting it to a glass slide with crystal bond. The glass slide is then held to the disc cutter stage using double-sided tape. Acetone is used to remove the crystal bond from the sample after cutting.

2. The disc is then thinned by hand using a lapping fixture. The sample is mounted face-down (i.e. the implanted side down) to a metal stage using crystal bond. The sample is then thinned with figure-eight motions to \(~100 \mu m\) determined by finger touch and visual inspection. A 15\(\mu m\) slurry of aluminum oxide (Al\(_2\)O\(_3\)) and water is used for abrasion on a glass plate. Acetone is again used to clean crystal bond off the sample.

3. Specimens are then mounted face-down to a Teflon stage using hot wax, leaving only a small portion of the backside uncovered. The sample is then further thinned using an acid etch of 25% hydrofluoric acid (HF) and 75% nitric acid (H\(_3\)NO\(_3\)). The sample is etched until a small bright spot is visible through the entire sample surrounded by a reddish area.

4. The etched samples are carefully removed from the Teflon stage and soaked in heptane overnight or until all wax has been removed from the sample.

2.3 PTEM Analysis and Data Extraction

The images generated from the PTEM can be seen in Appendix A. The defect densities are simply the count of defects in the observed area. Negatives are scanned into a .bmp file using an Epson Perfection 3490 Photo scanner at 300dpi. Using Adobe Photoshop, a 4cm x 4cm grid, or larger for lower defect densities, is laid over the image. The image is zoomed to an appropriate level for easy viewing, and the grid overlay maintains its scale. The defects are then counted within a grid square and divided by the area to determine the defect density. The negatives are enlarged by a scale of 50,000x by the TEM, so an appropriate factor of 50k\(x^2\) for area enlargement is included in the defect counts. The results are averaged over at least 5 squares on the negatives for each implant and anneal condition. There is an intrinsic +/- 20% error in this method. For the longer anneals, as fewer defects are counted, the error goes up as the number of samples are reduced and less data is available. This source of error could dramatically change the endpoints and the slope of the fitted curve if the curve is fit to the error range instead of
the data point. For example, in counting the 2e15, 5keV implant at 60 minutes, the number of defects per square was found to be anywhere from zero to twelve, but only four different areas could be counted due to the size of the squares, which was four times as large as the areas used for the five minute images. So, for this example, the defect density of 2.2e9 defects/cm² was found by counting an average of 5.5 defects in an area of 2.5e-9 cm² (6.25 cm² on the viewed image with the magnification).

Data extraction consists of using Microsoft Excel to fit an exponential curve of the form $y = A e^{x}$, where $x = -t/\tau$. In this equation, $t$ is the anneal time and $\tau$ is rate of decay. Other methods are also used to explore the effects of certain variables on $\tau$. For example, the prefactor $A$ is averaged for all implants and then the data forced to fit a curve with this new term. In addition, the effect of the 20% error was explored by changing the values of the 5 and 60 minute anneals to both +20% and -20% of the observed value. The changes are then fit with an exponential curve to see the change in the decay rate. The entire data set is also graphed and fit to a curve to find the ‘average’ value of the decay rate, and to determine if dose, energy, or both have an effect on the decay rate of defects. Comparisons are also made to previous work by Gutierrez [14].

2.4 Procedures for Simulation Experiments

For the work done using simulations, FLOOPS (FLorida Object Oriented Process Simulator) was used along with a defect evolution model by Law and Jones [27]. In the first experiment, the surface reaction rate which controls interstitial recombination was shifted. The resulting effect on {311} defect dissolution was investigated for a Si⁺ implant into a Silicon substrate for 40, 80, and 160 keV energies. The value was changed from 1e-11 to 1e-2 cm/s.
For the second simulation experiment, code developed by Seebauer was incorporated into the model [29]. This code affects the surface potential using a modified Poisson equation, setting up an electric field pointing into the bulk. The code added into FLOOPS for these simulations can be found in Appendix B. The effects of the electric field on \{311\} dissolution was investigated.
CHAPTER 3
DOSE AND ENERGY DEPENDENCE EXPERIMENT

This chapter discusses the results of the investigation of defect dissolution dependence on the dose and energy of the pre-amorphizing implant.

3.1 Overview

The purpose of this experiment was to further investigate the energy and dose studies previously done by Gutierrez [14]. Implants were chosen to compliment the $1e15$ cm$^{-2}$ implants at 5 and 10keV and the 5keV implants at $5e14$ cm$^{-2}$ and $3e15$ cm$^{-2}$ which Gutierrez studied. Implants in this experiment were performed at 10keV for $5e14$ cm$^{-2}$, $2e15$ cm$^{-2}$, and $5e15$ cm$^{-2}$, and at 5keV for $2e15$ cm$^{-2}$ and $5e15$ cm$^{-2}$. Table 3.1 lists the implants performed in this work and the relevant implants performed by Gutierrez.

Gutierrez has previously reported that these low energy implants follow a specific evolutionary pathway that results in small, unstable dislocation loops [14]. These loops dissolve quickly after approximately 60 minutes with an anneal temperature of 750° C [14]. Data in this chapter will be shown to be in agreement with previous work.

3.2 Results for 750° C Anneals

The data for the defect counts from each implant condition can be viewed in figures 3.1-3.5. These figures plot the defect density (in #/cm$^2$) against time on a log-linear scale. Data for each figure can be found in Appendix C. In addition, the PTEM images for each annealed implant can be seen in Appendix A, images A.1 through A.5. The images show that the defect types formed are small interstitial clusters and dislocation
loops. No \{311\} defects were observed at any time point. The evolution of the dislocation loops followed an Ostwald-ripening mechanism but did not coarsen greatly.

As the graphs show, the defects that are formed in these low-energy implants are not stable. The average decay rate was approximately 20 minutes. From this average, and by visual inspection of the PTEM images, it can be concluded that the small dislocation loops formed are almost completely dissolved by the 60 minute time point for all implant conditions. Table 3.2 lists the decay rate and $R^2$ for each implant taken from the exponential curve fit to the data.

