SYMPOSIUM J
Si Front-End Processing—Physics and Technology of Dopant-Defect Interactions III

April 17 – 19, 2001

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SESSION J1: FUTURE DEVICE ISSUES
Chair: Martin D. Giles
Tuesday 17 April 2001
Golden Gate A2 (Merrill)

8:30 AM *3.1.1 MOSFET DESIGN CONSIDERATIONS FOR THE SUB 75 NM TECHNOLOGY NODE
Dimitri A. Antoniadis, Microelectronics Technology Laboratories, Massachusetts Institute of Technology, Cambridge, MA.

Conventional MOSFETs have proven to be remarkably scalable to gate lengths around 30 nm, which are compatible with the 75 nm technology node. While typically the pace of scaling has been limited by lithography, other device design components are increasingly becoming limiting. While gate oxide thickness, channel doping and channel dielectric quality are critical, degradation in gate oxide quality is running out of thickness, the gate material, where the poly depletion region is becoming a significant part of the gate dielectric, channel doping, where profile abruptness and statistical dopant variation are both problematic, and source/drain doping and contacts where parasitic resistance is becoming comparable to channel resistance. In this paper I first review the scaling impact of these device design components on device figures of merit based on experiments and simulation through the use of inverse and forward device modeling. I then discuss novel MOSFET structures currently pursued to alleviate some or all conventional shortcomings. These include ultra-thin-film single- and double-gate SOI, Schottky source/drain and strained SiGe channel. At this point of process engineering, device specification may continue to meet the requirement of minimizing performance enhancement.

9:00 AM *3.1.2 DOPING PROCESS ISSUES FOR SUB 0.1 UM GENERATION MOSFETs

To meet the market demands for LSI’s with even higher performance, traditional scaling has been aggressively pursued and has won great success over 0.1 µm generations. To maintain continued growth in CMOS performance beyond 0.1 µm generation, key issues originating from the traditional scaling will be discussed. From the point of doping process (channel engineering, ultra-shallow junction, highly-activation) in this paper. To meet the acceleration in gate length miniaturization, short channel effects should be suppressed with aggressive channel engineering. A channel impurity profile must be optimized two-dimensionally, not uniformly or one dimensionally. We will demonstrate channel engineering using tilted channel implantation with Indium impurity. SOL-NMOSFETs for sub-0.1 µm will be demonstrated with well suppressed SCEs and competitive electrical characteristics. Traditional scaling results in large variation of threshold voltage due to the statistical impurity variation in a channel region. We studied effect of above channel profile on threshold voltage fluctuation due to statistical dopant variation by measurement and simulation. It will be discussed that the two-dimensionally optimized channel profile enhances threshold voltage fluctuation even if implantation process variation is negligible. As CMOS device scales, reduction of channel resistance becomes important for high-performance operation. Resistance at extension edge and contact resistance at silicon-Si interface are dominant factors. The traditional approach is to use a higher RIA temperature and a shorter RIA time. The ultimate RIA is laser annealing. We will demonstrate the laser annealing process with an ultra-low contact resistance of 0.4 x 1.68 ×10^−6 Ω·cm² and shallow extension simultaneously. By integrating the above technologies, in addition to ultra-thin gate insulators and gate-depletion from source/drain, we can establish front-end process for sub-0.1 µm generations.

9:30 AM *3.1.3 ADVANCED IMPLANTATION TECHNOLOGY FOR HIGH PERFORMANCE TRANSISTORS

Defect control in shallow source and drain and precise dose control in channel are important issues in high performance transistors of 0.1 to 0.13 micron regime. With shrinkage of junction depth, the thermal budget of annealing after ion implantation becomes smaller in order to suppress impurity diffusion. On the other hand, it becomes difficult to recover the channel by small deep junction annealing. Therefore, the annihilation of defects by annealing with small thermal budget is a key issue for 0.1 to 0.13 micron regime. We have developed a process module combined with cryo-implantation and rapid thermal annealing in order to minimize defects in source and drain regions. It was found out that the pn junction depth could be shallower as compared with RT implantation and pn junction leakage current was successfully decreased and applied to Co SALICIDE process. Precise dose control is indispensable in channel region of high performance MOSFETs. In order to improve the precision of implanted dose, dose size implantation technology without photore sist mask was developed. In this technology, chip-by-chip implantation can be carried out by step-and-repeat wafer stage, and different implantation conditions are available in the same wafer independent of wafer size. In this paper, the implantation results are reviewed and the some applications are presented. REFERENCES: [1] A. Murakoshi et al., MRS 2000 spring meeting abstract B38.05. [2] T. Shibata et al., IEDM 2000 Late News to be presented.

SESSION J2: ADVANCES IN DOPANT PROFILING
Chair: Anthony T. Foiy
Tuesday, April 17, 2001
Golden Gate A2 (Merrill)

10:30 AM *3.2.1 STATISTICAL CHARACTERISATION OF MOSFET MATCHED PAIRS: A POWERFUL TECHNIQUE FOR STUDYING MICROSCOPIC TRANSISTOR PROPERTY FLUCTUATIONS

As transistor minimum dimensions continue to shrink, microscopic device property fluctuations are seen to become significant compared to the overall process/device performance spread observing CMOS technology. Recent research has demonstrated that random local phenomena such as dopant fluctuations and gate polycrystalline grain boundaries cause local variations in MOSFET threshold voltage. However, the inherent independence of global process spread, pairs of closely spaced identical transistor(paired) prove to be very suitable test structures for studying these effects. After an introduction on the possible impact of random microscopic device property fluctuations on the performance of MOSFETs, requirements for statistical MOSFET matching characterization techniques will briefly be reviewed. Subsequently, our paper will discuss several examples of the impact of mismatch on CMOS transistor matching. More in particular we will reveal the impact of dopant fluctuations and boron penetration by measuring their correlation with the activation RIA as well as poly-silicon morphology. Furthermore we have demonstrated the validity of applying Poisson statistics for describing dopant fluctuations. This was done by comparing threshold voltage fluctuations of transistor pairs that received a Boron channel implantation with pairs that received a Deboronation implantation. More general, statistical characterization studies are necessary to provide the required information on device performance spreading that electronic circuit designers have to take into account for performance and yield optimization. But moreover, statistical studies provide important insights into microscopic device properties that, due to their statistical nature, cannot be obtained through other physical characterization techniques such as TEM, SEM, SIMS, etc.

11:00 AM *12.2 SSM AND SCM OBSERVATION OF MODIFIED LATERAL DIFFUSION OF DIS, BP AND Bi IN doubly SPACED SPACERS

Initial studies (using Scanning Spreading Resistance Microscopy) on the lateral diffusion of Si and As have shown an important influence of the thickness of nitride spacers. The latter phenomenon was tentatively ascribed to stress enhanced diffusion under the spacer region. This study has been complemented with Scanning Capacitance Microscopy (SCM), measurements, which confirm the SSM results. In fact both techniques show a similar increase in lateral diffusion with increasing spacer thickness (~0.2 nm/spacer thickness), whereby no effect is observed on the vertical diffusion. When using spacers with or without TEOS-liner, fairly similar enhancements could be seen. Micro-Raman and CIVB stress measurements for these cases do however show a large reduction in stress when a TEOS-liner is used, suggesting that the correlation (at least to the lateral) stress is not properly justified. A possible explanation could however be that the lateral diffusion occurs before the stress relaxation within the thermal treatment. In order to elucidate the diffusion mechanism, initial
stresses, interstitials, hydrogen incorporation, TED, ... we have expanded the experimental matrix with a vacancy diffuser such as Si and simulated the effects of hydrogen incorporation and the nitride deposition by an hydrogen anneal. Moreover we also have studied the impact of TED by splits with RTP anneals before the nitride deposition.

11:15 AM J2.3
DIRECT IMAGING OF THE DEPLETION REGION OF AN OPERATING PN JUNCTION WITH CONDUCTANCE MAPPING.
Jeong Y. Park, Dept. of Physics, University of Maryland and Laboratory for Physical Sciences, College Park, MD; D. J. Bruno, Dept. of MISiC, University of Maryland and Laboratory for Physical Sciences, College Park, MD; E. D. Williams, Dept. of Physics, University of Maryland and Laboratory for Physical Sciences, College Park, MD.

It is known that depletion zone related features on oxidized-grown Si pn junctions can be imaged by Scanning Tunneling Microscopy (STM), mainly due to the induced band bending [1]. It is also known that the incorporation of both electronic and topographical information make it difficult to get quantitative information about the dopant profile from STM images. In this study, dual scanning of conductance imaging and constant current mode STM imaging have been used to characterize the depletion zone of a Si pn junction over a range of reverse bias conditions. Conductance has been obtained by adding a modulation signal to voltages applied in p and n region, and by demodulating the tunneling current with lock-in amplifier. Our images show a pronounced dependence on reverse bias at electrically different regions (n, p, and depletion zone), and in agreement with the conductance from tunneling spectra measured across pn junction. This suggests that conductance mapping can exclusively give the electrical information of microdevice with high lateral resolution. We will also show a measurable time-dependent response when operated within inversion conditions for the tip-grown sample metal insulator semiconductor (MIS) junctions. [1] M. Pendl, R. J. Phaneuf, and E.D. Williams, Appl. Phys. Lett. 72, 3314 (1998).

11:30 AM J2.4

Applied Materials, Santa Clara, CA; Baxter Cross Inc, Menlo Park, CA.

The 2003 source/drain doping requirements in the International Technology Roadmap for Semiconductors (ITRS) are 3-4 nm deep, 240-675 nm2 sheet resistance, and 2.7 nm/decade abruptness. All are labeled as having “no known solutions.” The doping tools will have to perform in a very narrow process window over a 300 mm wafer diameter, creating a parallel metrology requirement to guarantee process stability. Existing methods such as SIMS, with a throughput too low for uniformity measurement or in-line use, may be insufficient to provide requirements for process control. Recently, junction characterization methods based on Carrier Illumination (CI) technology have shown depth resolution and throughput consistent with shallow junction process control requirements. This paper will outline the discussion of fabrication and characterization of advanced layers formed with low energy (LE) implants and spike anneals. Using careful process optimization, it is shown that this process module can meet or exceed the ITRS requirements. The ability to achieve high quality junctions is indeed a viable candidate for near- and mid-term doping requirements. Characterization of these same layers using CI methods shows junction depth resolution better than 1%, meaning that it is possible to achieve metrology performance consistent with process control requirements. Further details of these processes and their characterization will be presented.

In addition to the implant plus spike anneal solution, rapid progress is being achieved in ion implantation methods such as Laser Induced Annealing (LIA). The paper will close with a comparison of the current state of the art of the implant/anneal and LIA doping solutions and the application of the CI method to characterization and process optimization of LIA layers.


11:45 AM J2.5

Hydrogen is known to cause the passivation of boron acceptor after such processing steps as wet etching, reactive ion etching, sputter deposition of metal contacts, and Ar ion beam etching. The previous study of this effect employed CV profiling, spreading resistance profiling, SIMS measurements on samples diffused with deuterium. These methods are either destructive to the Si surface or require deposition of metal contact. In the present study we used a non-contact small signal ac surface photovoltage technique, currently available in commercial diagnostic tools. The simultaneous measurements of the semiconductor surface barrier, Vb, and the semiconductor capacitance of the surface depletion layer, Cb, allow calculating the concentration of boron atoms in submicron distances from Si surface or Si/SiO2 interface. The technique has proven very successful in monitoring low dose implants and also near surface doping in oxidized wafers. In bare silicon wafers the method occasionally indicated surface boron concentration noticeably below the bulk value. We found such unusually low values after the chemical cleaning, used to prepare hydrogen terminated surface. Thermal annealing at temperatures from 150°C to 200°C reactivates boron dopant. We will discuss the effect of various cleaning and annealing conditions on passivation and reactivation of boron dopant in the near surface region. The results obtained with the non-contact SPV technique show excellent agreement with previous studies. They also provide a basis for reliable measurement of the boron concentration free of the interference from hydrogen passivation.

SESSION J3: DOPANT DIFFUSION ISSUES
Chair: Lutieh Pechar and Peter A. Scalici
Tuesday, April 17, 2001
Golden Gate A2 (Marriott)

1:30 PM J3.1
DOPANT SELF-SPUTTERING DURING ULTRA-LOW ENERGY ION IMPLANTATION. Aditya Agarwal, Axxela Technologies, Inc., Tokyo, JAPAN.

The phenomenon of sputtering of the target during ion implantation has been known about and studied for several decades. Only recently, however, with the advent of ultra low sub-kV energy ion implantation, this phenomenon has become relevant to front-end semiconductor processing. At ultra-low implant energies (sub-kV for B, and sub-keV for As) a significant fraction of the intended dose can be lost due to sputtering of the dopant during the implantation process itself. Such an effect will combined with the difficulty of achieving high and low dose implants, can become a deciding factor in the choice of dopant implant energies. This paper presents several recent measurements of the dopant self-sputtering effect from implantation of boron,boron fluoride,deuterated boron, and arsenic silicon and silicon dioxide. These data, collected using nuclear reaction analysis, Rutherford backscattering or secondary ion mass spectroscopy, allow for the first time the calculation of the yield of the sputtering yield of these various dopant species from silicon, silicon dioxide. The experimental determined sputtering yields are an order of magnitude larger than what is predicted by theory.

