List of Figures

Figure 1.1 Two-dimensional schematic representations of (a) the kick-out interstitial diffusion mechanism and (b) the interstitialcy diffusion mechanism. 3

Figure 1.2 Two-dimensional schematic of the vacancy diffusion mechanism. 4

Figure 2.1 Process flow for reduced OED study. (a) n-type starting material, boron/arsenic epi growth, oxide deposition, and lithography. (b) High-dose Si^{28} implant. (c) Oxide etch, 1050˚C, 1 minute RTA. (d) Wafers cleaved in halves. Half saved for initial profile (left side) and half oxidized in pyrogenic steam (right). 9

Figure 2.2 SIMS data before (Curves #1 and #2) and after (Curves #3 and #4) oxidation for the 900˚C, 2 hour oxidized sample. The solid lines are the profiles underneath a region with defects, and the dotted lines are the profiles underneath a region without defects. The curves are numbered following the convention in Figure 2.1(d). 10

Figure 2.3 Plan-view TEM analysis samples (a) before and (b) after the 900˚C, 2 hour wet oxidation. 12

Figure 2.4 (a) Interstitial flux diagram during the wet oxidation. J_{total} is the flux due to the oxidation, J_{loops} is the flux into the extended defects, and J_{bulk} is the flux into the bulk of the substrate that enhances the diffusion of the boron buried layer. (b) Time-averaged interstitial supersaturations at various depths which are used to calculate J_{total} and J_{bulk}....13

Figure 2.5 Schematic representation of the torus surrounding the stacking fault along with the interstitial concentrations of interest. r is the radius of the stacking fault, and r_t is the radius of the torus surrounding the stacking fault. C_C is the interstitial concentration on the surface of the torus, C_I^{∞} is the interstitial concentration far away from the dislocation loop, C_I^* is the bulk equilibrium interstitial concentration, and $C^*_{I,loop}$ is the equilibrium interstitial concentration within the torus surrounding the stacking fault. 19

Figure 2.6 Equilibrium interstitial concentration surrounding a dislocation loop as a function of loop radius at 900ßC. 20

Figure 2.7 Comparison of the optimized, simulated boron profile versus SIMS data for the case of normal OED without extended defects. 23

Figure 2.8 Comparison of the optimized, simulated boron profile (using the model for loop growth) versus SIMS data for the case of reduced OED. 24

Figure 2.9 Final simulated interstitial supersaturations for the case of (a) normal OED, (b) reduced OED, and (c) diffusion-limited growth of the dislocation loops. 25

Figure 2.10 Final simulated boron profiles for the case of reaction and diffusion-controlled (solid line) and diffusion-limited only (dotted line) growth of dislocation loops compared to SIMS data. 26

Figure 2.11 Optimized values for θ as a function of oxidation temperature. The open circles are the optimized values, and the solid line is the best-fit Arrhenius expression to all the data. 31

Figure 2.12 Optimized values for K_{loop} as a function of oxidation temperature. The open circles are the optimized values, and the solid line is the best-fit Arrhenius expression to all the data. 32

Figure 2.13 Plan-view TEM micrographs (a) before oxidation, (b) after 850ßC, 3 hour wet oxidation, (c) after 950ßC, 45 minute wet oxidation, and (d) after 1000ßC, 30 minute wet oxidation. The magnification in all pictures is 66,000X. 33

Figure 2.14 Comparison of experimental data for uphill phosphorus diffusion from [26] to a SUPREM-IV simulation using the model for dislocation loop growth. 35

Figure 2.15 Comparison of uphill boron diffusion from [31] to simulations using SUPREM-IV and the model for the growth of dislocation loops. 36

Figure 2.16 Initial interstitial concentration used in the simulation that generated the final boron profile shown in Figure 2.15. 37

Figure 2.17 Process flow for reduced IED study. (a) After epitaxial growth, oxide deposition, and lithography. (b) $1x10^{13}$ cm^{-2} or $2x10^{15}$ cm^{-2}, 100 keV Si^{28} implant. (c) After oxide etch

and 1050ßC, 1 minute rapid thermal anneal. (d) Second Si^{28} implant, $2x10^{14}$ cm^{-2}, 70 keV. (e) After final oxide deposition. (f) Wafers cleaved in half. Half saved for initial profiles (left side) and half furnace annealed at either 750ßC for 2 hours or 900ßC for 30 minutes in an argon ambient (right side). 42

Figure 2.18 Bevel-and-stain result on sample H2 (a) before final anneal, (b) after 750ßC, 2 hour inert anneal....44