From the table below, the data shows a strong fit for all but one of the curves, $5e15 \text{cm}^{-2}$ with $5\text{keV}$ energy. Similarly, only one implant, $2e15 \text{cm}^{-2}$ with $10\text{keV}$ energy, is not within one standard deviation of the average. As mentioned before, the amount of error goes up with fewer defects since the amount of statistical data is less. This could improve the $R^2$ value if the data is fit with larger error bars on the 60-minute data points.

**3.3 Discussion and Analysis**

Further statistical analysis was performed on the data to determine the trends. Figure 3.6 shows in graphical form the decay rates of the five implants together. From this figure it can be seen that no trend exists either by dose or by energy of the implant. There are $5\text{keV}$ implants with decay rates larger than the $10\text{keV}$ implants, as well as a smaller dose implant ($2e15 \text{ cm}^{-2}$) with a larger decay rate than that of the largest dose implants. One would assume that any trend, if present, would indicate that higher energy and higher dose would lead to more damage and longer dissolution time.

The data set as a whole was also graphed and fit to a curve. This graph can be seen in Figure 3.7. The decay rate from this curve was found to be 19.12 minutes with an $R^2$
value of 0.778. Comparing this value with a curve fit to an average value at each time point we get a decay rate of 20.79 minutes but an R² value of 0.9913.

In comparison to previous work by Gutierrez, the same trend is noticeable in each data set with the exception of one 5e14 5keV implant by Gutierrez which exhibits a spontaneous combustion beginning around the 45-minute time point and then rapidly dissolving by 60 minutes. Figure 3.8 shows both data sets together on the same graph up to the 60 minute anneals. It should be noted that Gutierrez’s original data was not available, so it was extracted from the graphs available in [14]. Also of note is that Gutierrez performed sub-5 minute anneals using an RTA furnace. That data is included in Figure 3.7.

In his thesis, Gutierrez also concluded that dose does not have a significant qualitative or quantitative effect on defect evolution at low energy [14]. The data presented here supports and affirms that conclusion. Gutierrez does state that there is a heavy dependence on energy for defect behavior [14]. However, there are two regimes for the dependence, and 5-10keV energies exhibit the same behavior, whereas 30+keV energies form different defect morphologies. From the PTEM micrographs in Appendix A and in [14], it is shown that {311}’s do not form in the low-energy regime; only small, unstable dislocation loops. Previous work has suggested a pathway for the defect evolution for these low energy Germanium implants, as in Figure 3.9.

3.4 Summary

This chapter has presented the data obtained through the defect counts performed on the anneals of amorphizing Ge⁺ implants into silicon wafers. The data shows no trend in defect dissolution time in line with increasing dose or energy. The lack of trends is in
agreement with earlier experiments by Gutierrez [14]. In addition, only small point defects and unstable dislocation loops were observed.

![Defect density dissolution and curve fit for 5e14 10keV implant. The curve equation is listed on the graph.](image)

Figure 3.1 Defect density dissolution and curve fit for 5e14 10keV implant. The curve equation is listed on the graph.
Figure 3.2 Defect density curve for $2 \times 10^{15}$ 10keV implant. The curve equation is listed on the graph.
Figure 3.3 Decay curve for 2e15 5keV implant. The curve equation is listed on the graph.

\[ y = 7E+10e^{-t/15.7\text{min}} \]
Figure 3.4 Dissolution curve for 5e15 5keV implant. The curve equation is on the graph. Note that this curve has the smallest $R^2$ value (.7456) of the five implants.
Figure 3.5 Dissolution curve for 5e15 10keV implant. The curve equation is listed on the graph.

Table 3.1 List of implants done in this work and relevant previous work by Gutierrez. A starred (*) condition indicates work done by Gutierrez.

<table>
<thead>
<tr>
<th>Implant Dose (cm⁻²)</th>
<th>Implant Energy (keV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>5e14*</td>
<td>5*</td>
</tr>
<tr>
<td>5e14</td>
<td>10</td>
</tr>
<tr>
<td>1e15*</td>
<td>5*</td>
</tr>
<tr>
<td>1e15</td>
<td>10*</td>
</tr>
<tr>
<td>2e15</td>
<td>5</td>
</tr>
<tr>
<td>2e15</td>
<td>10</td>
</tr>
<tr>
<td>3e15*</td>
<td>5*</td>
</tr>
<tr>
<td>5e15</td>
<td>5</td>
</tr>
<tr>
<td>5e15</td>
<td>10</td>
</tr>
</tbody>
</table>
Table 3.2 Decay rates and $R^2$ values (a measure of how well the curve fits the data) for each implant.

<table>
<thead>
<tr>
<th>Implant</th>
<th>Decay Rate (min)</th>
<th>$R^2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>5e14 @ 10keV</td>
<td>15.43</td>
<td>.9706</td>
</tr>
<tr>
<td>2e15 @ 5keV</td>
<td>15.7</td>
<td>.938</td>
</tr>
<tr>
<td>2e15 @ 10keV</td>
<td>28.99</td>
<td>.9587</td>
</tr>
<tr>
<td>5e15 @ 5keV</td>
<td>22.12</td>
<td>.7454</td>
</tr>
<tr>
<td>5e15 @ 10keV</td>
<td>18.8</td>
<td>.9028</td>
</tr>
<tr>
<td>Average</td>
<td>20.21</td>
<td>5.61 min (std dev)</td>
</tr>
</tbody>
</table>

Figure 3.6 Decay rates for each implant condition. Note that there is no apparent trend in dose or energy.
Figure 3.7 Graph of data set for all implants together. Curve fit equation and $R^2$ value is on the graph. Note that a fit of the average value at each anneal time yields about the same decay rate but an $R^2$ value of 0.9913.
Figure 3.8 Comparison of data from this work and previous work by Gutierrez [14]. The data sets follow similar trends with the exception of the 5e14 5keV implant by Gutierrez. The reader is referred to Table 3.1 for which implants were performed for this work.
Figure 3.9 Germanium implant defect evolution tree [14]. This is an alternate path to the high energy implants which form stable loops and \{311\}'s. The highlighted grey path is the observed path both here and by Gutierrez.
CHAPTER 4
EFFECTS OF THE SURFACE ON SIMULATED END-OF-RANGE DAMAGE

4.1 Overview

This chapter details experiments made using FLOOPS to investigate the effects of the free Silicon surface on end-of-range damage, specifically \{311\} defects. In the first experiment, the model by Law and Jones [27] was used to simulate damage from multiple energy implants and a subsequent 750°C anneal. For the second set of simulations, a model by Seebauer et al. [28, 29 30, 31, 32] was incorporated into the Law and Jones model to create an electric field on the free surface and explore the effects on \{311\} evolution, if any. Code for the Seebauer model can be found in Appendix B.