2:00 PM J3.2

There is an increasing interest in the use of In as an alternative p-type dopant for silicon device processing. For instance, recent investigations indicate that replacing B with In as a channel dopant improves advanced NMOS devices. Advantages such as these have been related to the physical properties of In in Si, in particular as compared to B. Nevertheless, In has been studied least of all practical Si dopants and its properties remain controversial, e.g. the improved performance of In-channel devices is attributed to the "absence of diffusion". In this paper we report on a comprehensive study of the diffusional properties of In in Si as well as in SiO2, i.e. diffusion, segregation, solubility. We used In implanted with an energy of 210 keV into bare Si or Si covered with 50 and 500 nm of SiO2 to doses of 1015 to 1016 cm-2. This placed the In profile either fully in SiO2, or Si in the Si bulk. It was also incorporated into In by MBE of doping-super-lattices. Oxides were prepared either by annealing of bare Si wafers in dry oxygen or in oxygen containing a
small percentage of Cl (chlorinated oxides). Various post-implant annealing steps, followed by SIMS, RBS and TEM were then carried out. In Si, Cl diffuses and, in SiGe, OED and TED. In all also diffuses in the oxides; diffusion, in fact, is quite rapid although non-Fickian with retrograde diffusion occurring at certain times. This is true in both, dry and chlorinated oxides, although quantitative differences exist between Si and SiO$_2$ and we have determined the segregation coefficient directly from the In concentrations in SiO$_2$ and Si at the interface. Solubilities in Si were determined from the shoulder that develops after annealing in the depth profiles of high dose implants.

2:15 PM J.3

**SELF-DIFFUSION IN EXTRINSIC SILICON USING ISOTO-CALY ENRICHED 30Si SILICON**

Yukio Nakabayashi, Hirman I. Osamu, Toru Segawa, Kazuma Sato, Sauro Minamoto, Kio Univ., Dept. of Electronics and Electrical Engineering, Yokohama, JAPAN; Junichiro Matsuo, Takashi Uni, Resp. Inst. of Electrical Communication, TOTTORI, JAPAN; Kevin A. Aspnes, Massachusetts Institute of Technology, Dept. of M$\&$E, Cambridge, MA; Takuo Abe, Sin-Etsu Handcuff Co, Isobe R&D Center, Gunma, JAPAN.

Dopant atoms diffuse by interaction with point defects and self-diffusion in Si can be viewed as a limiting case of dopant atom diffusion. Thus the study of self-diffusion is stringent important for understanding of diffusion mechanism of dopant atoms. In the past, Si self-diffusion experiments were carried out with the short half-life (2.6 h) radioactive tracer $^{30}$Si. It limits such experiments to a narrow high-temperature range near the melting point. An approach for solving this problem is direct evaluation of Si self-diffusivity using stable isotope $^{30}$Si. Isotope heterogeneity has been used in order to investigate the silicon self-diffusion. It consists of pure $^{30}$Si epitaxial layer on natural Si. However, there is no report about Si self-diffusion using the epitaxial layer. A heterostructure of $^{30}$Si/natural Si enables us to investigate both the doping effect and isotope mass effect on self-diffusion in Si. In this work, we studied Si self-diffusion using isotoically enriched $^{30}$Si layer grown on natural Si substrate. The effects of doping and isotope mass on self-diffusion have been investigated. $^{30}$Si epitaxial layer was grown by gas source molecular beam epitaxy (GS-MBE). It was grown at 700°C on four different substrates in this experiment. The three of these substrates were heavily doped with $^{30}$Si/B or $^{30}$Si/Pb and the other is lightly doped with $^{30}$Si/B. These samples were annealed simultaneously in a resistance heating furnace in pure Ar (99.9995%) at 900°C for 360 h. The concentrations of the respective Si isotopes and dopant atoms in the Si substrate were measured with secondary ion mass spectrometry (SIMS). The each diffusion was extracted by numerical fitting process by solving Fick’s equation. The Si to B concentration of lightly doped sample $[\text{Si}] = 1 \times 10^{16}$ cm$^{-3}$ is much smaller than the intrinsic carrier concentration at 900°C, its sample is referred as intrinsic silicon. Comparing the $^{30}$Si profile in heavily B-doped Si with that of intrinsic $^{30}$Si, the $^{30}$Si diffusion in heavily B-doped Si is found to be enhanced and its enhancement ratio is about twice. The effects of $^{30}$Si and Si self-doped $^{30}$Si on self-diffusion profiles are hardly different from the profile of intrinsic Si. Doping effect on $^{30}$Si self-diffusion is similar to that of $^{30}$Si. For both intrinsic and extrinsic silicon, the $^{30}$Si self-diffusion coefficients are higher than that of $^{30}$Si. The measured rates of $^{30}$Si to $^{30}$Si are about 0.82. It means that self-diffusion coefficient varies with almost $m^{-3}$ where $m$ is the mass of the diffusing atom.

2:30 PM J.3.4

**A NEW MODEL FOR BORON DIFFUSION RETARDATION IN SiGe-STRAINED LAYERS ACCOUNTING FOR THE MECHANISM OF BORON TRAPPING/DETRAPPING BY Ge ATOMS.**

Victor Koldyev, P&F Solutions, San Jose, CA.

The Boron diffusion in the strained pseudomorphic SiGe layers on Si is of great interest from the scientific and practical point-of-views. A phenomenon known as Ge-atom trapping/detrapping effects in strained SiGe diffusion retardation in such layers was proposed by N. Counin in 1994. This model describes the B diffusion from SiGe layers. However, this approach fails when describing the B diffusion into strained SiGe. The B diffusion model predicts the continuous B concentration at the interface of SiGe having different slopes of the profiles from the Si-side and the SiGe-side. Different slopes are result of the different B diffusivities in Si and SiGe layers providing there is no B accumulation at the interface and there is no free flux of boron through the interface. Our experimental study of the B diffusion into the SiGe layer from the Si side one shows a segregation process of B into SiGe-layers is happening. The model of more complicated mechanism of B diffusion through the interface and in SiGe occurs. There is the electric field across the interface due to the band discontinuity and not ideally abrupt Ge concentration decrease at the interface but quantitation of the electric field can provide a twice of the high the diffusion which is not enough to agreed the experimental and simulated profiles. An assumption about the segregation processes which is due to capturing B in the SiGe-layer can provide the exact agreement between the B and Ge diffusion.

Microscopic theory of the capturing which has been developed allows us to decompose the total B diffusion retardation in SiGe-layer into two components: about 45% of the total diffusion retardation is due to the strain and about 50% is due to boron capturing resulting in an effectively less value of the total diffusion. We believe that the driving force for such a capturing is the attractive interaction between the large Ge atoms carrying the compressive strain with the small Boron atoms carrying the tensile strain around.

2:45 PM J.3.5

**SHALLOW-TYPE JUNCTIONS FOR SUB-100NM CMOS.**


The achievement of shallow, low-resistance junctions is seen as one of the important prerequisites for enabling the scaling of CMOS technology into the sub-100nm generations. In current practice, p-type junctions are formed by the implantation of B followed by thermal activation. In this case, shallow junctions are difficult to achieve due to the enhanced diffusion and clustering of boron dopants during thermal processing. In recent years, ion-beam pre-amorphization combined with spike annealing has been proposed as a means to extend the classical way of junction formation into the deep submicron era. In the present study, we have explored the optimum conditions for Ge pre-amorphization (dose, energy) for making shallow junctions with 1 keV B implants. By tuning Ge/B co-implantation and spike annealing conditions, 30 nm deep p-type junctions without any resistances as low as 400 Ohms/square. To our knowledge, these are the best shallow junction parameters reported until now for p-type junctions formed with ion implantation and annealing. The optimized junction fabrication scheme has been integrated into a full process flow (including gate lengths down to 50 nm), allowing an electrical assessment of the junction performance in terms of series resistance, underdiffusion, overcapacitance and parasitic leakage.

3:30 PM J.3.6

**THE ROLE OF ION MASS ON END-OF-RANGE DAMAGE IN SHALLOW PRE-AMORPHIZING SILICON.**

Mark J. Cohn, University of Florida, Dept. of M$\&$E, Gainesville, FL; Kevin J. Jones, University of Florida, Dept. of M$\&$E, Gainesville, FL; Tony E. Hanes, Oak Ridge National Laboratory, Oak Ridge, TN; Charles J. Barbour, Sandia National Laboratories, Albuquerque, NM; Ebrahim Andleeb, Intel Corporation, Portland, OR.

Pre-amorphization is commonly used in the shallow junction formation of silicon CMOS devices. The purpose of this experiment was to study the effects of the pre-amorphizing ion species mass on the intentional concentration at the end-of-range region. Isoelectric species of Si, Ge, Sn and Pb were compared. Silicon wafers with a CVD grown-in buried boron marker layer (5000 A deep) were amorphized using ions of 1 MeV /u Si, 1 MeV /u Ge, 1 MeV /u Sn and 1 MeV /u Pb. The amorphous layer thickness at the end-of-range of Si is approximately 0.82, meaning that self-diffusion coefficient varies with almost $m^{-3}$ where $m$ is the mass of the diffusing atom.

Post-implantation anneals were performed at 750°C for times ranging from 15 to 240 minutes. Plan-view transmission electron microscopy (PTEM) and Transmission Scanning Electron microscopy (XTEM) and Spectroscopic Ellipsometry were used to measure amorphous layer depths (approximately 100 A). Pre-amorphization damage was reduced by a factor of 9, ranging from 2 to 207 AMU. This result is consistent with the observed reduction in intrinsic injection and TED.
as al [APL 54, 1427 (1989)] report much higher diffusivity values. In this work we report measurements of the silicon diffusion coefficient in silicon dioxide and also in an isochronally etched silicon dioxide layer that enables relatively low $^{35}$Si concentration measurements to be performed using Secondary Ion Mass Spectrometry. Two types of experiments are made. $^{35}$Si atoms are introduced in excess in a stoichiometrically pure silicon dioxide layer either by an implantation or by a predeposition technique. Annealing of implanted profiles is performed from 1050 to 1150°C for durations of some hours to many days. The diffusivity is calculated from fitting the silicon ion concentration profiles using a constant diffusivity value. For the predeposition experiments special structures were prepared. The final structure is a Si crystalline layer that contains the $^{35}$Si isotopes in their natural abundance on top of an isochronally pure SiO$_2$ layer. SIMS measurements were performed using the same procedure as described above. The concentration profiles measured are three orders of magnitude higher than reported direct measured values with an estimated activation energy of 5 eV. Possible mechanisms for the diffusion of silicon in the oxide will be discussed.

4:00 PM 13.8
THE EFFECT OF TRIPLE WELL IMPLANT DOSE ON PERFORMANCE OF NOS TRANSISTORS
Konstantin K. Bourdeau, Samir Chaudhury, Jerome Chu, Bell Laboratories, Lucent Technologies, Orlando, FL.

The application of triple well structures provides important advantages to different types of silicon devices. Those include analog CMOS [noise and cross-talk reduction], digital CMOS [fabrication of low threshold voltage n-channel transistors to improve circuit speed] and memory devices (higher density and faster speeds). In a triple well technology an addition of one moderate dose high energy phosphorus implant allows the creation of a separate p-channel transistor which is isolated from the substrate. In this work we study the dependence of NOS device performance and leakage current in dice test structures on the dose of 1 MeV phosphorus triple well implant (TWI). The devices were fabricated using 0.25 μm CMOS process. We observed that initial increase in TWI dose leads to increase in threshold voltage of the devices with a peak at a dose of about 1×10$^{14}$ cm$^{-2}$. With further increase in dose threshold voltage decreases: the decrease corresponds to the onset of Si amorphization induced by 1 MeV phosphorus implant. We interpret the data in a framework of a model that incorporates the suppression of transient enhanced diffusion of boron (in the channel region) by the formation of buried amorphous layer. Using a PROPHET simulator we were able to reproduce the experimental I-V data. The data on dose dependence of leakage current in large area junction diode structures are explained by the formation of tunneling dislocations. This interpretation is supported by the defect etch and transmission electron microscopy measurements.

4:15 PM 13.9
PHOSPHORUS INTRINSIC DIFFUSION IN PURE EPITAXIAL SILICON. Jens S. Christensen, Andrew Yu, Konnoret, Henry H. Badman, The Royal Institute of Technology (KTH), Dept. of Electronics, Stockholm, SWEDEN; Bengt G. Svensson, University of Oslo, Physics Department/Physical Electronics, Oslo, NORWAY.

Epitaxial silicon layers with a box-shaped phosphorus profile produced by low pressure chemical vapor deposition (LP-CVD) were used to study phosphorus diffusion in silicon. The samples were annealed in an inert nitrogen atmosphere, in the temperature range of 810 - 1100°C. The concentration of phosphorus was chosen so that it was lower than the intrinsic carrier concentration, even at 810°C. The diffused phosphorus profiles were determined by secondary ion mass spectrometry (SIMS) and compared with the as-grown profile to extract the diffusion coefficient of phosphorus ($D^p$). It was found that ($D^p$) follows an Arrhenius dependence with the activation energy $E_a = 2.74 ± 0.07$ eV and the prefactor ($8.5± 5.4) 10^{23} cm^3/s$. The activation energy and the prefactor differ considerably from the previously reported and widely accepted literature values (3.0±0.6 eV and 3.84 10$^{23}$ cm$^3$/s respectively). Phosphorus diffusion in silicon was studied extensively during the 70-80s, and is commonly believed to be well understood. Most of the studies have been, however, performed in bulk Czochralski (Cz) grown silicon with a low concentration of competing traps for silicon self-interstitials, which is considered as the main vehicle mediating phosphorus diffusion. In contrast, LP-CVD epitaxially grown silicon contains substantially smaller concentrations of such impurities as carbon and oxygen. In the present paper we compare our results with literature data and discuss microscopic/atomistic mechanisms for phosphorus diffusion in pure epitaxial silicon.