Figure 2.19 SIMS boron data of sample H2 which was first implanted with $2x10^{15}$ cm^{-2}, 100 keV Si^{28}, RTA annealed, implanted again with a low-dose of Si^{28}, then furnace annealed at 750ßC for 2 hours. The solid lines are data taken from a masked region and the dotted lines are from an open region....45

Figure 2.20 SIMS boron data of sample H3 which was initially implanted with $1x10^{13}$ cm^{-2}, 100 keV Si^{28}, RTA annealed, implanted again with a low-dose of Si^{28}, then furnace annealed at 750ßC for 2 hours. The solid lines are data taken from a masked region and the dotted lines are from an open region....46

Figure 2.21 SIMS boron data of sample H5 which was initially implanted with $2x10^{15}$ cm^{-2}, 100 keV Si^{28}, RTA annealed, implanted again with a low-dose of Si^{28}, then furnace annealed at 900ßC for 30 minutes. The solid lines are data taken from a masked region and the dotted lines are from an open region....47

Figure 3.1 Schematic cross-section of the experimental structure used to study the effects of implantation damage below and above the amorphization threshold....55

Figure 3.2 Channeling RBS measurements for the samples implanted with silicon at $1x10^{15}$, $2x10^{15}$, and $4x10^{15}$ cm^{-2} at 50 keV along with a random RBS measurement....58

Figure 3.3 Channeling RBS measurements for the samples implanted with silicon at $1x10^{16}$ cm^{-2}, 50 keV and $2x10^{15}$ cm^{-2} at 100 keV along with a random RBS measurement. 58

Figure 3.4 Channeling RBS measurements for the samples implanted with silicon at $1x10^{14}$, $2x10^{14}$, $4x10^{14}$ and $8x10^{14}$ cm^{-2} at 80 keV along with a random RBS measurement. 59

Figure 3.5 Channeling RBS measurements for the samples implanted

with silicon at $8x10^{14}$ and $2x10^{15}$ cm^{-2} at 80 keV along with a random RBS measurement. 59

Figure 3.6 Bevel-and-stain measurement for the $2x10^{15}$ cm^{-2}, 100 keV silicon implanted sample after annealing at 750ßC for 10 minutes. The left-hand side is underneath a region masked from the silicon implant while the right-hand side is underneath an implanted region. 60

Figure 3.7 SIMS data and optimized SUPREM-IV simulation for the $2x10^{15}$ cm^{-2}, 100 keV silicon implanted, 750ßC, 30 minute annealed sample. The initial silicon implant profile (calculated using a BTE solver [27],[28]) shows the spatial separation of the implant from the diffusing layer. The enhancement in boron diffusivity for this case is 1975X. 61

Figure 3.8 Extracted time-averaged boron diffusivity enhancements for various silicon implants, all above the amorphization threshold, annealed at 750ßC. The solid circle represents a $4x10^{15}$ cm^{-2} implanted sample, RTA annealed for 2 minutes at 745ßC and the solid square represents a $4x10^{15}$ cm^{-2} implanted sample preannealed at 550ßC for 30 minutes before final annealing. 63

Figure 3.9 Extracted time-averaged boron diffusivity enhancements for several implant doses and energies, all above the amorphization threshold, annealed at 800ßC. 64

Figure 3.10 Extracted time-averaged boron diffusivity enhancements for the $1x10^{14}$ cm^{-2} (below amorphization) and the $8x10^{14}$ cm^{-2} (above amorphization) samples annealed at 750ßC for various times. 64

Figure 3.11 Extracted time-averaged boron diffusivity enhancements for the $1x10^{14}$ cm^{-2} (below amorphization) and the $8x10^{14}$ cm^{-2} (above amorphization) samples annealed at 800ßC for various times. 65

Figure 3.12 Effect of silicon implant energy on <D>/D* for the 750ßC anneals. 65

Figure 3.13 Effect of silicon implant energy on <D>/D* for the 800ßC anneals. 66

Figure 3.14 Profiles for the $1x10^{14}$ cm^{-2} and $8x10^{14}$ cm^{-2}, 80 keV silicon implants calculated using a Boltzmann Transport Equation solver [27],[28]. The integrated dose beyond the amorphous layer for the $8x10^{14}$ cm^{-2} implant is still $1.9x10^{14}$ cm^{-2}. 67

Figure 3.15 Enhancements in boron diffusivity for identical high-dose silicon implants ($4x10^{15}$ cm^{-2}, 50 keV) annealed at 750ßC and 800ßC. 68

Figure 3.16 Comparison of low-dose enhancements from [11] versus the high-dose enhancements from this study after 750ßC furnace annealing. The dotted lines represent data for sub-amorphizing implants and the solid lines represent data for amorphizing implants. 69

Figure 3.17 Comparison of low-dose enhancements from [11] versus the high-dose enhancements from this study after 800ßC furnace annealing. The dotted lines represent data for sub-amorphizing implants and the solid lines represent data for amorphizing implants. 70