4.2 Surface Reaction Rate Effects on \{311\}’s

This first simulation experiment explores the effects of the value of the variable “ksurf” on \{311\} evolution. The variable “ksurf” is a measure of how quickly silicon interstitials and di-interstitials recombine at the surface. It is important to know this effect, since during an annealing step, when \{311\}’s begin to dissolve, they release interstitials which contribute to TED [15, 33]. The interstitials eventually recombine back into the lattice at the surface or interact with a vacancy to fill a lattice site. The default value of “ksurf” is

\[
4\pi*2.7e^{-8}*0.138 \exp(-1.37eV/kT)\times
\{0.51e14 \exp(2.63eV/kT)/(1.0e15 + 0.51 \exp(2.63eV/kT)}\]
\]

which is \(4\pi\) multiplied by the lattice spacing which makes up a capture radius for the defects, default interstitial diffusivity, and kink-site density, and where k is Boltzmann’s
constant and T is temperature. The kink-site density is limited by the denominator inside the braces \{\}. It represents a limit to the number of capture sites available at the surface and the energy required to reincorporate an interstitial. The default value for “ksurf” is set at 6e-19 cm/s for interstitials flowing to a silicon/silicon dioxide interface. This value is greatly increased for this experiment to observe its effects.

The physics behind the “ksurf” variable can be thought of as a Deal-Grove type kinetic model with relation to the surface which is similar to the linear-parabolic model of silicon oxidation. Using this model, the “ksurf” variable can be thought of as controlling the limiting process in \{311\} dissolution just as oxide thickness is the limiting step in oxide growth [1]. In other words, when “ksurf” is very large, the dissolution rate is limited by the source of the interstitial, i.e. the defect population. In this regime, the release of interstitials from the defects is the limiting step in defect dissolution, since they will immediately diffuse to the surface and recombine. For very deep damage layers, dissolution also depends on the diffusion length to the surface, which could be a competing factor to interstitial release for the limiting step. This is comparable to the linear oxidation regime in which surface reaction is the limiting step. When “ksurf” is small, the limiting factor for interstitial recombination at the surface is the diffusion length and the recombination rate, meaning that interstitials will not necessarily be able to recombine as soon as they reach the surface. In this case, however, the interstitials are likely diffusing more into the bulk than toward the surface, which would be an even greater limiting step. For this reason, the decay rates for the different energies are very close. This behavior is comparable to the parabolic oxidation regime where diffusion to the silicon/oxide interface limits oxide growth. It is, therefore, comparable to change
“ksurf” to vary the distance to the surface, which is thought to control the dissolution rate of \{311\} defects [15, 25, 34].

The model addresses \{311\} evolution and sub-micron interstitial clusters (SMIC’s) which influence TED [4, 15, 23, 27, 33]. The model is based on experimental data by Law and Jones, and the observations that \{311\} defects dissolve at a nearly constant rate (2.3nm/min at 770°C) due to the constant end-size of the defect, and that the population decays proportionally to the interstitial loss rate and inversely to the size of the defect. In addition, the defect size is not dependent on energy. The dissolution rate is a function of the interstitial release rate rather than interstitial diffusion to the surface [27].

The model specifically solves for the number of trapped interstitials in the defects and the total number of defects, referred to as \(C_{311}\) and \(D_{311}\), respectively. The defects begin nucleation during the implant, and are simulated using UT-Marlowe and the kinetic accumulation damage model. The defects begin as small \{311\}’s or SMIC’s, and then either grow in the case of \{311\}’s or dissolve to the surface for SMIC’s. The capture and release of interstitials by \{311\}’s happens only at the end of the defect and is therefore proportional to the number of defects in the population, \(D_{311}\), hence the nearly constant dissolution rate. Moreover, this means that the dissolution rate is also dependent on defect size for a given number of trapped interstitials, \(C_{311}\), since a larger defect population has fewer defects and therefore fewer ends at which interstitials can be released. The following equations model the described behavior.

\[
\frac{dC_{311}}{dt} = \frac{D_{311}(C_1 - C_{311\ Eq})}{\tau_{311}} \quad 4.2 \\
\frac{dD_{311}}{dt} = \frac{-D_{311}*C_{311\ Eq}/\tau_{311}}{D_{311}/C_{311}} \quad 4.3
\]
\[ \frac{dC_{SMIC}}{dt} = C_{SMIC}(C_i - C_{SMIC_{Eo}})/\tau_{SMIC} \]

The above equations use energetics proposed by Cowern [35], and the SMIC’s have a dissolution energy of 3.1 eV and the total dissolution energy for the \{311\}’s is 3.77 eV. The final term in equation 4.3 is the inverse of the average size which accounts for the observation of the smaller defect populations dissolving faster. For comparisons to experimental data the reader is referred to [27] and the data included in [23].

The model was used for simulations of 40, 80, and 160 keV Si+ implants into silicon and a subsequent anneal of 135 minutes at 750°C. Of interest is the value for \(\tau_{311}\) which is the decay rate constant.

The data trends can be seen in Figure 4.1. From this graph, a slight decrease in dissolution time can be observed when “ksurf” is increased to 1e-6 cm/s. The data can be found in Table 4.1. At this point, all the implants undergo a rapid decrease in dissolution times. Simulations were also performed for “ksurf” with values of 1e-20 and 1e10 for several of the implants. That data is not included in the figure to improve the scale, and because the values are very close in value to the value at the presented endpoints.