4:30 PM 13.10
DIFFUSION OF NITROGEN IMPLANTED INTO SILICON AT AMORPHIZING DOSES. Lukh Shakh Adam, Lance Robertson, Mark E. Low, Software for Advanced Materials and Processing (SWAMP) Center, Univ. of Florida, Gainesville, FL; Suri Hegde, Omer Dokumaci, Semiconductor Research and Development Center, IBM Corporation, Hopewell Junction, NY.

Nitrogen implantation is used in multi-gate oxide thickness processing. Previous studies have reported on the diffusion behavior of implanted nitrogen in silicon at amorphizing doses. Most of these studies showed that nitrogen diffuses rapidly towards the surface at 750°C. The present study looked at the diffusion behavior of nitrogen implants at amorphizing doses of $5\times10^{14}$ N$^+$ and $2\times10^{15}$ N$^+$ at 40 keV. XTEM images generated in highest dose forms a continuous amorphous layer to a depth of about 8000 Å while the lower dose forms a buried amorphous layer between 1000 Å and 6000 Å from the surface. After implantation, the samples were furnace annealed at 750°C for times from 12 min to 4 hours in multiple steps. This should form either a monolayer of range (EOR) or Type II defects for the higher dose and Type IV defects (where the amorphous layer most likely occurs) in addition to EOR at the original amorphous-crystalline interfaces for the lower dose. For the case of a continuous amorphous layer, the medium energy of the implant results in the formation of EOR defects at depths sufficient to preclude surface interaction with the EOR defects. SIMS studies on these samples show that at the higher dose of $2\times10^{15}$ N$^+$, the nitrogen segregates towards the EOR defects (at about 8000-9000 Å) up to the longest annealing time. However, in the case of the lower dose of $5\times10^{14}$ N$^+$, the profile shrinks with time, and the peaks are pinned at about 500 Å. This is in contrast to the non-amorphizing case where the peaks shift towards the surface with time. Further, the nitrogen implanted at this dose diffuses towards the surface upon annealing. The extent of this diffusion is much less than that observed in the non-amorphizing case. In the extent of this diffusion could be possibly explained by a surface site density limit as suggested by current nitrogen diffusion models, this would still have to be investigated further. Diffusion effect at these doses for the varied times and correlated to EOR, SIMS results. Currently, investigation is in progress to couple an existing loop evolution/dissolution model into an already developed nitrogen diffusion model to predict the diffusion of nitrogen at amorphizing doses.

SESSION 14: POSTER SESSION
Thursday Evening, April 17, 2001
8:00 PM
Salon I-7 (Marriott)

J4.1
EFFECTS OF MULTIPLE NONMULTI LAYER PULSES ON BORON IMPLANTED IN SILICON. Susan Eagles, Mark Low, Kevin Jones, Univ. of Florida, SWAMP Center, Sarasota, Florida, Vedanta, San Jose, CA, Sean Corcoran, Intel, Portland, OR.

The effects of multiple nonmulti laser pulses on boron implanted silicon have been studied. The energy of the implanted boron varied from 3keV to 250keV at nominal doses of 1x10$^{15}$ to 5x10$^{15}$ ions/cm$^2$. The samples received one to 1000 laser pulses at a constant energy low enough not to melt the silicon. Furnace anneals and RIE followed by Hall Effect, Four-point probe, SIMS, and PL and PC TEM were then done to study the activation, diffusion, and microstructure of the boron implanted silicon. SIMS results indicate that the samples processed with a laser anneal prior to the RIE diffuse less than the samples receiving just the RIE. The resistivity of the samples is also shown to decrease as the number of laser pulses is increased.

J4.2
THE EFFECT OF CHLORINE ON DIFFUSION AND ACTIVATION OF NITROGEN IMPLANTED BORON IN SILICON. K.A. Galble, L.S. Robertson, K.S. Jones, Univ of Florida, Dept of MSE & GE, Gainesville, FL.

The interaction between boron and silicon interstitials caused by ion implant damage is a physical process which hinders the formation of ultra-thin, low resistivity junctions. The possibility of mitigating this interaction between boron and interstitials has been explored by co-implanting chlorine with ion implanted boron in silicon. It has been investigated. Amorphization of a n-type Czochralski wafer was achieved using a series of Si implants of 40 keV and 150 keV, each at a dose of 1x10$^{11}$ cm$^{-2}$. The N$^+$ implants produced a 2800Å deep amorphous layer, which was then implanted with 8 keV $^{35}$Cl$^+$ ions ranging from 30 to 90 keV and doses ranging from 5x10$^{14}$ to 2x10$^{15}$ cm$^{-2}$. The energies of the chlorine implants were chosen such that the damage and ion profiles of the
chlorine were contained within the amorphous layer. This allowed for the chemical species effect to be studied independent of the implant damage caused by the ion itself. To prevent the oxidation of Si implanted in air, the implantation experiment was performed in a vacuum at 750°C and in a RTA at 1050°C. Secondary ion mass spectrometry was used to monitor the dopant diffusion after annealing. Hall effect measurements were used to study the dopant activation. Transmission electron microscopy (TEM) was used to study the end-of-range defect evolution. The addition of chlorine has significant effects on the boron diffusion, boron activation, and extended defect evolution. Under certain conditions the chlorine content resulted in improvement in the boron junction characteristics. Detailed chemical and microstructural analysis will be presented to explain the observed phenomenon.

3.4.3 Vacancies and Oxygen Behavior in Highly Carbon Doped Silicon

Carbon and oxygen are the two major electrically inactive impurities of Si and have been studied separately for 20 years. High carbon concentrations in silicon gained some interest recently due to the beneficial role of carbon in suppressing transient enhanced diffusion. Carbon, when incorporated well above its solubility in silicon ([Si < 10^18 cm^-3 at melt temperature] changes the silicon point defect equilibrium. Solitary interstitials are consumed in the carbon diffusion process leading to their underconsumption whereas vacancies become oversaturated. After annealing, it appears also that the oxygen concentration increases locally in carbon rich areas. To explain this carbon oxygen interaction in taking silicon vacancies into account. The interaction of vacancies with carbon and oxygen will be discussed. The precipitation of carbon will also be discussed.

3.4.4 Modeling of Threading Dislocation Loops


High energy boron implantation into silicon generates severe lattice defects in the region near the projected range. These defects can be dislocation loops. [311] or threading dislocation loops (TDLs). TDLS are long dislocation loops that can grow up to the surface. The formation of TDLS as a function of implant conditions is studied in boron implanted silicon for various implant doses (1e13 to 5e14 cm^-2). Experiments show that TDLS density increases dramatically with increasing dose to a maximum at a dose of 1e14 cm^-2. At doses beyond 1e14 cm^-2, TDLS density decreases rapidly. In a study, a statistical point defect based model for the nucleation and evolution of TDLS is developed. However, in the point of the different Process Simulates (FLOOPS), modeling results are in agreement with the experimental results. The model assumes that all the nucleated loops come from [311] unfaulted loops, and that loop density follows a log normal distribution. Oxidation rimming becomes dominant when excess interstitial density drops to the values close to equilibrium interstitial concentration. Loops whose radius close to their distance from the surface are considered as TDLS.

3.4.5 Characterization of Damage Induced by Cluster Ion Implantation

Takashi Ake, Jire Masao, Gikun H. Tsukada, Ion Beam Engineering Lab., Kyoto Univ., Kyoto, JAPAN.

As the scale of LSI device decreases, the formation of ultra shallow p-type junction becomes more important. Cluster ion implantation using small boron cluster, deca boron (B12H4), has been introduced as a candidate for ultra shallow junction formation. Both experiments and molecular dynamics (MD) simulations of small B cluster and monomer implantation were performed in order to study the difference between cluster and monomer ion implantation. When a cluster, with the size below 10 and the energy of several hundreds eV per atom, impacts on Si substrate, the cluster breaks up in the substrate and each B atom penetrates into the substrate independently. Therefore, the depth profile of B atoms by cluster implantation is the same as those by B monomer ion with same energy per atom. In the case of the damage mechanisms, there are huge differences between cluster and monomer. For both cases of the impact of B monomer and cluster, the number of displaced Si atoms induced by one B atom is almost the same as that of the impinging ion. However, the damage recovery process is different, depending on cluster size. Damage induced by B12 recoveres more slowly than those by B1 ions. Compared to the B1 ion impact, there were several times larger number of displaced Si atoms by the B12 cluster. These displaced lattice atoms by B12 clusters concentrate in the near surface region of the impact point. The property of damage by cluster impact is different from that by monomer ions, so that different recovery processes are expected during annealing.

3.4.6 Atomistic Modeling of Carbon-Boron Interactions


Ab inito calculations were carried out to investigate carbon-boron interactions in Si at the atomic scale with a focus on the C-B split interstitial pair. The initial results for such a C-B pair include morphology and orientation, binding energies, an estimate of migration energy, and the electrical activity of the C-B pair. Charge states and Fermi-level effects were taken into account for these calculations. It was found that the <110> C-B split interstitial is relatively stable compared with the <111> and <111> C-B pairs. We find that the C-B can break up by C diffusing away in a similar fashion to the C-Si split interstitial pair, and the break-up energy is on the order of ~2.2 eV. We find the electrical activity of the C-B pair depends on the Fermi level. In addition, the migration energy of C in Si was also calculated to be 0.56 eV using the nudged elastic band method, comparable with previous ab inito results and in reasonable agreement with experiment. Implications of these results on understanding of the effect of C-B diffusion in Si will be briefly discussed.

3.4.7 Computer Simulation of Decaborane ImaPLantation in Silicon, Annealing and Re-Crystalization of Silicon

Zinetsu Inagawa, Ito Yumada, Lab. of Adv. Sci. & Technology, Himeji Inst. of Technology, JAPAN.

Phenomenological and computational models of Decaborane ion implantation into Silicon, Rapid Thermal Annealing (RTA), and amorphous Silicon recrystallization have been developed. The B and Si atomic positions for irradiation with many Decaborane ions, with energy up to a few keV per B and Si ion, were determined, with monomer B ions were obtained by MD simulations. The size of the basic cell was determined by Boron implantation dose of 10^13 -10^14 ion/cm^2. The main difference between monomer and Decaborane ion implantation with the same doses is the formation of a large amorphized area in a subsurface region for the Decaborane case. Almost all Boron atoms were trapped within the amorphous region. Two types of activation processes with different activation energies were studied for B diffusion. The activation energy at a higher temperature, typical for the RTA, was obtained to be close to the equilibrium activation energy of B dopants in Si. This result is comparable with the results of other groups. The diffusion activation energy was significantly smaller in a low temperature region suggesting a new B diffusion mechanism for this region. Re-crystallization of amorphized Silicon areas containing Boron atoms has been studied in detail at various temperature and pressure regimes. According to our computer simulation results, we have suggested a new mechanism of Boron diffusion that may occur during the Silicon re-crystallization process. This new effect has analogy with the Soret effect for crystallization from liquid.

3.4.8 Effect of the Ge Preamorphization Dose on the Thermal Evolution of End of Range Defects

Benjamin Colombeau, Gérard Ben Assayag, Alain Chassard, CéTemes/CNRS, Toulouse, FRANCE; Jean Christophe Maré, Fuccio Cristino, LAAS/CNRS, Toulouse, FRANCE.

To realize ultra shallow junctions compatible with advanced CMOS technology, it is now admitted that preamorphization of the wafer prior to low energy implantation has several advantages. After annealing of such preamorphized implants, End of Range (EOR) defects are formed below the n+p interface. As these defects strongly influence dopant diffusion, it is necessary to know how process parameters such as the preamorphization dose affect their thermal evolution. In this paper, we study the effect of the Ge preamorphization dose on the thermal evolution of EOR defects upon annealing. In other words, we investigate the influence of the amplitude of the initial supersaturation of Si interstitials ([Si]_s) found below the n+p interface on the kinetics of EOR defects. Amorphizations were carried out by implanting Ge at 150 keV for doses ranging from 1x10^15 ions/cm^2 to 8x10^15 ions/cm^2. Rapid Thermal Annealing (RTA) was performed for various temperature combinations in nitrogen ambient. Plan view transmission electron microscopy under specific imaging conditions was used to measure the size distributions and densities of the EOR.
defects. For a fixed thermal budget, the increase of the Ge ion dose results in the increase of the defect density but has no effect on the defect size distribution. This means that the number (N_d) of Si atoms bound to the EOR defects is a monotonically increasing function of the Ge ion dose. Furthermore, we find that N_d is directly proportional to the number of Si atoms in excess to the vacancies found below the interface as calculated by Monte Carlo simulation. This is consistent with the excess interstitial model which explains the origin of the EOR defects. In summary, we have found that the passivation ion dose has no effect on the defect size distribution. This investigation is of great importance with respect to the initial supersaturation introduced in the matrix is an expected characteristic of a conservative Ostwald ripening mechanism.

34.10 KINETICS OF STACKING FAULT ANNihilation IN BORON IMPLANTED SILICON


In an incising incidence x-ray diffuse scattering study of ion implantation damage in silicon we have found a clear signature of stacking faults forming during neutron annealing at temperatures 800 - 1100°C. Stacking faults are manifest by rods of diffuse scattered intensity normal to [111] planes in reciprocal space around Bragg reflections. The rod intensity is a measure of the stacking fault density while the width of the rod is a measure of their average size. Theoretical calculations of scattering intensity will be compared to the experimental data in order to support our interpretation. Upon annealing we find that in the initial stages the rod intensity and size grows for a while, however at characteristic times depending on the temperature the intensity begins to decrease until it vanishes completely after longer annealing. Simultaneously the average size of the faults at first increases, peaks and then decreases again with the decrease in intensity. Previous estimates of integrated intensity and halfwidth based on radial x-ray scans suggest a dissolution based annihilation mechanism for the stacking faults. Recent more accurate transverse x-ray scans of integrated intensity and half-width based on intensity of the second order Bragg peak do not support this mechanism. Kinetics of the growth and shrinkage of the faults will be discussed based on these findings.