Figure 3.18 Comparison of SIMS data and optimized SUPREM-IV simulation for the epitaxially grown boron marker layer annealed at 800ßC for 112 hours. For the optimized SUPREM-IV simulation, D_B^* was scaled by 0.81X. 73

Figure 3.19 Comparison of SIMS data and optimized SUPREM-IV simulation for the epitaxially grown boron marker layer annealed at 850ßC for 48 hours. For the optimized SUPREM-IV simulation, D_B^* was scaled by 0.66X. 74

Figure 3.20 Comparison of SIMS data and optimized SUPREM-IV simulation in FZ material annealed at 800ßC for 112 hours. For the optimized SUPREM-IV simulation, D_B^* was scaled by 0.71X. 74

Figure 3.21 Comparison of SIMS data and optimized SUPREM-IV simulation in FZ material annealed at 850ßC for 48 hours. For the optimized SUPREM-IV simulation, D_B^* was scaled by 0.73X. 75

Figure 4.1 Time-averaged enhancements between time points for the $4x10^{15}$ cm^{-2}, 50 keV silicon implanted samples annealed at 750ßC for 10, 30, and 120 minutes. The best-fit exponential decay is represented by the dotted line and the parameters are given in the plot. 81

Figure 4.2 Comparison of best-fit exponential decay in the enhanced boron diffusion to the 10, 30, and 120 minute SIMS data. 82

Figure 4.3 BTE simulation of a $1x10^{14}$ cm^{-2}, 80 keV silicon implant showing the intersititial and vacancy Frenkel pairs created as well as the as-implanted +1 profile. 88

Figure 4.4 Comparison of simulation results using Packan s model and the full +1 approach compared to experimental data for a $4x10^{15}$ cm^{-2}, 50 keV silicon implanted sample annealed at 750ßC for 2, 10, 30, and 120 minutes. C_I^{max}/C_I^* was set to 15,025 in this simulation. The remaining simulation parameters are from [23] and are listed in Table 2.2 on page 27. 91

Figure 4.5 Comparison of simulation results using Packan s model and the scaled +1 approach compared to experimental data for a $4x10^{15}$ cm^{-2}, 50 keV silicon implanted sample annealed at 750ßC for 2, 10, 30, and 120 minutes. C_I^{max}/C_I^* was set to 15,025 in this simulation and the remaining simulation parameters are from [23] and are listed in Table 2.2 on page 27. The scaled +1 dose used was $3x10^{12}$ cm^{-2}. 93

Figure 4.6 Comparison of the time-averaged enhancements in boron diffusivity between time points for the $4x10^{15}$ cm^{-2}, 50 keV silicon implanted samples annealed at 750ßC for 2, 10, 30, and 120 minutes to the simulated interstitial supersaturation at a depth of 0.6 µm using Packan s model and the scaled +1 approach. 94

Figure 4.7 Comparison of the time-averaged enhancements in boron diffusivity between time points for the $4x10^{15}$ cm^{-2}, 50 keV silicon implanted samples annealed at 750ßC for 2, 10, 30, and 120 minutes to the simulated interstitial supersaturation at a depth of 0.6 µm using Park and Law s model and the scaled +1 approach. Parameters from Park and Law [72] were used in this simulation except K_{BI}, the equilibrium boron/interstitial pairing constant, was decreased to $6x10^{-18}$ cm^3. A scaled +1 dose of $1.1x10^{12}$ cm^{-2} was used as the initial interstitial profile.....97

Figure 4.8 Comparison of simulation results for the $4x10^{15}$ cm^{-2}, 50 keV silicon implanted samples annealed at 750ßC for 2, 10, 30, and 120 minutes using Park and Law s model and an initial interstitial profile of $6x10^{12}$ cm^{-2}. D_I=$2.15x10^{-11}$ cm^2/s, D_V=$1x10^{-11}$ cm^2/s, and K_{BI}=$2.15x10^{-20}$ cm^3. K_B, $D_IC_I^*$, $D_VC_V^*$, and D_I/K_S^I are taken from Table 4.2. 98

Figure 4.9 Comparison of simulation results for $2x10^{13}$ cm^{-2}, 35 keV silicon implanted samples annealed at 750ßC using the same parameter set as in Figure 4.8 except a scaled +1 dose of $3x10^{13}$ cm^{-2} was used. SIMS data from Crowder [74]. 99

Figure 4.10 Comparison of simulation results for the $4x10^{15}$ cm^{-2}, 50 keV silicon implanted samples annealed at 750ßC for 2, 10, 30, and 120 minutes using the two.dim model and an initial interstitial profile of $3.5x10^{12}$ cm^{-2}.....100