4.3 Effects of a Surface Field on \{311\}’s

This set of simulations uses a modified version of the model found in section 4.2. The defect kinetics for the \{311\} and SMIC type defects remains unchanged. What is added is a new effect of band-bending at the surface that is a result of the silicon/oxide interface [28, 29, 30, 31, 32]. Figure 4.2 shows how the band-bending functions in p-type silicon. The band-bending is attributed to defects created at the interface which lead to bond rupture [28]. The resulting degree of band-bending is about 0.5 eV at a maximum [28, 29]. The band-bending persisted for all annealing times and temperatures performed by Seebauer at al [29]. The band-bending is used to explain the pile-up of electrically
active boron within 1nm of the interface as well as deepening of the junction depth because the near-interface electric field repels charged interstitials. For more detail on the behavior of boron in this model, the reader is referred to work in [28, 29, 30, 31, 32].

Of interest in this model are two important aspects. The first is the changes to the surface modeling using new terms to determine a surface annihilation probability for interstitials. The second is a new form of Poisson’s equation with new boundary conditions to set up the near-surface band-bending.

For the surface modeling, a new fraction \( f \) controls the ability of the surface to act as either a reflector or sink. The fraction \( f \) is then incorporated into a parameter \( S = 1-f \) which is an annihilation probability [29]. The nature of the surface is then controlled by the following equation.

\[
-D_j \frac{dC_{j,x=0}}{dx} = D_j \frac{(S*C_{j,x=\Delta x})}{\Delta x} = kr * C_{j,x=\Delta x}
\]

where \( \Delta x \) represents a point in the bulk and \( C_j \) is the concentration of the dopant species. For this equation, a value of \( f = 1 \) (\( S = 0 \)) corresponds to a perfect reflector and \( f = 0 \) (\( S = 1 \)) corresponds to a perfect sink. \( S \) was modeled as a constant to be fit to experimental data [29]. The conclusions of Seebauer et al. was that experiments with band-bending present exhibit a much lower annihilation probability than experiments at flat band [29].

New boundary conditions for Poisson’s equation represent an approximation that the interface Fermi energy is located 0.5eV above the \( E_v \) level of the silicon side of the interface. The approximation is made for computational simplification [29]. The new boundary conditions are detailed below in the following equations.

\[
\Psi(x = 0,t) = \Psi_s
\]

\[
\Psi(x = 0,t) = E_v (T)/ q + (0.5eV )/ q
\]
Both equations are presented by Seebauer et al. in [29]. Two regimes were observed: the first in which band-bending increases to 0.56 eV between 300°C to 500°C, and the second in which band-bending decreases to zero above roughly 750°C. A temperature ramp was performed to see the effects of the low-temperature regime, but temperature was never increased past 750°C for simulations performed in this work. The variable of interest is the ‘pin’ value, which sets the potential in electron volts at the surface. The default value of this variable is 0.2 eV.

The results of the simulations can be seen below in Figures 4.3 and 4.4. Figure 4.3 is a graphical representation of the potential produced by the Seebauer modifications. A very low energy B implant was used as the electrically active species to produce this curve. For figure 4.4, the 40 keV implant condition was used from the previous section with a “ksurf” value of 1e-6 cm/s. As can be seen, the pin value has no trend in its effect on the dissolution rate of the {311} defects. All values fall within two standard deviations of the average value of 67.6 minutes. This result is not surprising, since the modifications are intended to influence electrically active dopants, not silicon interstitials released from {311}’s. This is not much different than the value for the simulations without the new Poisson equation and boundary conditions, which was a value of 64.03 minutes.

**4.4 Summary**

This chapter has presented several surface effects on the {311} defect population. The varying of the “ksurf” variable, which controls the recombination rate of interstitials and di-interstitials at the surface, was varied for implants of 40, 80, and 160 keV implants at a dose of 1e15 cm⁻². There was little change in the 40, 80, and 160 keV implants until a “ksurf” value of 1e-6 cm/s, when a sharp drop occurred but leveled out for larger values.
For the second set of simulations, a near-surface electrical field was introduced and the pinned potential value at the surface varied for the 40keV implant condition with a “ksurf” value of 1e-6 cm/s. The \{311\} dissolution time had no apparent influence from the surface field or a changing pin value at the surface.

![Ksurf vs Tau](image)

Figure 4.1 Effect of changing “ksurf” for each implant energy on the dissolution time of \{311\} defects.

<table>
<thead>
<tr>
<th>ksurf (cm/s)</th>
<th>40 keV</th>
<th>80 keV</th>
<th>160 keV</th>
</tr>
</thead>
<tbody>
<tr>
<td>1e-20</td>
<td>104.14</td>
<td>125.2</td>
<td>n/a</td>
</tr>
<tr>
<td>1e-11</td>
<td>112.82</td>
<td>140.71</td>
<td>206.55</td>
</tr>
<tr>
<td>1e-10</td>
<td>109.82</td>
<td>138</td>
<td>208.34</td>
</tr>
</tbody>
</table>
Figure 4.2  Schematic of band bending energy diagram for p-type silicon showing a narrow space-charge region and its influence on charged particles [29].
Figure 4.3  Potential curve created from a low energy B implant into silicon.
Figure 4.4 Effect of surface pinning value on the dissolution rate of \{311\}’s created by a $10^{15}$ cm$^{-2}$, 40keV Si$^+$ implant into silicon. There is no apparent trend in the effect of the surface pin on the dissolution time.
CHAPTER 5
CONCLUSIONS AND FUTURE WORK

5.1 Overview

The purpose of this work is twofold: to further explore the effects of the surface on \{311\} defect evolution, and to flesh out previous work by Gutierrez [14] regarding the defect evolution of low-energy amorphizing Ge\(^+\) implant into silicon. The exploration of \{311\} defect evolution is important because \{311\}’s are the major contributing source of interstitials to TED [1, 4, 15, 23, 33, 36]. By understanding the evolution more accurately, modeling of the process flow becomes more exact and therefore more useful. Investigation of the defect evolution resulting from a Ge\(^+\) PAI is important since Ge\(^+\) is becoming a popular species for amorphization since it achieves amorphization of the substrate at lower doses and energies than silicon self-implantation. Understanding the morphology and evolutionary behavior of these defects is a key step in modeling them.