34.11 DIFFUSION IN SILICON AND THE PREDICTIVE POWER OF AB-INITIO CALCULATIONS II. Weigang Windl, Xiong-ying Liu, Roland Stumpf and Michael P. Murakami, Computational Materials Group, Motorola, Inc. Austin, TX, and Los Alamos, NM. Blas P. Urrutia and Hanne Jonsson, Dept of Chemistry, Univ of Washington, Seattle, WA.

First-principles calculations of diffusivities and reaction constants of dopant atoms and native defects in semiconductors can be a very useful input to improve semiconductor process simulations, provided adequate methods are used and the "right" quantities are calculated. This paper presents work done at the Computational Materials Group of Motorola, which includes multiscale modeling of boron-interstitial clustering, the influence of boron on the formation of extended interstitial defects, and ab-initio numbers for defect and dopant diffusion that really help to discriminate between the contradictory experimental diffusivities and their use in process simulations.

34.12 ULTRA-SHALLOW Sb-DOPED LAYER FORMATION IN SiC[001] BY ARGON RECOIL IMPLANTATION. Kurt E. Dali, David T. Vosk and Robert J. Cullis, Department of Physics and Astronomy, Arizona State University, Tempe, AZ. Ultra shallow Antimony doped layers in Si[001] were produced by recoil implantation. The ultra shallow layers were produced first by depositing a thin Si film. The deposition is followed by high-energy positron annihilation ion and ion implantation. In the last step, the structure undergoes a final chemical etching of the residual Si film. The thickness of the doped layers is found to be less than 2.8 nm. The final Si concentration is found to be weakly dependent on the initial Si layer thickness. T. Michael was supported by National Foundation grant DMR-9898056 for Research Experience Undergraduates (REU) while working on this project.

34.13 A MOLECULAR DYNAMICS STUDY OF DAMAGE IN A VICINAL (100) SILICON SURFACE: EFFECTS OF LOW-ENERGY IMPLANTS OF ARGON AND BORON. A.M. Maznev, CNRS, Bologna, ITALY.

In these recent years considerable experimental and theoretical effort has been concentrated on the structural properties of the silicon surface. These studies have shown that a nominally flat (100) surface contains monatomic steps with an alternating dimerization direction. The atoms in the steps are weakly bonded and the step morphology may be significantly altered by the presence of a dopant impurity, by applying a mechanical or thermal stress, or by electron or ion irradiation. Seminal studies at atomistic level have shown the effects of the steps on adatom deposition and film growth in epitaxial growth. In this study of similar accuracy seems to be available on the effect of an implant on the step morphology and evolution. In this work implantation of argon and boron with kinetic energy in the range from 2 eV to 30 eV into a silicon stepped surface has been studied with molecular dynamics simulation with classical forces. The damage structures resulting from these implants consist on point defects and lattice relaxation. We analyze the dependence of these effects on the ion type and energy and on the step structure.


Homogeneously contaminated silicon samples were implanted with helium ions at 1.6 MeV at a fluence of 5 10^16 cm^-2. Both Ni and Pt were used as impurities. Since Ni is a fast diffuser and Pt is a hybrid, only differences in their behavior could be observed. The influence of the impurities on the nature and evolution in the damaged area. Pt has been already used for the profiling of vacancies. An annealing at 1050°C for 2 hours was then used to grow some and impurities to them. After the annealing, the width of the damaged zone shrinks down from 0.5 μm to 0.2 μm and depends essentially in carbon 10 to 100 nm in size. These carbon are faceted mainly along [111], but also along [110] and [100] planes as provided by high resolution electron microscopy. Secondary ion mass spectroscopy (SIMS) on the samples exhibit a shoulder shape with a maximum at the projected range. These measurements demonstrate that the carbons are very efficient sinks for any impurities regardless their nature. Nevertheless, the width of the MSB peak was found to be about five times larger than that of the cavity chain for all impurities used. The broadening and the shoulder of the gettering band have also been reported by RBS measurements. This demonstrates that MeV helium implantation induces not only well known and expected carbons but also a variety of defects located mainly before the projected range. These defects seem to be sensitive to the gettering of both fast and hybrid diffusers. In addition, an unexpected defect evolution was found when the growth of carbons and the diffusion of impurity take place during the same annealing.
The need for very shallow junctions (tens of nm) in future generations of MOS devices requires implantation of B at very low energy (<1 keV), where space charge effects limit the attainable beam current. Implantation of decaboron ions, consisting of ten B atoms and a few H atoms, may be an attractive alternative to ultra low energy implantation of B ions. Such cluster ions can be implanted at higher energy since their kinetic energy is partitioned among the constituent atoms. Moreover, there is only one charge state for ten B atoms. While there is a growing interest in decaboron implantation and more experimental results are being reported, the understanding of the fundamental procedure remains quite rudimentary. Theoretical studies of these ions are still lacking. We have applied the computational methods involving Molecular Dynamics Simulation and Monte Carlo, to the study of decaboron ion implantation in Si. These methods were used previously to investigate the effects of cluster ions of argon on a variety of materials. Of particular interest in the case of decaboron ions were implantation range, damage amorphization, and sputtering. Comparison with available experimental data is reported.

**J4.20**

**PHOTOLUMINESCENCE STUDY OF DEFECTS INDUCED BY B12H14 IONS. Noriaki Toyoda, Massachusetts Institute of Technology, Cambridge, MA.**

B12H14 ion implantation is one of the candidates for the ultra shallow junction formation below 5nm. However, the defect formation mechanisms induced by low-energy ion have to be clarified to understand the Transient Enhanced Diffusion (TED) of dopant. The kick-out and enhanced diffusion of boron is caused by excess Si interstitial, which is believed to be supplied by extended defects on the (311) habit plane. The interstitial Si aggregates formation is the first step for the (311) extended defects. In this study, interstitial aggregates formation by B12H14 decaborane was studied with photoluminescence measurements. In the PL spectra, we focused on the W-line (1019meV). From the recent first-principle calculations, the W-line is originated from interstitial Si aggregates. This W-line was observed in implanted Si with B12H14 ion implantation over the implant energy of 10keV. The W-line intensity increased with the implant energy. From the SIMS profile, TED was negligible when the W-line was not observed in PL spectra. Therefore, it is expected that excess Si interstitial would be low by low-energy (<3keV) B12H14 implantation, and TED is suppressed at this energy. The W-line in PL spectra would be a signature of interstitial Si formation induced by ion implantation damage.

**J4.21**

**SURFACE Fermi LEVEL PINNING: AN ELECTRICAL “VALVE” IN TRANSIENT ENHANCED DIFFUSION. Michael Y.L. Jung, Rudranto Gunawan, Richard D. Branz, Edmund G. Seebauer, Dept of Chemical Engineering, Univ of Illinois-CU, IL.**

Here we discuss surface effects in the modeling of transient-enhanced diffusion (TED) after ion implantation during ultrashallow junction formation by rapid thermal annealing. Simulations were performed for boron using a modified version of FLOOPS, and included the heteroepitaxial neglected phenomenon of surface Fermi level pinning. We find that such pinning greatly reduces dose loss, induces pileup of electrostatically-active boron within 1 nm of the surface, and leads to noticeably deeper junctions. The effects occur even when the surface functions as an excellent sink for interstitial of all types. The mechanism is that pinning sets up an electric field in the space charge region that opposes the diffusion of interstitials assisted by the Fermi level. In addition, applications of AFM/SCM in process control and failure analysis will be discussed and presented.

**J4.22**

**AB Initio Study of Self-Interstitial Clusters. Maxime Chickine, Merilyn De Sousa, De Montfort Univ, Emerging Technologies Centre, UNITED KINGDOM.**

The formation of silicon self-interstitial clusters has been investigated using ab initio total energy pseudopotential method. The clusters up to size 12 were studied employing supercells up to 128 atoms. The growth of the clusters is self-consistent. Larger models are obtained from the smaller ones capturing a single interstitial. This single interstitial can be low energy (110) split interstitial or high energy (100) split interstitial. The electronic structure of the clusters beyond size 2 is featured by the presence of low energy electronic levels at the bottom of the valence band and defect localized orbitals corresponding to these levels. The energetics of the investigated models shows the non-monotonic dependence of the binding energy with cluster size.

**J4.10**

**MODELING OF BORON IMPLANTATION WITH DECABORANE IONS. Zinetella Inagaki, Lab of Adv Sci & Technology, Himeji Inst of Technology, JAPAN; Mikao Sonowski, NJIT; Hisashi Yamada, Lab of Adv Sci & Technology, Himeji Inst of Technology, JAPAN.**

The need for very shallow junctions (tens of nm) in future generations of MOS devices requires implantation of B at very low energy (<1 keV), where space charge effects limit the attainable beam current. Implantation of decaboron ions, consisting of ten B atoms and a few H atoms may be an attractive alternative to ultra low energy implantation of B ions. Such cluster ions can be implanted at higher energy since their kinetic energy is partitioned among the constituent atoms. Moreover, there is only one charge state for ten B atoms. While there is a growing interest in decaboron implantation and more experimental results are being reported, the understanding of the fundamental procedure remains quite rudimentary. Theoretical studies of these ions are still lacking. We have applied the computational methods involving Molecular Dynamics Simulation and Monte Carlo, to the study of decaboron ion implantation in Si. These methods were used previously to investigate the effects of cluster ions of argon on a variety of materials. Of particular interest in the case of decaboron ions were implantation range, damage amorphization, and sputtering. Comparison with available experimental data is reported.
An increasing interest is nowadays devoted to the comprehension and modeling of damage related phenomena in c-Si. The continuous shrinking of electronic devices has encouraged experimental and simulation studies to better understand the interaction of defects with dopants during device operation. In this context, we present new results related to the defect generation and activation during the dopant implantation. The aim of this work is to review the experimental data and provide a unique interpretation of damage evolution in c-Si. To this purpose, we compare the experimental results of the electrical, optical and structural characterization of the residual damage in a kinetic lattice Monte Carlo (KLMC) simulations. Experimental data were taken as a function of implantation conditions and using different dopants Si and B were implanted on epitaxial and Czochralski-type and p-type Si with energies of 0.6-1.2 MeV and doses of 1x10^{14}-1x10^{15} cm^{-2}. Samples were characterized from the as-implanted state up to annealing temperatures of 1500 °C. Low temperature (300-500 °C) annealing causes the formation of L-defects. At high temperatures, the L-defects are destroyed and other point defect types are formed. In the intermediate temperature range (450 °C-600 °C) the concentration of L-defects is reduced and the concentration of point defects is increased.

9:00 AM 15.2

The defect evolution measured in samples processed by KLMC simulations is in good agreement with the experimental data. The simulations predict the formation of L-defects at low temperatures and the destruction of L-defects at higher temperatures. The activation energy for the destruction of L-defects is also in good agreement with experimental data. The simulations predict a decrease in the defect concentration with increasing temperature and a decrease in the defect concentration with increasing dose.

In previous studies, the effect of arsenic on (311) nucleation and dislocation was studied at 750 °C using x-ray diffraction. The results showed that the arsenic atoms are preferentially incorporated into the silicon lattice, forming arsenic interstitials. In a follow-up experiment, the interstitial flux released from the arsenic implantation region was studied using x-ray nuclear magnetic resonance spectroscopy and it was determined that the arsenic is reducing the number of arsenic interstitials.

In the present study, we used the KLMC simulations to study the formation and evolution of arsenic-interstitial clusters (AICs). The simulations predict the formation of AICs at low temperatures, with a maximum concentration at around 450 °C. The AICs are then destroyed at higher temperatures, with a decrease in the defect concentration. The simulations also predict a decrease in the defect concentration with increasing dose.

In conclusion, the KLMC simulations are in good agreement with the experimental data and provide a unique interpretation of damage evolution in c-Si. The simulations predict the formation of L-defects at low temperatures and the destruction of L-defects at higher temperatures. The simulations predict a decrease in the defect concentration with increasing temperature and a decrease in the defect concentration with increasing dose.

9:15 AM 15.5

In the development of MOS LSI, the electrical activation of impurities is the key issue in ultra-shallow junction formation. The electrical activation of impurities is important for the performance of the device. We have investigated the electrical activation of impurities in Si using ion implantation and ion channeling in combination with nuclear reaction analysis (NRA). Boron implanted Si at an energy of 10 keV with a dose of 5 x 10^{14} cm^{-2} (low dose) and implanted Si at 1000 °C for 10 seconds (RFA) or 800 °C for 10 minutes (FA) was annealed. The activation ratio of these samples was estimated from the B atomic concentration in the low dose RFA samples and in the high dose RFA sample. The activation ratio of B in the low dose RFA sample is around 90%. The activation ratio of B in the high dose RFA sample is around 60%. These results indicate that the activation ratio of B in the high dose RFA sample is higher than in the low dose RFA sample.

In conclusion, the KLMC simulations are in good agreement with the experimental data and provide a unique interpretation of damage evolution in c-Si. The simulations predict the formation of L-defects at low temperatures and the destruction of L-defects at higher temperatures. The simulations predict a decrease in the defect concentration with increasing temperature and a decrease in the defect concentration with increasing dose.
model is developed in the Florida Object Oriented Process Simulator (FOOPS) using the single set of extracted parameters. The nucleation of defects is controlled by a limited competition for excess interstitials between PIA and SIA clusters. Once formed, the release of interstitials in driving TED is driven by crystal dislocation. Modeling results show a strong correlation to those experimentally observed data. A SIA cluster in the specific domain, demonstrating the improved predictive capabilities with respect to dopant activation, TED, and dose loss. This work confirms the overwhelming importance of accounting for dopant-defect clustering during phosphorus diffusion simulations.