Figure 4.11 Comparison of simulation results for the $4x10^{15}$ cm^{-2}, 50 keV silicon implanted samples annealed at 800ßC for 5, 10, and 30 minutes using the two.dim model and an initial interstitial profile of $3.5x10^{12}$ cm^{-2}.....101

Figure 4.12 Comparison of simulation results for $2x10^{13}$ cm^{-2}, 35 keV silicon implanted samples annealed at 750ßC using a scaled +1 dose of $2x10^{12}$ cm^{-2} and the parameters from Table 4.2. SIMS data from Crowder [74]. 102

Figure 4.13 Comparison of simulation results for the $1x10^{14}$ cm^{-2}, 80 keV silicon implanted samples annealed at 750ßC for 30, 120, and 210 minutes using the two.dim model and an initial interstitial profile of $5x10^{12}$ cm^{-2}.....104

Figure 4.14 Comparison of simulation results for the $1x10^{14}$ cm^{-2}, 80 keV silicon implanted samples annealed at 800ßC for 30 and 120 minutes using the two.dim model and an initial interstitial profile of $5x10^{12}$ cm^{-2}.....104

Figure 4.15 Comparison of simulation results for the $1x10^{14}$ cm^{-2}, 80 keV silicon implanted samples annealed at 850ßC for 30 minutes using the two.dim model and an initial interstitial profile of $5x10^{12}$ cm^{-2}.....105

Figure 4.16 Comparison of simulation results for the $2x10^{15}$ cm^{-2}, 100 keV silicon implanted samples annealed at 750ßC for 10, 30, and 120 minutes using the two.dim model and an initial interstitial profile of $4x10^{12}$ cm^{-2}.....105

Figure 4.17 Comparison of simulation results for the $2x10^{15}$ cm^{-2}, 100 keV silicon implanted samples annealed at 800ßC for 5, 10, and 30 minutes using the two.dim model and an initial interstitial profile of $4x10^{12}$ cm^{-2}.....106

Figure 4.18 Enhanced diffusion after a $1x10^{15}$ cm^{-2}, 40 keV phosphorus implant. The enhanced diffusion saturates within 15 seconds during the 900ßC RTA. However, additional motion occurs for a subsequent, 850ßC, 1 hour furnace anneal (Reproduced from Kim et al. [81]). 108

Figure 4.19 Interstitial evolution using the dislocation loop model to mimic cluster dissolution. The clusters become less than 10

in radius in less than 1 second. The clusters were centered at 0.175 μm from the surface with an initial radius of 11 and a density of $4.5x10^9$ cm^{-2}. K_{loop} was set to 0.5 in this simulation. 111

Figure 4.20 Interstitial evolution using the dislocation loop model to mimic cluster dissolution. The initial radius in this case was 25 . All other parameters were identical to Figure 4.19. 112

Figure 4.21 Simulation fits to the $4x10^{15}$ cm^{-2}, 50 keV implanted samples annealed at 750ßC using the scaled +1 approach and the model for dislocation loops. A $5x10^{12}$ cm^{-2} scaled +1 profile was used. The loops were centered at 0.175 μm, the initial radius of the loops was 10 , the density of the loops was $1.35x10^{10}$ cm^{-2}, and K_{loop} was 0.35. 113

Figure 4.22 Simulation fits to the $1x10^{14}$ cm^{-2}, 80 keV implanted samples annealed at 750ßC using the scaled +1 approach and the model for dislocation loops. An $8x10^{12}$ cm^{-2} scaled +1 profile was used. The loops were centered at 0.175 μm, the initial radius of the loops was 10 , the density of the loops was $1.35x10^{10}$ cm^{-2}, and K_{loop} was 0.35. 114

Figure 4.23 Simulation fits to the $2x10^{15}$ cm^{-2}, 100 keV implanted samples annealed at 750ßC using the scaled +1 approach and the model for dislocation loops. A $7x10^{12}$ cm^{-2} scaled +1 profile was used. The loops were centered at 0.175 μm, the initial radius of the loops was 10 , the density of the loops was $1.35x10^{10}$ cm^{-2}, and K_{loop} was 0.35. 115

Figure 4.24 Comparison of the time-averaged enhancements in boron diffusivity between time points for the $4x10^{15}$ cm^{-2}, 50 keV silicon implanted samples annealed at 750ßC for 2, 10, 30, and 120 minutes to the simulated interstitial supersaturation at a depth of 0.6 μm using the scaled +1 approach with the model for loop dissolution. Parameters from Table 4.2 were used in this simulation and a scaled +1 dose of $5x10^{12}$ cm^{-2} was used as the initial interstitial profile. 116