5.2 Dose and Energy Dependence Experiment

Silicon wafers were implanted with 5keV and 10keV Ge\(^+\) at doses of 5e14 cm\(^{-2}\), 2e15 cm\(^{-2}\), and 5e15 cm\(^{-2}\). They were subsequently annealed at 750°C for 5-60 minutes, and the defect densities were counted using PTEM micrographs, which can be seen in Appendix A along with the counting data. All observed defects were small interstitial clusters and small dislocation loops, both of which were unstable at the anneal temperature. The defect dissolution was fit to an exponential decay curve for each implant condition as well as for the data set as a whole. There was no observed dependence or trend with regards to energy or dose. All decay constants were within two
standard deviations of the average decay constant of 20.21 minutes. The defects were almost completely dissolved by 60 minutes. The data is in general agreement with previous work by Gutierrez [14] and the comparison of curves can be found in Figure 3.8. One aspect of note, however, was that the spontaneous combustion observed by Gutierrez for the 5keV, 5e15 cm⁻² implant condition was not observed for similar conditions in this work.

5.3 Simulated Effects of the Surface on {311} Evolution

Simulations were performed using FLOOPS and model of {311} evolution by Law and Jones [27] based on experimental data by Saleh et al. [23]. For a detailed explanation of the model, please refer to Chapter 4. The value of the variable “ksurf” which represents a surface reaction rate was varied to see the effect on {311} dissolution from 1e-10 cm/s to 1e-2 cm/s. This was done as an alternative to changing the distance to the surface since {311} dissolution is thought to depend on the distance of the damage layer to the surface [25]. The simulations were performed on implants of 1e15 cm⁻² Si⁺ into silicon with energies of 40, 80, and 160 keV. All implants showed little effect until “ksurf” was raised to 1e-6 cm/s, when a steep drop was observed until 1e-2 cm/s where the values leveled off.

Additional simulations were performed using the same model but with modifications by Seebauer et al. [29] which uses an electrical field at the surface to explain both dopant pile-up and junction broadening of boron implants. The simulations were performed on the 40keV Si⁺ implant by setting “ksurf” to 1e-6 cm/s and changing the pin value which controls the fixed value of the electrochemical potential at the silicon/oxide interface. The simulations showed no trend or dependence on the effect of the pin value in {311} dissolution. All values were consistent with minor variations and
very close to the value obtained in the simulations without the modifications by Seebauer et al. This is not surprising since the modifications were developed to effect charged ion species and not silicon interstitials.

### 5.4 Future Work

Several experiments can be performed in order to make both parts of this work more conclusive. For the energy and dose dependence study, an attempt to recreate the conditions of Gutierrez’s $5 \times 10^{14}$ cm$^{-2}$ 5keV implant and the observed spontaneous combustion around 30 minutes is needed to prove if that condition is anomalous or if a new regime for defect evolution starts with that condition. Additionally, annealing of the implant conditions at 825°C would provide more data to compare to work by Gutierrez [14] and King [13].

For the simulation part of this work, some minor additions could be added to increase the amount of data available for analysis. The simulations with “ksurf” and with the pin value could be re-run at a lower temperature, to see if the band-bending has more effect and to compare at other values of “ksurf”. In addition, the simulations with the electric field could be run for other energies, but it is unlikely that these simulations would show any trend or influence on the \{311\} evolution.
Figure A.1 PTEM micrographs of a 5e14 10keV implant and 750°C anneal. Each image is approximately 20μm across. A) 5 minutes, B) 15 minutes C) 30 minutes D) 45 minutes, E) 60 minutes.
Figure A.2 PTEM micrographs for a 2e15 5keV implant annealed at 750°C. Each image is approximately 20μm across. A) 5 minutes, B) 15 minutes C) 30 minutes, D) 45 minutes, E) 60 minutes.
Figure A.3 PTEM micrographs for a $2 \times 10^{15}$ 10keV implant and 750°C anneal. Each image is approximately 20μm across. A) 5 minutes, B) 15 minutes, C) 30 minutes, D) 45 minutes, E) 60 minutes.
Figure A.4 PTEM micrographs of a 5e15 5keV implant annealed at 750°C. Each image is approximately 20μm across. A) 5 minutes, B) 15 minutes, C) 30 minutes, D) 45 minutes, E) 60 minutes.
Figure A.5 PTEM micrographs for a 5e15 10keV implant annealed at 750°C. Each image is approximately 20μm across. A) 5 minutes, B) 15 minutes, C) 30 minutes, D) 45 minutes, E) 60 minutes.

<table>
<thead>
<tr>
<th>time (min)</th>
<th>5e14 10keV</th>
<th>2e15 10keV</th>
<th>2e15 5keV</th>
<th>5e15 10keV</th>
<th>5e15 5keV</th>
<th>data average</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>6.89E+10</td>
<td>7.57E+10</td>
<td>5.49E+10</td>
<td>4.51E+10</td>
<td>1.36E+11</td>
<td>7.61E+10</td>
</tr>
<tr>
<td>15</td>
<td>3.43E+10</td>
<td>4.53E+10</td>
<td>3.80E+10</td>
<td>3.21E+10</td>
<td>5.93E+10</td>
<td>4.18E+10</td>
</tr>
<tr>
<td>30</td>
<td>2.14E+10</td>
<td>2.43E+10</td>
<td>6.53E+09</td>
<td>2.59E+10</td>
<td>1.42E+10</td>
<td>1.85E+10</td>
</tr>
<tr>
<td>45</td>
<td>4.12E+09</td>
<td>1.81E+10</td>
<td>3.10E+09</td>
<td>2.20E+10</td>
<td>1.05E+10</td>
<td>1.16E+10</td>
</tr>
<tr>
<td>60</td>
<td>2.14E+09</td>
<td>1.05E+10</td>
<td>2.20E+09</td>
<td>2.40E+09</td>
<td>7.40E+09</td>
<td>4.93E+09</td>
</tr>
</tbody>
</table>

Table A.1 Data set used for graphing figures 3.1-3.8.
APPENDIX B
FLOOPS MODIFICATIONS BY SEEBAUER ET AL.

Note that the real portion of interest is the end of the code which sets the boundary conditions and the changes to the Poisson Equation.