10:30 AM 15.6
A NEW KINEMATIC MODEL FOR THE NUCLEATION AND GROWTH OF SELF-INTERSTITIAL CLUSTERS IN SILICON. Christophe Ortiz, PHASE/CNRS Laboratory, Strasbourg, FRANCE and ECTM Laboratory, Delf University of Technology, THE NETHERLANDS; Daniel Mathiot, PHASE/CNRS Laboratory, Strasbourg, FRANCE.

Nowadays, Transient Enhanced Diffusion (TED) of dopants is of importance in IC fabrication. As process simulation has become an essential part of new technology development in the silicon IC industry, it is important to have a good understanding of physical mechanisms controlling TED in order to provide models which are as predictive and efficient as possible. To do so, a considerable effort has been devoted in the last few years to the understanding of the annealing kinetics of Dislocation Loops (DL). Several defects and even of small self-interstitial clusters, which all maintain an interstitial supersaturation and thus play an important role in TED. Nevertheless, almost nothing is known about small precursor clusters. In this paper, we propose a new kinetic model based on thermodynamic considerations for the nucleation and growth of self-interstitial clusters in silicon. This model accounts for the attachment and detachment of interstitials to clusters of different sizes (up to a few hundred atoms) and includes the interstitial recombination at the surface. On this basis we will show that, according to this model, the binding energy of an Si atom in a given cluster depends not only on the cluster size (as accounted for in existing models) but also on the local free interstitial supersaturation. On the other hand, it will be shown that using only four physical parameters, our model accounts for most experimental results on TED found in the literature. Physical parameters such as the interstitial diffusion coefficient and solid solubility will be fitted on experimental results.

10:45 AM 15.7
EFFECTS OF CLUSTERING AND PRECIPITATION ON THE INTERSTITIAL CONCENTRATION IN HIGH-DOSE As+ IMPLANTED SILICON. Michelle Gregg, University of Florida, Dept. of Electrical and Comp. Engineering, Gainesville, FL; Kevin Jones, Mark Clark, University of Florida, Dept. of Material Sci. and Engineering, Gainesville, FL; Mike Rendón, Motorola Corporation, Phoenix, AZ; Bob Marto, SEMATECH International, Austin, TX; Ron Arvelo, Mary Dignard, Varian Semiconductor Equipment, Gloucester, MA.

Arsenic is the most common dopant in silicon due to its high solubility and low diffusivity. Ultra-shallow junctions formed by highly doped As layers often have As concentrations which exceed solid solubility. At a critical concentration, dependent upon anneal temperature, As clustering occurs. When the As concentration exceeds a critical value greater than that of clustering, monolonic SIA\textsuperscript{+}s precipitation then occurs. This investigation includes the effects of clustering and precipitation from the effects of end-of-range (EOR) damage on the interstitial population in high concentration. As-implanted silicon. Silicon with a CVD grown boron marker layer was implanted with either As or Ge at doses of 2x10\textsuperscript{14}, 7x10\textsuperscript{14}, 2x10\textsuperscript{15}, and 4x10\textsuperscript{15} cm\textsuperscript{-2}. The Ge implants result in EOR damage as well as clustering and precipitation (2x10\textsuperscript{14} and 4x10\textsuperscript{15} cm\textsuperscript{-2}) after a 1500°C RTA spike anneal. Change in the interstitial concentration as a result of EOR damage and As clustering or precipitation was observed as an movement of the B marker layer diffusion compared to diffusion observed for the samples with EOR damage only (Ge implants). There was a slightly observable difference in marker layer diffusion between the cluster and precipitation (As implants) was observed as an movement of the B marker layer diffusion compared to diffusion observed for the samples with EOR damage only (Ge implants). The data shows that the As implants do not produce defects that are visible in the SIMS data. The As implants were performed to verify the extent of EOR damage from implants.

11:00 AM 15.8
DETERMINING THE RATIO OF THE PRECIPITATED VersUS SUBSTITUTED ARSENIC BY XAFS AND SIMS IN HEAVY DOSE ARSENIC IMPLANTS IN SILICON. M. Schirmer, S.W. Noack, Ch. Koetz, J. Wojsik, NIST, Gaithersburg, MD; J. Liu, Varian Semiconductor Equipment Associates, Gloucester, MA; V. Krishnamoorthy, Department of MSE, University of Florida, Gainesville, FL.

Doping silicon with arsenic by ion implantation above the solid solubility level leads to As clusters and/or precipitates in the form of monolonic Si\textsuperscript{+}s creating a wide temporal and spatial domain in which the As concentration is above the solid solubility level. Information on the local structure around the As atom, and the As concentration profile is important for the implantation and annealing process in order to reduce the precipitated As and minimize the electrically active As. In this work, we determined the local As structure and the precipitated versus substituted As for As implants in Cz [001] Si wafers, with implant energies between 20 keV and 100 keV, implant doses ranging from 1 x 10\textsuperscript{14} cm\textsuperscript{-2} to 1 x 10\textsuperscript{16} cm\textsuperscript{-2}. The samples are selected to different annealing conditions. We used standard x-ray mass spectrometry (SIMS) and UT-MARLOWE simulations to determine the region where the As-concentration is above the solubility level. By x-ray absorption fine structure spectroscopy (XAFS), we probed the structure of the local environment around As. XAFS being capable of probing the short-range order in crystalline and amorphous materials provides information on the number, distance and chemical identity of the neighbors of the main absorbing atom. Using Fourier analysis, the coordination numbers (N) and the nearest-neighbor distances (R) to As atoms in the first shell were extracted from the EXAFS data. When As is precipitated as monolonic Si\textsuperscript{+}s, the nearest-neighbor distances and coordination numbers are ~2.37 Å and ~3. As with substitutional is nonvolatile and can not be detected. Based on this information, the critical implant dose where the precipitation/clustering of As starts, and the ratio of the substitutional versus cluster/precipitate form As in the samples are determined.

11:15 AM 15.9
PARALLEL REPlica SIMulations FOR GROWTH MODELING OF Si SELF-INTERSTITIAL CLUSTERS. Stefan Birner, Jeongnim Kim, John W. Wilkins, Dept of Physics, Ohio State University, OH; Thomas Lenosky, Lawrence Livermore National Laboratory, Livermore, CA; Arthur F. Voter, Los Alamos National Laboratory, NM.

We discuss the energetics of small Si\textsuperscript{+} clusters containing n = 1 to 44 cluster. Small and medium sized clusters (n ≤ 31) are known to form flat Energy Minima (EM) of high stability at low temperature. However, larger clusters can also form non-flat low-energy configurations. Our previous calculations\textsuperscript{7} showed that compact interstitial clusters are favored for n ≤ 34, while elongated clusters are energetically favorable for larger clusters. We perform extensive atomistic simulations using Modified Embedded Atom Method (MEAM),\textsuperscript{3} tight-binding (TB) and ab initio Hamiltonians to determine the interstitial-energy and capture radii for small clusters. For each cluster, we performed parallel replica minimization using MEAM to identify 10-50 possible low-energy configurations that are further investigated by TB and ab initio potentials. We determine the critical size n at which smaller interstitial clusters transform from compact to elongated structures. The presence of the clusters and interstitial-cluster diffusion is investigated by parallel replica method\textsuperscript{4} using MEAM and TB potentials.

11:30 AM 15.10
MODELING OF ANNEALING OF HIGH CONCENTRATION AS PROFILES. Pavel Fastek, Scott T. Dunham, Electrical Engineering Department, University of Washington, Seattle, WA.

In this paper we will describe our approach to model diffusion and activation of high concentration arsenic implants. The formation of shallow low-resistance junctions requires implantation of high doses of As\textsuperscript{+}s with heavy energy. At present, simulation models are not capable of predicting accurately junction depth and resistivity of high concentration arsenic profiles. The standard approach for simulation As\textsuperscript{+} implants would consider amorphization of surface layer and include (311) loops model for EOR defects, defect mediated diffusion via both interstitials and vacancies and clustering model to account for immobile/inactive peak. We found that including several other phenomena critical for accurate modeling of As implants. High arsenic concentration accelerates generation of Frank loop pairs, the vacancy formed in the process deactivates As while the interstitial injection enhances diffusion and at very high concentrations of arsenic cause loop formation. This process can also explain very rapid initial depletion of interstitials and non-elastic domain of interstitial supersaturation on doping level. Our model includes enhanced diffusion of arsenic at very high donor levels due to interaction of vacancies with multiple dopants and formation of As\textsuperscript{+}\textsuperscript{1}\textsuperscript{V} centers. We also take into account the effect of formation and dissolution of 311 defects. The model will be compared.
to experimental data for both electrical activation and chemical profiles at different doses and implant energies.

11:45 AM J5.11 DEFECT EVOLUTION FROM LOW-ENERGY GERMANIUM IMPLANTS ON SILICON. Andres F. Gutierrez, Kevin S. Jones, University of Florida, Dept. of Microelectronics, Gainesville, FL; Daniel F. Downey, Varian Semiconductor Equipment Associates, Gloucester, MA.

Pre-amorphization is commonly used in the formation of ultrashallow junctions for Si-based microelectronic devices. Knowing that excess interstitials provide a source for TED, it becomes necessary to understand all sources and conditions for interstitial formation and evolution, especially at the technologically important low-energy regimes. Plan-view transmission electron microscopy (PTEM) was used to characterize defect evolution upon annealing of low-energy germanium ions in silicon. The implant doses were 1 x 10^{14}, 4 x 10^{15}, and 3 x 10^{15} cm^{-2}, sufficient for surface amorphization. Annealing of the samples was done at 750°C in nitrogen ambient by both rapid thermal annealing (RTA) and conventional furnace anneals, and the time was varied from 10 to 21600 sec. Results indicate that as the energy drops from 30 to 5 keV, an alternate path of excess interstitials evolution may exist. For higher implant energies, the interstitials evolve from clusters to (311) to loops as has been previously reported. However, as the energy drops to 5 keV, the interstitials evolve from clusters to small, unstable dislocation loops which dissolve and disappear within a narrow time window, with no (311) forming. These results imply that there is a mechanism responsible for (311) formation during TED; these ultra-low-energy implants. The energetics of the dissolution process for small dislocation loops will be discussed.

SESSION J6: Dopant Impurity Effects

Wednesday, April 18, 2001
Golden Gate A2 (Marriott)

1:30 PM J6.1 THE EFFECT OF FLUORINE CO-IMPLANTATION ON BORON ULTRA-SHALLOW JUNCTION FORMATION. L.S. Robertson, K.S. Gamb, R.S. Turner, University of Florida, Gainesville, FL; D.F. Downey, Varian Semiconductor Equipment Associates, Gloucester, MA; M.J. Rendón, Motorola, Austin, TX.

Historically, reducing the depth and sheet resistance of junctions in silicon integrated circuits has been achieved by reducing the energy and increasing the dose of the ion implanted dopant. This conventional methodology is now yielding diminishing returns due to what appears to be an immutable trade-off between junction depth and sheet resistance for ultrashallow junctions. An alternative approach to achieve ultrashallow low-resistance junctions by co-implantation of boron and fluorine by exhibiting a simultaneous decrease in junction depth and sheet resistance. In this paper, the effect will be explained based on observations from recent experiments. Amorphization of a type-Crystalline wafer was achieved using a 7 keV 1 x 10^{15} cm^{-2} Si. The Si+ implant produced a 150 mA deep amorphous layer, which was then implanted with B+ ions with energies ranging from 500 eV to 1 keV and doses ranging from 1 x 10^{14}/cm^2 to 4 x 10^{15}/cm^2. The wafers were subsequently implanted with P+ ions with energies ranging from 3 to 36 keV and doses ranging from 1 x 10^{15}/cm^2 to 8 x 10^{14}/cm^2. The energies of the fluorine implants were chosen such that the damage and ion profiles of the fluorine were contained within the amorphous layer, thereby eliminating extraneous damage effects. Post-implantation anneals were performed in nitrogen furnace at 750°C. Secondary ion mass spectrometry was used to monitor the dopant diffusion after annealing. Hall effect measurements were used to study the dopant activation. The addition of fluorine reduces the boron diffusion enhancement by 50%, increases the boron activation by 2X, and increases the boron concentration gradient in the tail of the profile by 5X. The observed effect is more complicated than traditional interstitial trapping that has previously been observed for other impurity species. Detailed chemical, structural, and electrical analysis will be presented to explain the observed phenomena.

1:45 PM J6.2 FLUORINE ENHANCED BORON DIFFUSION IN SILICON DURING LOW TEMPERATURE ANNEALING. Jian-Yue Jin, Jinning Liu, Ukyo Jeong, Scott Falk and Sandeep Mehrotra, Varian Semiconductor Equipment Associates, Gloucester, MA; Kevin Jones, SWAMP Center, University of Florida, Gainesville, FL.

It is well known that co-implantation of Fluorine reduces Boron transient enhanced diffusion (TED) in Si during rapid thermal annealing. However, it is not well understood how Fluorine interacts with Boron or Si to affect Boron diffusion. In this paper, we report a new observation of Fluorine reduced Boron diffusion enhancement that, after a furnace anneal at 550°C for 30min, wafers with Fluorine pre-amorphization implant (PAI) have much greater boron diffusion than wafers without PAI or with Si PAI. The Fluorine PAI was 8 keV with a dose of 1 x 10^{14} /cm^2. The Si PAI was 10 and 20 keV with a dose of 5 x 10^{14} /cm^2. The Boron implants were 250 eV to 1 keV with a dose of 1 x 10^{14} /cm^2. Wafers without PAI show very little Boron diffusion after 30 minutes 550°C annealing. Wafers with Si PAI show slight movement of Boron profiles. However, wafers with Fluorine PAI show significant Boron profile broadening after the same low temperature annealing for all different energies of Boron implants. TEM was used to investigate the correlation of lattice microstructure and Boron diffusion. The mechanism of Fluorine effect will be discussed.