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```tcl
proc SurfConc {Sol} {
    set y [lindex [lindex [print.1d name=$Sol] 1] 1]
    return y
}

proc TEDspike {EBi EI Eko Eki Edis clEa2 clEa3 clEa4 clEa5 Emix Btrap Strap Ebb rate T fudge Name} {
    # Initializing
    init inf=grid3.str
    sel z=1.0 name=f2 store
    sel z=1.0 name=f3 store
    sel z=1.0 name=f4 store
    sel z=1.0 name=f5 store
    sel z=1.0 name=BsBi store
    sel z=1.0 name=BsI store
    sel z=1.0 name=BsBiI store
    sel z=1.0 name=BsI2 store
    sel z=1.0 name=BsBiI2 store
    sel z=1.0 name=BsI3 store
    sel z=1.0 name=BsBi2I store
    sel z=1.0 name=BsI2I2 store
    sel z=1.0 name=BsBiI3 store
    sel z=1.0 name=BsI4 store

    # Choosing Poisson Eqn and its boundary condition
    pdbSetBoolean Silicon Potential TEDmodel 1
    pdbSetBoolean Silicon Potential Pin 0

    # define the species to be simulated
```
solution name=MyBi solve !damp !negative add
solution name=MyBs solve !damp !negative add
solution name=MyI solve !damp !negative add

# define all the parameters (diffusivity, rate of reaction, etc)

# Common parameters (note: Ea is binding energy)
set tempK [pdbDelayDouble tempK]
term name=kb add Silicon eqn = "8.617383e-05"
term name=pi add Silicon eqn = "3.14159e0"
term name=captr add Silicon eqn = "2.73e-8"
term name=alpha add Silicon eqn = "kb*$tempK"
term name=Eg add Silicon eqn = "(1.17e0-(4.73e-4*$tempK*$tempK)/($tempK+635.0e0))" 
term name=ni add Silicon eqn = "4.84e15*($tempK^1.5)*exp(-Eg/(2.0e0*kb*$tempK))"
term name=nu add Silicon eqn = "6.1e12"

# Energy levels
term name=Ei add Silicon eqn = "-Potential"
term name=Ev add Silicon eqn = "-Eg/2.0e0-Potential"
term name=Ec add Silicon eqn = "Eg/2.0e0-Potential"
term name=EF add Silicon eqn = "0.0"

# Asumme equilibrium electron and hole concentration
term name=Myn add Silicon eqn = "ni*exp((EF-Ei)/(kb*$tempK))"
term name=Myp add Silicon eqn = "ni*exp((Ei-EF)/(kb*$tempK))"

# Trap energies
term name=ESi add Silicon eqn = "((Eg/1.170e0)*$Strap)+Ev"
term name=EBi add Silicon eqn = "((Eg/1.170e0)*$Btrap)+Ev"

# population of charged species

# +2 Si interstitial
term name=thlp2 add Silicon eqn = ”1/(1+0.5e0*exp((EF-ESi)/(kb*$tempK)))”
# Neutral Si interstitial
term name=thln1 add Silicon eqn = ”1/(1+2e0*exp((ESi-EF)/(kb*$tempK)))”
# +1 Boron interstitial
term name=thBip add Silicon eqn = ”1/(1+exp((EF-EBi)/(kb*$tempK)))”
# -1 Boron interstitial
term name=thBin add Silicon eqn = ”1/(1+exp((EBi-EF)/(kb*$tempK)))”

# Diffusivity
term name=diffBi add Silicon eqn = ”1.0e-3*exp(-$EBi/(kb*$tempK))”
term name=diffI add Silicon eqn = ”1.0e-3*exp(-$EI/(kb*$tempK))”
# Necessary terms to make diffusion equations readable by Floops

# For +/- Boron interstitial
# term name=Bi1 add Silicon eqn = "grad(Potential*thBip*MyBi)-grad(Potential*thBin*MyBi)"
# term name=Bi2 add Silicon eqn = "(thBip-thBin)*MyBi*grad(Potential)"
# term name=Bi3 add Silicon eqn = "Potential*(grad(thBip*MyBi)-grad(thBin*MyBi))"

# For +/- Boron interstitial
term name=Bi1 add Silicon eqn = "grad(Potential*thBip*MyBi)"
term name=Bi2 add Silicon eqn = "(thBip)*MyBi*grad(Potential)"
term name=Bi3 add Silicon eqn = "Potential*(grad(thBip*MyBi))"

# For 2+/0 Si interstitial
term name=I1 add Silicon eqn = "2.0e0*grad(thIp2*Potential*MyI)"
term name=I2 add Silicon eqn = "(2.0e0*thIp2*MyI)*grad(Potential)"
term name=I3 add Silicon eqn = "Potential*grad(2e0*thIp2*MyI)"

# define the diffusion equations
pdbSetString Silicon MyBi Equation "ddt(MyBi)-diffBi*(grad(MyBi)+0.5e0/alpha*(Bi1+Bi2-Bi3))"
pdbSetString Silicon MyBs Equation "ddt(MyBs)"
pdbSetString Silicon MyI Equation "ddt(MyI)-diffI*(grad(MyI)+0.5e0/alpha*(I1+I2-I3))"

#BsI intermediate
solution name=BsI solve !damp !negative add
term name=Kassoc add Silicon eqn = "4*pi*captr*(diffI)"
term name=Kko add Silicon eqn = "nu*exp(-$Eko/(kb*$tempK))"
term name=Kdis add Silicon eqn = "6.1e12*exp(-$Edis/(kb*$tempK))"
term name=Kki add Silicon eqn = "nu*exp(-$Eki/(kb*$tempK))"

term name=Rk1 add Silicon eqn = "Kassoc*MyI*MyBs-Kdis*BsI"
term name=Rk2 add Silicon eqn = "Kki*MyBi-Kko*BsI"
pdbSetString Silicon BsI Equation "ddt(BsI)-Rk1-Rk2"
set Bieqn [pdbGetString Silicon MyBi Equation]
set Ieqn [pdbGetString Silicon MyI Equation]
set Bseqn [pdbGetString Silicon MyBs Equation]
pdbSetString Silicon MyI Equation "$Ieqn+Rk1"
pdbSetString Silicon MyBi Equation "$Bieqn+Rk2"
pdbSetString Silicon MyBs Equation "$Bseqn+Rk1"

# Cluster Evolution
term name=Ea2 add Silicon eqn = "$cEa2"
term name=Ea3 add Silicon eqn = "$cEa3"
term name=Ea4 add Silicon eqn = "$cEa4"
term name=Ea5 add Silicon eqn = "$cEa5"

#Interstitial Clusters
solution name=f2 solve !damp !negative add
solution name=f3 solve !damp !negative add
solution name=f4 solve !damp !negative add
solution name=f5 solve !damp !negative add

term name=KI add Silicon eqn = "4*pi*captr*diffI"
term name=Kf1b add Silicon eqn = "nu*exp(-Ea2/(kb*$tempK))"
term name=Kf2b add Silicon eqn = "nu*exp(-Ea3/(kb*$tempK))"
term name=Kf3b add Silicon eqn = "nu*exp(-Ea4/(kb*$tempK))"
term name=Kf4b add Silicon eqn = "nu*exp(-Ea5/(kb*$tempK))"

term name=R1 add Silicon eqn = "2*KI*MyI*MyI-Kf1b*f2"
term name=R2 add Silicon eqn = "KI*MyI*f2-Kf2b*f3"
term name=R3 add Silicon eqn = "KI*MyI*f3-Kf3b*f4"
term name=R4 add Silicon eqn = "KI*MyI*f4-Kf4b*f5"

pdbSetString Silicon f2 Equation "ddt(f2)-R1+R2"
pdbSetString Silicon f3 Equation "ddt(f3)-R2+R3"
pdbSetString Silicon f4 Equation "ddt(f4)-R3+R4"
pdbSetString Silicon f5 Equation "ddt(f5)-R4"
set Ieqn [pdbGetString Silicon MyI Equation]
pdbSetString Silicon MyI Equation "$Ieqn+2*R1+R2+R3+R4"

# Boron Cluster
solution name=BsBi solve !damp !negative add

term name=KBi add Silicon eqn = "4*pi*captr*diffBi"
term name=KB1b add Silicon eqn = "nu*exp(-Ebb/(kb*$tempK))"
term name=RB1 add Silicon eqn = "KBi*MyBi*MyBs-KB1b*BsBi"
pdbSetString Silicon BsBi Equation "ddt(BsBi)-RB1"
set Bieqn [pdbGetString Silicon MyBi Equation]
set Bseqn [pdbGetString Silicon MyBs Equation]
pdbSetString Silicon MyBi Equation "$Bieqn+RB1"
pdbSetString Silicon MyBs Equation "$Bseqn+RB1"

# Mixed Boron Interstitial Cluster
sel z=1.0 name=BsBi1 store
sel z=1.0 name=BsI2 store
sel z=1.0 name=BsBi2 store
sel z=1.0 name=BsI3 store
sel z=1.0 name=BsBi2I store
sel z=1.0 name=BsBi2I2 store
sel z=1.0 name=BsBiI3 store
sel z=1.0 name=BsBi3I store
sel z=1.0 name=BsI4 store

solution name=BsBi2I solve !damp !negative add
solution name=BsI2 solve !damp !negative add
solution name=BsBi2I2 solve !damp !negative add
solution name=BsI3 solve !damp !negative add
solution name=BsBi2I solve !damp !negative add
solution name=BsBi2I2 solve !damp !negative add
solution name=BsBiI3 solve !damp !negative add
solution name=BsBi3I solve !damp !negative add
solution name=BsI4 solve !damp !negative add

term name=Km3 add Silicon eqn = "nu*exp(-Ea3/(kb*$tempK))"
term name=Km4 add Silicon eqn = "nu*exp(-Ea4/(kb*$tempK))"
term name=Km5 add Silicon eqn = "nu*exp(-$Emix/(kb*$tempK))"
term name=G1 add Silicon eqn = "KI*MyI*BsBi-Km3*BsBiI"
term name=G2 add Silicon eqn = "KBI*MyBi*BsI-Km3*BsBiI"
term name=G3 add Silicon eqn = "KI*MyI*BsI-Km3*BsI2"
term name=G4 add Silicon eqn = "KBI*MyBi*BsI2-Km4*BsBi2I"
term name=G5 add Silicon eqn = "KI*MyI*BsI2-Km4*BsI2I"
term name=G6 add Silicon eqn = "KI*MyI*BsI2-Km4*BsI3"
term name=G7 add Silicon eqn = "KBI*MyBi*BsBiI2-Km4*BsBi2I2"
term name=G8 add Silicon eqn = "KBI*MyBi*BsBi2I-Km5*BsBi3I"
term name=G9 add Silicon eqn = "KI*MyI*BsBi2I-Km5*BsBi2I2"
term name=G10 add Silicon eqn = "KBI*MyBi*BsBi2I2-Km5*BsBi2I2"
term name=G11 add Silicon eqn = "KBI*MyBi*BsBiI2-Km5*BsBiI3"
term name=G12 add Silicon eqn = "KBI*MyBi*BsI3-Km5*BsBiI3"
term name=G13 add Silicon eqn = "KI*MyI*BsI3-Km5* BsI4"

pdbSetString Silicon BsBiI Equation "ddt(BsBiI)-G1-G2+G5+G7"
pdbSetString Silicon BsI2 Equation "ddt(BsI2)-G3+G4+G6"
pdbSetString Silicon BsBiI2 Equation "ddt(BsBiI2)-G4-G5+G10+G11"
pdbSetString Silicon BsI3 Equation "ddt(BsI3)-G6+G12+G13"
pdbSetString Silicon BsBi2I Equation "ddt(BsBi2I)-G7+G8+G9"
pdbSetString Silicon BsBi2I2 Equation "ddt(BsBi2I2)-G9-G10"
pdbSetString Silicon BsBiI3 Equation "ddt(BsBiI3)-G11-G12"
pdbSetString Silicon BsBi3I Equation "ddt(BsBi3I)-G8"
pdbSetString Silicon BsI4 Equation "ddt(BsI4)-G13"

set Bieqn [pdbGetString Silicon MyBi Equation]
set Ieqn [pdbGetString Silicon MyI Equation]
set BsBieqn [pdbGetString Silicon BsBi Equation]
set BsIeqn [pdbGetString Silicon BsI Equation]

pdbSetString Silicon MyBi Equation "$Bieqn+G2+G4+G7+G8+G10+G12"

pdbSetString Silicon MyI Equation "$Ieqn+G1+G3+G5+G6+G9+G11+G13"

pdbSetString Silicon BsBi Equation "$BsBieqn+G1"