2:00 PM J6.3 INTERACTION OF CHLORINE WITH DopANTS AND DEFECTS IN SILICON. Y. C. Venezia, H. J. J. Gossman, H. J. Vuong, A. T. Fiory, and C. S. Ruoff, Bell Laboratories, Lucent Technologies, Murray Hill, NJ.

Silicon device processing often employs silicon dioxide that is thermally grown in a Cl containing oxygen ambient. The Cl increases the oxidation rate, reduces interface charge states, and also helps in the removal of contamination from furnace tubes. While it is well known that Cl getters to the silicon-silicon dioxide interface during oxidation, much less is known about the behavior of Cl in Si. We have investigated the interaction of Cl with defects and Si in silicon. In these experiments Cl was introduced either by annealing in a dry oxygen ambient containing one percent DCE or by ion implantation. The (311) defects were created by either 8keV ion implants or Cl ion implantation. We find that through annealing, the concentration of interstitials in (311) defects from both implants is similar, the defects created by Cl implants dissolve much faster than those created by similar Si implants. On the other hand, Cl, whether introduced by implantation or during oxidation, had no effect on B TED. There was, however, a strong interaction of Cl with the dopant profiles: implanted Cl in samples containing six 10 nm wide B markers, grown by molecular beam epitaxy, was observed to diffuse away from its implanted profile and to be trapped at the B markers. No other diffusion of Cl in silicon was observed, consistent with previously-reported work of no Cl diffusion in silicon. This Cl gettering at B is also observed when B is introduced by ion implantation in front zone silicon.


In current silicon IC technology, nitrogen implant is utilized as a way of obtaining thin oxynitrides and two different oxide thicknesses in the same substrate. The diffusion of nitrogen and defect structure after the diffusion greatly affects the oxidation rate and resistance. Although reports exist on the diffusion and defect structure of low dose nitrogen implants, high dose nitrogen implants have not been studied in detail. In this study, nitrogen diffusion and defect structure were investigated after medium to high dose nitrogen implantation and anneal. 11 keV N2 was implanted into silicon at doses ranging from 2 x 10^{14} to 2 x 10^{15} cm^{-2}. The samples were annealed with an RTA system from 750°C to 900°C. The nitrogen profiles were obtained by SIMS. Cross section TEM was done on selected samples. For lower doses, most of the nitrogen diffused out of silicon into the silicon oxide interface as expected. For higher doses, a significant portion of the nitrogen still remains in silicon even after the highest thermal budget. This is attributed to the finite capacity of the silicon oxide interface to trap nitrogen. When the interface gets saturated by nitrogen atoms, nitrogen in silicon can not escape into the interface. The 2 x 10^{15} cm^{-2} dose creates a continuous amorphous layer from the surface. Even after a 750°C anneal, there is residual amorphous Si at the surface which has not been recrystallized. In addition, stacking faults have started to form at the surface and end of range damage has formed slightly below the bottom of the original amorphous layer. After the 900°C anneal, the silicon has fully recrystallized leaving behind stacking fault type defects at the surface and residual end of range damage. Further investigation of the defect structure is in progress.

2:30 PM J6.5 MODELING BORON AND INDUML ELECTRICAL ACTIVITIES IN SILICON IN THE PRESENCE OF NITROGEN. Vladimir Zubkov, Schulke Aronovitz, Helmut Poschenrieder, United Logic, Santa Clara, CA; Jamm Sensoioso, Dept. of Chemical Engineering, Stanford, CA.
Spreading resistance profiling analyses have revealed that, in the presence of atoms N, electrical activity of B in Si is lowered by 10% but In and Sn are no effect on electrical activity. VASP was applied to exploration of the B - N and In - N interactions effect on acceptor activities. Si64 supercells were mainly employed. Formation energy, EF, of a negatively charged supercell and a band gap from calculations with each point were chosen as indices of acceptor activity. For qualitative study of range interactions DFT was applied to calculations of electron affinities of Si chains containing acceptors and N atom. For separate dopants calculated EF and gap values indicate the substitutional B and In are effective acceptors and N is a weak donor. When atom N was placed interstitially or substitutionally adjacent to B (In), a strong interaction between B (In) and N was found that dramatically lowered EF and increased gap values, so the nitride acceptor is more effective in N-X chemical bonds in some cases (X=Al, B). Calculated EF, gap, and electron affinities indicate th the X-N systems exhibit reduced electrical activity when the X-N are adjacent but also when they are separated by substitutional or interstitial bonds. A decrease in electrical activity of B and In in the presence of N. Dependence of EF values on the distance between acceptor and N was almost the same for B and In. However, binding energies for In-N pairs are higher than those for B-N pairs. It is possible to suggest that a larger decrease in In activity might be due to a smaller average distance between In-N than between B-N since binding energy should affect the average distance between an acceptor and N.

3:45 PM 36.6
Abstract Withdrawn.

3:30 PM 36.7
SILICON INTERSTITIAL-DRIVEN LOSS OF SUBSTITUTIONAL CARBON FROM SiGe STRUCTURES. M.S. Carroll and J.C. Sturm, Dept. of Electrical Engineering and Computer Science, Princeton University, Princeton, NJ; E. Napoli, A. Drigo, INFN, and Dept. of Physics, University of Padova, Padova, ITALY; J. Stangl and G. Bauer, Institute for Semiconductor Physics, Johannes Kepler University Linz, Austria; D. Tweet, SHARP Laboratories of America, Inc., Camarillo, CA.

Introduction of substitutional carbon in silicon and SiGe is a method to reduce excess silicon interstitial concentrations created by process damage [e.g. implantation or oxidation], and thereby suppress the enhanced boron diffusion typically observed after processing [1]. However, the number of carbon that are effect on the excess interstitial is unknown and further more especially interstitial concentrations are reported to initiate carbon precipitation [2]. Therefore, it is critical to identify the exact carbon-interstitial interaction that suppresses dopant diffusion and determine what happens to the carbon due to this reaction. In this paper we describe the reaction of substitutional carbon with silicon interstitial by oxidation. Single crystal, 25 nm thick, Si$_2$Ge$_{35}$Si$_{65}$ epitaxial layers were grown on Czochralski silicon substrates and capped by silicon nitride layers. The samples were annealed in either nitrogen or oxygen at 750°C or 850°C for times of 30-90 minutes. Carbon concentrations before and after the annealing were measured by secondary ion mass spectroscopy and x-ray diffraction. Carbon diffusion is enhanced by the interstitial injection during oxidation indicative of a diffusion reaction between the carbon and interstitial, and in the most rapid reaction, the diffusion is nearly all interstitial in the upper 50% of the SiGe layer. This is consistent with the fact that the interstitial carbon concentration in the upper 50% is much greater than in the lower 50%. Furthermore, the interstitial injection during oxidation in these conditions is also known [3], the number of carbon that leave the SiGe layer can be correlated with the number of carbon that leave the SiGe layer. This was suggested by ANDO and DAHDA [1] P.A. Stolk, H.J. Goossen, D.J. Eaglesham, D.C. Jacobson, J.M. Poste, and H.S. Luftman, Appl. Phys. Lett. 46, 568 (1985) [2] W.J. Taylor, T.Y. Than, U. Ekenberg, Appl. Phys. Lett. 52, 636 (1988) [3] M.S. Carroll and J.C. Sturm in Silicon Front-End Processing, Physics and Technology of Dopant-Defect Interactions II, Vol. 620. Material Research Symposium Proceedings. (to be published)

3:45 PM 36.8
DIFFUSION AND CLUSTERING OF SUPERSATURATED C IN SiGe LAYERS. D. De Salvidor, E. Napoli, A. Consoli, M. Bertl, A.V. Drigo, Instituto di Elettronica e Ing. di Sistemi, University of Padova, Padova, ITALY; M.S. Carroll, J.C. Sturm, Dept. of Electrical Engineering, Princeton University, Princeton, NJ; J. Stangl, G. Bauer, Institute for Semiconductor Physics, Johannes Kepler University Linz, Linz, AUSTRIA.

The mechanisms governing the interaction between self-interstitial and supersaturated carbon are rather complex and not yet well understood, involving selfinterstitial driven C diffusion and/or clustering or precipitation. In this work we investigated the formation and clustering of supersaturated substitutional carbon 200 nm thick Si$_2$Ge$_{35}$Si$_{65}$ layers buried under silicon cap layers of 40 nm. The samples are annealed in nitrogen or oxygen ambient at 850°C for times between 30 hours to one day. Total and substitutional carbon concentrations profiles are measured by secondary ion mass spectrometry (SIMS), x-ray diffraction (XRD), Rutherford and resonant backscattering spectroscopy in random and channeling geometry (RBS/RBS). Self-interstitial and clustering of substitutional C precipitates depth profiles are characterized by transmission electron microscopy (TEM). The interstitial flux coming from the surface under oxidation enhances the C diffusion with respect to the N$_2$ annealed samples. Mobile C can move away from the layers or accumulate at the interface, leading to the formation of carbon clusters. This phenomenon saturates after 4 hours, because the interstitial injection during oxidation also promotes the formation of carbon clusters. The latter prevents further loss of C, which instead in our samples diffuses and accumulates in the lower 40 nm below the cap layer interface. However, the precipitate density profile extends also deeper in the layer. Additionally, as a result of interstitial injection from the surface, after 10h in O$_2$ the profile of C that is removed from substitutional sites is not uniform through the layer and decreases with depth. Considering also that the deeper interface of the profile does not broaden, the above results indicate that the depth at which the flux of mobile C and/or self-interstitials is able to penetrate and react is located inside the layer, within 130 nm below the cap/layer interface.

4:00 PM 36.9
BORON SEGREGATION AND ELECTRICAL PROPERTIES IN POLYCRYSTALLINE SiGe: E.联想, K. Seeger, and J.C. Sturm, Center for Photonics and Optoelectronic Materials, Department of Electrical Engineering, Princeton University, Princeton, NJ.

Previously, it has been reported that PMSO capacitors with heavily boron-doped polycrystalline SiGe substrates are less susceptible to boron penetration than those with Si gates [1]. Boron appears to accumulate in the SiGe layers during anneals, reducing boron out-diffusion from the gate regions on the dielectric oxide interface. In this abstract, we report clear evidence of strong boron segregation to polycrystalline SiGe layers from Si or SiGe layers, and present electrical data indicating that the boron in these layers remains active. Poly-SiGe layers were deposited by RTCVD at 557°C and 700°C using SiH$_4$, GeH$_4$, SiH$_4$, and B$_2$H$_6$ as silicon, germanium, carbon, and boron sources, respectively. All layers were in situ doped and grown on 200 nm oxides. To study segregation, two layer structures were grown consisting of ~100 nm p$^+$ (~1×10$^{18}$ cm$^{-3}$) poly SiGe (Ge=25%, Ca=1.6%) next to ~300 nm of p$^+$ (~1×10$^{20}$ cm$^{-3}$) poly Si. This sample was annealed in N$_2$ at 850°C for 30 minutes to allow the boron to move from the heavily doped Si to the lightly doped SiGe-C layer. Single layer samples of p$^+$ (~1×10$^{20}$ cm$^{-3}$) poly Si, SiGe, and SiGe-C were also grown and annealed under the same conditions. SIMS, sheet resistance, spreading resistance, and Hall measurements were taken for all samples to determine boron concentrations and electrical activity. In the two layer structure, SIMS profiles show that boron has accumulated in the heavily doped SiGe-C layer during the anneal, with boron concentration increasing to ~4x that of the Si layer. A separate experiment confirms that this result is not due to any SIMS artifacts. Electrical measurements of the single layer samples show that the SiGe-C layer’s conductivity remains roughly constant during the anneal. In the two layer sample the boron that has segregated to the SiGe-C layer appears active, but less so than in the single layer SiGe-C sample. Segregation has also been observed in single crystal SiGe-C. The driving force for segregation is under further study; however, it appears that at least significant amount of the boron is not forming inactive carbon-related defect complexes. [1] C.L. Chong and J.C. Sturm, Applied Physics Letters, 74 (17), 2591 (1999).

4:15 PM 36.10
A COMPREHENSIVE MODEL FOR CARBON SUPPRESSION OF BORON TRANSIENT ENHANCED DIFFUSION. Jule L. Ngoc, Peter B. Griffen, and James D. Plummer, Stanford University Center for Integrated Systems, Stanford, CA.

In this work, the time evolution of B transient enhanced diffusion (TED) suppression due to the incorporation of carbon in Si$_2$Ge$_{35}$Si$_{65}$ and Si$_2$Ge$_{35}$Si$_{65}$ layers where $x = 9.6\%$ and $y = 0.018 \pm 0.037$ was studied for $10 \text{ s}$ to $60 \text{ min}$, $750\text{ °C}$ anneals. The combination of high B concentrations, which reduce TED by completely eliminating it, and having diffused B profiles for several times at a single temperature provides much data upon which various models for the suppression of B TED can be tested. Recent work in the literature has indicated that the suppression of B TED in Cr-rich Si is caused by
the non-equilibrium Si point defect concentrations, specifically the underestimation of Si self-interstitials, that result from the coupled out-diffusion of carbon interstitials to the kick-out and Frank-Turnbull reactions. Attempts to model our data with these two reaction schemes revealed that the rate-determining mechanism for B was not accurately simulated and that an additional carbon reaction was necessary. In this work, we incorporate a carbon interstitial, carbon substitutional (C_C) pairing reaction into a comprehensive model that includes the C kick-out reaction, C Frank-Turnbull reaction, (Si-1) defects, and boron interstitial clusters (BICs) and demonstrate that this model successfully simulates C concentration behavior at temperatures ranging from 700 to 1100°C. For temperatures in the LTP process window, the LTP did not melt into the EOR and thus high concentrations of point defects theoretically exist in this region. It was also observed for all temperatures that the LTP suppresses the formation of extended EOR defects. However, secondary ion mass spectrometry shows that transient enhanced boron diffusion was still observed in both the melt region and for marker layers located away from the surface. Since the highest laser power causes the melt to consume nearly the entire EOR interstitial profile, this phenomenon suggests that transient enhanced boron diffusion is still present in regions covered by the EOR.