pdbSetString Silicon BsI Equation "$BsIeqn+G2+G3"

# Boundary Conditions
if {{[pdbGetBoolean Silicon Potential Pin]}} { 
  pdbSetBoolean Gas_Silicon Potential Fixed_Silicon 1
  pdbSetString Gas_Silicon Potential Equation_Silicon "1e20*(Potential_Silicon-
  0.2+((1.17e0-(4.73e-4*$tempK*$tempK)/($tempK+635.0e0))/4))" 
}

pdbSetString Gas_Silicon MyI Equation_Silicon "(-1.0e-3*exp(-$EI/(8.617383e-
0.05*$tempK))*$fudge*MyI_Silicon)/5e-9"

pdbSetString Gas_Silicon MyBi Equation_Silicon "(-1.0e-3*exp(-$EBi/(8.617383e-
0.05*$tempK))*$fudge*MyBi_Silicon)/5e-9"

# Annealing profile
  temp_ramp clear
  temp_ramp name=flat1 trate=0.0 time=0.3333 temp=168 press=0.0
  temp_ramp name=up1 trate=135 time=(437-168)/(60.0*135) temp=168 press=0.0
  temp_ramp name=up2 trate=7.6 time=(492-437)/(60.0*7.6) temp=437 press=0.0
  temp_ramp name=up3 trate=22 time=(660-492)/(60.0*22) temp=492 press=0.0
  temp_ramp name=flat2 trate=0.0 time=0.1667 temp=660 press=0.0
  temp_ramp name=rampup trate=$rate time=($T-660)/(60.0*$rate) temp=660
  press=0.0
  temp_ramp name=down1 trate=-64 time=($T-810)/(60.0*64) temp=$T press=0.0
  temp_ramp name=down2 trate=-35 time=(810-600)/(60.0*35) temp=810 press=0.0
  temp_ramp name=down3 trate=-14 time=(600-450)/(60.0*14) temp=600 press=0.0

  foreach step {flat1 up1 up2 up3 flat2 rampup down1 down2} { 

    puts ""
    puts ""
    puts "!!!!!Doing $step!!!!!!"
    puts ""
    puts ""
    diffuse name=$step adapt init=1e-10
  }

  struct outf=$Name
}

# TEDspike {EBi EI Eko Eki Edis cIEa2 cIEa3 cIEa4 cIEa5 Emix Btrap Strap Ebb rate T
  fudge Name}
TEDspike 0.359 0.720 0.408 0.460 0.575 1.400 2.192 3.055 3.700 3.500 0.330 0.120
1.790 150 1050 1e0 up+0.2+0s1
TEDspike 0.359 0.720 0.408 0.460 0.575 1.400 2.192 3.055 3.700 3.500 0.330 0.120
1.790 150 1050 1e-1 up+0.2+0s0.1
TEDspike 0.359 0.720 0.408 0.460 0.575 1.400 2.192 3.055 3.700 3.500 0.330 0.120
1.790 150 1050 1e-2 up+0.2+0s1e-3
TEDspike 0.359 0.720 0.408 0.460 0.575 1.400 2.192 3.055 3.700 3.500 0.330 0.120
1.790 150 1050 1e-3 up+0.2+0s1e-4
TEDspike 0.359 0.720 0.408 0.460 0.575 1.400 2.192 3.055 3.700 3.500 0.330 0.120
1.790 150 1050 1e-4 up+0.2+0s1e-5proc PotentialEqns { Mat Sol } { 
    set pdbMat [pdbName $Mat]
    set Vti {[simGetDouble Diffuse Vti]}
    set terms [term list]
    if {![lsearch $terms Charge] == -1} {
        term name = Charge add eqn = 0.0 $Mat
    }
    set Poiss 0
    if {[pdbIsAvailable $pdbMat $Sol Poisson]} {
        if {[pdbGetBoolean $pdbMat $Sol Poisson]} {set Poiss 1}
    }
    set ni [pdbDelayDouble $pdbMat $Sol ni]
    if {! $Poiss} {
        set neq "0.5*(Charge+sqrt(Charge*Charge+4*ni*ni))/ni"
        term name = Noni add eqn = "exp( Potential*$Vti)" $Mat
        term name = Poni add eqn = "exp( -Potential*$Vti)" $Mat
        set eq "Potential * $Vti - log($neq)"
        pdbSetString $pdbMat $Sol Equation $eq
    } else {
        #set a solution variable
        set sols [solution list]
        if {![lsearch $sols Potential] == -1} {
            solution add name = Potential solve damp negative
        }
        term name = Noni add eqn = "exp( Potential*$Vti)" $Mat
        term name = Poni add eqn = "exp( -Potential*$Vti)" $Mat
set eps "([pdbDelayDouble $pdbMat $Sol Permittivity] * 8.854e-14 / 1.602e-19)"

if {{pdbGetBoolean $pdbMat $Sol TEDmodel}} {
puts "!!!!!Using TED Poisson model by Jung and Seebauer!!!!!"

# Our modification

  term name=Pos add $Mat eqn = "Myp+thBip*MyBi+2*thIp2*MyI"
# For +/-0 boron interstitial
  term name=Neg add $Mat eqn = "Myn+MyBs"
# For +/- boron interstitial
#  term name=Neg add $Mat eqn = "Myn+MyBs+thBin*MyBi"

  set eq "($eps*grad(Potential)+(Pos-Neg))"
}
} else {
puts "!!!!!Using Floops Poisson equation!!!!!"

  set eq "($eps*grad(Potential) + $ni * (Poni - Noni) + Charge)"
}

pdbSetString $pdbMat $Sol Equation $eq

proc PotentialInit { Mat Sol } {
  term name = Charge add eqn = 0.0 $Mat
}
LIST OF REFERENCES


42. Borucki, L., IEEE 1992, Honolulu. 27.


BIOGRAPHICAL SKETCH

The author was born in Nashville, TN, in 1981. After graduating from Montgomery Bell Academy in 1999, he attended the University of Florida, where he earned a B.S. in computer engineering in 2004. He continued his studies at UF in the graduate school of the Electrical and Computer Engineering department and received his M.S. in 2006.