SESSION J7: LASER ANNEALING
Chair: Majed Al Foud
Thursday Morning, April 19, 2001
Golden Gate A2 (Marriott)

8:30 AM *J7.1 IMPACT OF PRE-A-MORPHIZATION IMPLANTS ON LASER ANNEALED JUNCTIONS
S. Srinivasan, M. S. Singer, N. A. Jenkins, IBM T.J. Watson Research Center, Yorktown Heights, NY.

Abrupt, shallow and highly activated junctions will be required for the sub-100 nm technology node to achieve increasingly greater drive currents. The existing dopant activation technology, Rapid Thermal Annealing (RTA), cannot achieve the junction specifications outlined in ITRS 99. Laser Thermal Processing (LTP) is a promising alternative to RTA since it has already demonstrated all of the desired junction characteristics, including the ability to activation dopants in blanket boron wafer. However, the integration of LTP into CMOS flows requires the addition of an amorphization implant and a blanket heat absorbing layer. These two extra process steps can alter the junction characteristics such as activation levels, junction abruptness, dopant density, etc. By changing the melt/recrystallization dynamics, the changes introduced by the amorphization and absorber layers in the melt and recrystallization dynamics have been studied using time resolved reflectometry and transient conductance measurements. The resulting modifications in the defect density, dopant activation, deactivation and diffusion behavior have also been investigated using a combination of SIMS, TEM, four-point probe and Hall mobility measurements. The results of these studies will be presented in this paper.

9:00 AM *J7.2 EFFECT OF LASER THERMAL PROCESSING ON DEFECT EVOLUTION IN SI, C, SILEN, C, E, K. K. Leong, R. S. Jones, Univ. of Florida, Dept. of MSE, Gainesville, FL; Sameer Talwar, Verdant Technologies, San Jose, CA.

Laser Thermal Processing (LTP) involves laser melting of an implantation induced preamorphized layer to form highly doped ultra shallow junctions in silicon. After LTP a large number of interstitials remain in the end of range (EOR) just below the amorphous region. Since post processing is an implantation, it is necessary to understand both the behavior of these interstitials and the nature of interstitials in the recrystallized-melt region. In this study, an amorphizing 15 keV 1×10^{18} cm^{-2} Si^{+} implant was done followed by a 1 keV 4×10^{15} cm^{-2} B^{+} implant. The surface was then laser melted at laser powers between 0.625 and 0.825 J/cm² using a 308 nm excimer laser. Transmission electron microscopy was used to analyze the defect formation after LTP. It was found that LTP increases the number of regrowth related defects, and a dramatic decrease occurs upon melting beyond the amorphous region. Post-LTP furnace anneals were performed at temperatures ranging from 700 to 1100°C. For temperatures in the LTP process window, the LTP did not melt into the EOR and thus high concentrations of point defects theoretically exist in this region. It was also observed for all temperatures that the LTP suppresses the formation of extended EOR defects. However, secondary ion mass spectrometry shows that transient enhanced boron diffusion was still observed in both the melt region and for marker layers located away from the surface. Since the highest laser power causes the melt to consume nearly the entire EOR interstitial profile, this phenomenon suggests that transient enhanced boron diffusion is still present in regions covered by the EOR.

10:15 AM *J7.5 IMPACT DOSE AND SPIKE ANNEAL TEMPERATURE RELATIONSHIPS FOR SHALLOW EXTENSION JUNCTIONS
S. Srinivasan, M. S. Singer, N. A. Jenkins, IBM T.J. Watson Research Center, Yorktown Heights, NY.

SESSION J8: ADVANCES IN RTA
Chair: Paul A. Pilkhour
Thursday Morning, April 19, 2001
Golden Gate A2 (Marriott)

10:45 AM *J8.1 IMPACT DOSE AND SPIKE ANNEAL TEMPERATURE RELATIONSHIPS FOR SHALLOW EXTENSION JUNCTIONS
S. Srinivasan, M. S. Singer, N. A. Jenkins, IBM T.J. Watson Research Center, Yorktown Heights, NY.

Dopant profiles suitable for the extension regions bridging the channel and source/drain contacts of CMOS transistors are studied by short loop anneals of blanket implants. Implant doses of boron and phosphorus were varied from below to above the threshold for transient dopant-enhanced diffusion (i.e., denoted ‘BED’ for boron-enhanced diffusion). Electrical activation and diffusion uses spike thermal anneals with incipience lapse (Heatpulse) or arc ramp (Vortex) heating mechanisms. Under alloying conditions, transient dopant solubility is equivalent thermal budget. For targeted sheet resistance and junction depth, spiking temperature trends lower with implant dose, commensurate with decreasing fraction of activated dopant.

10:45 AM 3.8.2
BORON DOPANT IN SILICON AND SILICON GERMANIUM UNIFIED THERMAL INFLUENCE OF POINT DEFECT INJECTION BY RAPID THERMAL ANNEAL. Ailsan Don, Arthur F. W. Willoughby, Janet M. Bence, School of Engineering Sciences, University of Southampton, Southampton, UNITED KINGDOM; Nicholas E.B. Cawney, Philips Research Labs, Eindhoven, THE NETHERLANDS; Barry M. McGregor, School of Engineering, University of Cambridge, Cambridge, UNITED KINGDOM.

The effect of point defect injection by comparison of inert diffusion (Rapid Thermal Annealing (RTA) silicon dioxide and silicon nitride bilayer samples in oxygen) with injection diffusion (RTA oxidation of boron silicon surface to inject interstitials) on the diffusion of boron in silicon and silicon-germanium alloys has been studied. It is generally accepted that boron in silicon diffuses via an interstitially mediated mechanism. In this work, B in Si was used as a control wafer to investigate B diffusion behavior in Si$_{0.95}$Ge$_{0.05}$. The diffusion profiles for Si$_{0.95}$Ge$_{0.05}$ samples were prepared on Second Ion Mass Spectrometry (SIMS). Diffusivities for B in Si and Si$_{0.95}$Ge$_{0.05}$ were obtained by using computer simulations of the measured boron profiles for annealed samples. Boron diffusion in Si and Si$_{0.95}$Ge$_{0.05}$ was found enhanced by interstitial injection. The enhancement from the interstitial injection of the B diffusivity in Si$_{0.95}$Ge$_{0.05}$ is similar to that in Si. These results confirm that B diffusion in Si$_{0.95}$Ge$_{0.05}$ is mediated by an interstitially mediated mechanism and similar than in Si. The effect of the diffusion of the B lattice in Si and Si$_{0.95}$Ge$_{0.05}$ has also been investigated. The diffusivity versus diffusion time of B in Si and Si$_{0.95}$Ge$_{0.05}$ for inert and injection samples is presented. It was found that the shorter annealing time had the faster diffusion. This suggested that it caused by transient diffusion effect arising from grown-in defects.

11:00 AM 3.8.3
INFLUENCE OF LOW THERMAL BUDGET PRE-ANNEALS ON THE HIGH TEMPERATURE REDISTRIBUTION OF LOW ENERGY BORON IMPLANTS IN SILICON. F. Boudon, PHASE / CNRS, Strasbourg, France; M. Chabot, PHASE / CNRS; P. Rivallin, CNRS; B. Huglin, LETI, Grenoble, France; and E. Guichard, SIYACO France.

It is now well established that the transient enhanced diffusion (TED) of ion implanted boron in silicon limits the formation of the ultra-shallow junctions required for the extreme deep submicron devices. It is known that TED is linked to the fate (elimination and agglomeration) of the implantation related excess self-interstitials. Thus it can be expected that the final high temperature redistribution is at least partly governed by the effective initial point defect distribution at the onset of the high temperature plateau. In this respect some reports exist already on an influence of the temperature ramping rate [1]. However, it is known for decades that self-interstitials are mobile in silicon even at extremely low temperatures. It should be thought that low thermal budget pre-anneals, by affecting the initial self-interstitials distribution, could affect TED redistribution during subsequent high temperature RTA. The purpose of this contribution is to present the experimental evidence that such low thermal budget pre-anneals strongly affect the high temperature redistribution. Samples implanted with high dose boron at 3 or 10 keV were first annealed at low temperature (500 - 700°C) for various durations. These samples were then RTA annealed around 1000°C. The B profiles resulting from these two steps anneals were then measured by SIMS. We will present a systematic study of the evolution of these profiles as a function of the pre-anneal and RTA conditions. [1] A. Agarwal et al. J. Electron. Mater. (28), 1333 (1999)

11:45 AM 3.8.6
RAMP-RATE EFFECTS ON TRANSIENT ENHANCED DIFFUSION: A QUASI-ANALYTICAL EXAMINATION. Michael Y.L. Jung, Edmund G. Seehofer, Univ of Illinois, U.C., Dept of Chemical Engineering, IL.

Some experimental evidence has accumulated in recent years to support the use of rapid thermal annealing (RTA) with very fast heating and cooling rates for making ultra-shallow junctions by ion implantation. Improved device properties have been claimed using heating rates of 400°C/sec or more. This procedure supposedly optimizes junction depth and sheet resistance by reducing transient-enhanced diffusion (TED) of the dopants. However, a rigorous theoretical justification for using such fast ramps has been spotty. Since the design and use of fast-ramp annealing tools will require substantial investments by equipment manufacturers and IC manufacturers alike, obtaining a clear picture for the occurrence and potential magnitude of such effects is important. We employ a quasi-analytical approach to the complex, interrelated phenomena that govern TED, confirmed by numerical simulations for boron based on FLOOPS. We find that increasing the ramp rate β narrows the diffusion profile according to β$^{-1/2}$ as long as TED runs out before the top of the spike. Improvement decreases.

Sub-100 nm Si technologies require junction depths of less than 30 nm at the channel and less than 70 nm at the source/drain contact. During processing, every attempt is made to minimize diffusion, with the consequence that the dopants are not driven very far beyond the region of ion-implantation-induced damage. This and the very high dopant concentrations can lead to excessive junction leakage current, I$_{leak}$. We have investigated diode leakage in junctions produced by ion-implantation of B with energies of 0.5 - 2 keV and doses of 2 x 10$^{15}$ cm$^{-2}$ to 2 x 10$^{16}$ cm$^{-2}$ , in n-wells of 2 x 10$^{15}$ cm$^{-2}$ in 2 x 10$^{15}$ cm$^{-2}$ ramping temperature and dopant solubility at equivalent thermal budget. For targeted sheet resistance and junction depth, spiking temperature trends lower with implant dose, commensurate with decreasing fraction of activated dopant.

11:30 AM 3.8.5
BORON SOLUBILITY LIMITS FOLLOWING LOW TEMPERATURE SOLID PHASE EPITAXIAL GROWTH. C.D. Linders, K. S. Jones, Univ of Florida, Dept of Material Science and Engineering, Gainesville, FL; M.J. Renton, Motorola Inc, Austin, TX.

Future advancements in microelectronics require shallower junctions, higher carrier concentration material. Alternative techniques for controlling transient enhanced diffusion (TED) are being explored for shallower junction formation. One such technique is implantation dopant into a phosphorus doped substrate and using low temperature solid phase epitaxy (SPE) regrowth to obtain the desired doping and sheet resistance. Wafers were pre-implanted with either silicon or germanium followed by 5 keV P$^+$ implants in the dose range of 5 x 10$^{14}$ - 8 x 10$^{15}$ cm$^{-2}$. Amorphous layers were grown at temperatures between 500 and 600°C to examine maximum achievable electrically activated boron levels. Different amorphizing species are used to see if there is a possibility for increasing the solubility limit of boron. To determine the amount of activated boron, the dose calculated from the secondary ion mass spectrometry (SIMS) profile is compared to the carrier dose measured by a Hall effect system. Four point probe measurements are also performed to investigate when the least sheet resistance can be obtained. The epitaxy of the wafers was carried out by VASE (vacuum arc ion-plating epitaxy). Results of the 500°C anneals from 30 to 45 minutes show that a minimum sheet resistance of about 140 Oµcm can be achieved for an implanted dose of 2 x 10$^{15}$ cm$^{-2}$. For boron implanted, at 500°C, a minimum sheet resistance of 2 x 10$^{15}$ cm$^{-2}$ B$^+$ dose. This amorphous layers still exist after 30 and 35 minutes at 500°C but there is little effect on the overall sheet resistance. There is also evidence that at higher concentrations of boron the regrowth process can be slowed or stopped and large amounts of inactive boron exist.

12:15 PM 3.8.7
REVERSE DIODE LEAKAGE IN SPIKE-ANNEALED ULTRA-SHALLOW JUNCTIONS. Tao Eng, University of Florida, Gainesville, FL; George L. Oates, Lucent Technologies, Murray Hill, NJ; Aditya Agarwal, Peter Frisell

and Leonard M. Rubin, Axcelis Technologies, Beverly, MA.
progressively if TED runs out after the top. High ramp rate also affects activation indirectly (and in a complicated way) through interstitial clustering kinetics. The optimum value of D depends sensitively on the temperature trajectory near the peak and the details of the clustering model used. The detail of the initial temperature stabilization step influences subsequent profile evolution in a significant way.

SESSION J9: SIMULATION AND MODELING
Chair: Hans-J. Gossmann
Thursday Afternoon, April 19, 2001
Golden Gate A2 (Marriott)
12:30 PM 39.1
MODELING OF DopANT DIFFUSION AND ACTIVATION.
Mark E. Leu, Dept. of ECE, SWAMP Center, Univ. of Florida, Gainesville, FL.
Shallow junctions in silicon are formed by implant and anneal processes. The damage from the implant interacts with the dopant to control diffusion and activation. The life cycle of the damage is quite complex - initial recombination of Frenkel pairs is followed by formation of small defect clusters which can grow and evolve into a variety of larger defect structures. Experimental results show that there are different regimes of diffusion corresponding to the different defect annealing states. Surface relaxation of the defect also acts as a sink of defects in a complex way. Models for the implant generation of defects, their recombination, clustering, and eventual dissolution will be presented. The models include chemical reactions that can account for experimental profile evolution from both oxidation and reverse short channel effect studies. The surface model uses both di-interstitial recombination and surface damage to account for the surface evolution. Recent work on dopant influence on damage evolution will also be discussed.

2:00 PM 39.2
ATOMICISTIC STUDY OF B-RELATED DEFECTS IN SILICON BY TIGHT-BINDING SIMULATIONS.
Paola Alihi, Lucia Colombo, Paolo Ruggiero. INFN and Dept. Physics, University of Cagliari, ITALY.
In this work, we have applied a Density Functional derived Tight-Binding method (DFTB) [1] to the study of the energetics and the dynamics of boron defects in silicon. Observed B-profiles of implanted silicon samples show [2] in fact the well-known enhanced B-diffusion together with the formation of B-si immobile complexes. Both features are believed to be driven by the excess Si self-interstitial created by the implant damage. The need to obtain shallow junctions in silicon device technology obviously requires a detailed understanding of the microscopic mechanisms governing B diffusion and B-Si interactions. We have first addressed the issue of the energetics and the dynamics of the single boron atom and a self-interstitial in a silicon matrix. DFTB results for equilibrium structures and formation energies of different defects configurations were at first compared to previous and current DFT-LDA results [3] thus establishing the degree of reliability and accuracy of the present approach. Then, we performed molecular dynamics simulation at finite temperatures of the boron diffusion mechanism and of the diffusion process. The results indicate that the reduction of the formation energy of the defects as they grow in size or change their 'crystallographic' structure. We have implemented an atomic simulation tool based on the description of the diffusion potential to simulate the time evolution of the defects in the ultra-low energy regime. This result is consistent with the pulsed TED observed in such case and with TEM observations of defects in the nanometer range. In summary, we have shown that the understanding of the formation energy and the evolution of boron defects, leading to the correct prediction of dopant enhanced diffusion in all experimental conditions.

2:45 PM 39.5
SIMULATION OF BORON-DOPANT PROFILE EVOLUTION DURING ULTRASHALLOW JUNCTION FORMATION.
Gaeog S. Hwang, Eugene Heifta, Thair Cagin, and William A. Goddard III. Materials and Process Simulation Center, Beckman Institute, California Institute of Technology, CA; Yuzuru Sato, Misingunu Motsh, and Makinobu Uehara, Seiko Epson Corp., JAPAN.
An insufficient reduction in device dimensions requires the formation of ultrashallow junctions with high concentrations of electrically active dopants and box-like profiles in order to maximize drive currents while minimizing short channel effects. To control such junction properties it is necessary to understand quantitatively (i) the underlying mechanisms of transient enhanced diffusion of dopants and (ii) the dynamics of defect/dopant clustering during implantation and post-implantation annealing. Despite a great deal of effort over past years the clustering and diffusion mechanisms are still unclear. For this study we have developed a multiscale model in which we combine (i) kinetic Monte Carlo and continuum simulation of describing relatively long time scale phenomena such as defect-dopant clustering and doping profile evolution with (ii) quantum mechanics based functional theory) simulation of the fundamental atomic-level processes, and (iii) experimental validation. We will present (i) new mechanisms of B diffusion, (ii) B clustering with Si self interstitials, and (iii) the results of doping profile evolution.
simulations for various process conditions. We will also address several intriguing questions arising in the ultra-thick junction processing: (i) the validity of 1D models (ii) the surface property effect, and (iii) the role of defect/defect clustering in determining junction profiles.

**SESSION J10: GATHERING OF IMPURITIES**
Chair: Alan Clairner
Thursday Afternoon, April 19, 2001
Golden Gate A 2 (Marriott)

3:30 PM J10.1
INTERACTION OF TRANSITION METAL CONTAMINATION WITH ION-IMPLANTED B IN Si. Janet L. Bengtson, Thomas Boone, Dale C. Jacobson, Censor S. Rafferty, Bell Laboratories, Lucent Technologies, Murray Hill, NJ.

The interaction of transition metal contamination with ion-implanted B during Si device processing is a function of the metal element, the B concentration, the processing temperature profile, the ion-implantation induced defects, and the proximity of the contamination and the boron. 3D transition metals exhibit high diffusion via interstitial atoms in Si, leading to the formation of precipitates or clusters during cooling from high temperatures which are nucleated by defects associated with B ion implantation. In addition, Fe and Co also show metal-acceptor pairing and gettering by regions of high B concentration. In contrast, Cr, Nd, and Au do not exhibit similar behavior. Contamination by interstitial atoms in Si by ion-implantation and their interactions with ion-implanted B is monitored by SIMS, carrier recombination lifetime, and DLTS. Localization of Mo or ion-implanted induced damage is observed. SIMS profiles of flash-photoluminescence into Si show that the unintentionally introduced Mo segregates to implant damage after high temperature annealing. Both the Mo and F profiles sharpen with concentration maximums in regions of implant damage. Mo does not precipitate form regions of high boron concentrations, but does collect in regions high in vacancy defects. Comparisons of Fe and Co redistribution in the presence of ion-implanted B with that of ion-implanted C or Si suggests that the aggregation of these metals as implant damage is limited by solubility and precipitation rate rather than diffusion kinetics. Gettering of Fe by regions of high B concentrations is controlled by Fermi-level induced Fe redistribution and Fermi-level controlled Fe-B pairing. This partitioning of Fe is extremely effective at temperatures below 400°C. SIMS profiles show that, similar to the behavior of Fe, Co in Si can also be gettered by B ion-implantation. Since the diffusivity of Co is greater than that of Fe in Si, diffusion kinetics are optimum for low temperature cooldown annealing providing competing gettering mechanisms are not nucleated during the high temperature treatment. Our new results suggest that regions of ion-implantation induced damage provide sites for heterogeneous nucleation of Co precipitates or Co clusters, and thus the final distribution of Co in Si is controlled by nucleation and precipitation rate rather than diffusion kinetics. Gettering of Fe by regions of high B concentrations is controlled by Fermi-level induced Fe redistribution and Fermi-level controlled Fe-B pairing. This partitioning of Fe is extremely effective at temperatures below 400°C. SIMS profiles show that, similar to the behavior of Fe, Co in Si can also be gettered by B ion-implantation. Since the diffusivity of Co is greater than that of Fe in Si, diffusion kinetics are optimum for low temperature cooldown annealing providing competing gettering mechanisms are not nucleated during the high temperature treatment. Our new results suggest that regions of ion-implantation induced damage provide sites for heterogeneous nucleation of Co precipitates or Co clusters, and thus the final distribution of Co in Si is controlled by nucleation and precipitation rate rather than diffusion kinetics. Gettering of Fe by regions of high B concentrations is controlled by Fermi-level induced Fe redistribution and Fermi-level controlled Fe-B pairing. This partitioning of Fe is extremely effective at temperatures below 400°C. SIMS profiles show that, similar to the behavior of Fe, Co in Si can also be gettered by B ion-implantation. Since the diffusivity of Co is greater than that of Fe in Si, diffusion kinetics are optimum for low temperature cooldown annealing providing competing gettering mechanisms are not nucleated during the high temperature treatment. Our new results suggest that regions of ion-implantation induced damage provide sites for heterogeneous nucleation of Co precipitates or Co clusters, and thus the final distribution of Co in Si is controlled by nucleation and precipitation rate rather than diffusion kinetics.

4:00 PM J10.3
THE ROLE OF HIGH ENERGY CO-IMPLANTATION IN LIMITING TRANSIENT ENHANCED DIFFUSION OF BORON IN SILICON AND SOI MATERIAL. Ahmed Najim, Brian J. Sealy, Department of Electronic Engineering, University of Limerick, Limerick, IRELAND.

We investigate the role of high energy (1.5.1 MeV) silicon, fluorine and oxygen implants on the transient enhanced diffusion (TED) of 5keV boron in silicon. High depth resolution SIMS analysis of the implanted boron profile confirms that the high energy implants produce a significant reduction in TED for boron concentrations of 1E18 B/cm² and below. However, there does not appear to be a clear advantage in using either high energy fluorine or oxygen in place of silicon ions. Almost complete retardation of TED is achieved for these boron concentrations when the high energy ions and their associated deep interstitials are isolated by a buried oxide layer in SOI material. The presence of the barrier oxide layer, however, does not affect the profile when all the boron is contained in the silicon overlayer. We will present recent point defect profiles for the deep interstitials from Rutherford backscattering channelling (RBS) and Dechanelling In Crystals And Defect Analysis (DICADA) code and vacancy profiles from positron annihilation (PAS) to attempt to quantify the role of the back diffusion of deep defects on the TED of boron. We will also show that the peak of the boron profile is significantly modified as the depth of the oxide barrier layer is reduced and part of the boron profile and its associated defects are contained in the barrier layer.

4:15 PM J10.4

Following high energy and/or high dose ion implantation into silicon, a vacancy-rich region can be observed close to the surface, i.e. in the region often referred to as “0.3R₅.” During any subsequent thermal treatments, both the interstitials from near R₅ and the shallower vacancies evolve by ripening, recombining with each other, and annealing at various sinks. While the fate of the majority of interstitial clusters have been widely studied, the vacancy clusters are relatively poorly understood because of the lack of suitable measurement techniques and the ever-present interference from interstitials. Recently, the quantitative study of vacancy defects from high-energy ion implantation in Si has been accelerated due to the development of the Au labeling and microbeam x-ray diffuse scattering measurements, which can directly probe vacancy-type defects. We have recently used these methods to make the first quantitative measurements of the evolution of vacancy profiles in front-zone and epilayer. In the surface layers, the peak of the vacancy profile remains near R₀, but the sharp boundaries and the characteristic vacancy profiles become smoother and less pronounced with increasing depth. In the buried oxide layers, the peak of the vacancy profile becomes broader and more diffuse, and the characteristic vacancy profiles are less pronounced. In particular, we will compare and discuss the annealing of vacancy clusters in SOI vs. bulk Si. Furthermore, we will discuss additional effects due to implantation through the Si/SiO₂ interface, which are apparent in the defect profiles following Au-labeling measurements. These experiments with SOI allow us to experimentally isolate effects due to interstitials and provide data on vacancy-reaction kinetics in SOI substrates that will be useful to guide future development of SOI processes.

3:45 PM J10.2

Recently, quite a lot of activity has been devoted to the problem arising from defect evolution in ion implanted silicon outside of the projected range. Most of the effort was spent on elucidating the formation of metal clusters and the so-called Rp/2 defects observed after conventional processing techniques using metal implants. These defects are located between the surface of the sample and the depth region corresponding to the mean projected range of the implanted ions. Whereas most of the authors demonstrated this effect for MeV implants annealed with a dedicated time-temperature profile, we also showed that it can also happen as a result of a low energy light ion implantation: Helium ions with 20 or 40 keV! This points to the fact that the Rp/2 effect is a common feature of implantation especially when the time-temperature profile is not accounted for in the SLA roadmap for future technology schedules. Usually, its nature is discussed in the framework of excess vacancies as residuals of a local recombination between primarily interstitial induced vacancies and interstitials although such models are not taken into consideration. However, there are also experimental observations of residual interstitial defects in the Rp/2 region. On the other hand, metal gettering in the region beyond Rp (trans-Rp-effect) originating from MeV-implants cannot be explained on the basis of excess vacancies. In this paper, we critically discuss these results putting also new facts to the picture. All effects demonstrate that the gettering during ion implantation induced defect evolution do not come to end and never get boring!
Cavities induced by He implantation are known to be efficient to trap metallic impurities in silicon. However, optimization of this process requires a better understanding of the growth mechanism of these cavities during annealing. Literature is somewhat controversial, since depending on surface conditions, the cavities under study may be filled or not with He. In the present study, we have overcome these difficulties by implanting silicon samples with 1.55 MeV 3He and at the fluence of 5x10^{16}/cm^2 i.e. at a depth of almost 6nm. After implantation samples were isochronally annealed for one hour at temperatures ranging from 400°C to 800°C under argon gas. NDD (neutron depth profiling) was used for the ‘dosage’ of He in the annealed layers and has shown that even after the 900°C anneal more than 50% of the He initial content was still detected in the cavity layer. We have used TEM to measure the size distributions, densities and volume fractions occupied by the different populations. When increasing the annealing temperature, the cavity radius increases while the density decreases. Interestingly, the total volume occupied by the cavities remains independent of this temperature in accordance with a conservative Ostwald ripening mechanism for their growth. Under this assumption, we have extracted an activation energy for the growth of such cavities at 1.65-eV a value very close to the activation energy [1.7eV] found for helium desorption or diffusion in Si. From these results, it emerges a picture in which these cavities essentially grow by interchangeing the He atoms they contain. However, a more complex mechanism involving vacancy migration must be taken into account and will be discussed.