SYMPOSIUM J

Si Front-End Processing–Physics and Technology of Dopant-Defect Interactions III

April 17 – 19, 2001

Chairs

Kevin S. Jones
Dept of MS&E
Univ of Florida
SWAMP Center
Gainesville, FL 32611
352-392-9872

Martin D. Giles
Intel Corp
SC12-205
Santa Clara, CA 95052
408-765-8797

Peter A. Stolk
Philips Research Leuven
IMEC2/0.01
Leuven, 3000 BELGIUM
32-16-288324

Jiro Matsuo
Ion Beam Engr Experimental Lab
Kyoto Univ
Kyoto, 606-8501 JAPAN
81-75-753-5953

Erin C. Jones
IBM T.J. Watson Research Center
PO Box 218
Yorktown Heights, NY 10598
914-945-3622

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* Invited paper

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

8:30 AM *J1.1
MOSFET DESIGN CONSIDERATIONS FOR THE SUB-70-NM TECHNOLOGY NODES. Dimitri A. Antoniadis, Microsystems 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 70-nm technology node. While typically the pace of scaling has been limited by lithography, other device design components are increasingly becoming limiting. These include the gate dielectric, where silicon dioxide 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 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 designs, and strained Si/SiGe channels. One or more of these novel device design features will have to be adopted so that device scaling can continue to meet the requirement of miniaturization with commensurate performance enhancement.

9:00 AM *J1.2
DOPING PROCESS ISSUES FOR SUB-0.1 UM GENERATION MOSFETS. Toshihiro Sugii, Youichi Momiyama, Kenichi Goto, Takuji Tanaka, Hajime Kurata, Tomonari Yamamoto and Toshiro Futatugi, Fujitsu Laboratories Ltd., Atsugi, JAPAN; Masataka Kase, Fujitsu Ltd., Mie, JAPAN.

To meet the market demands for LSIs 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 addressed 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. SOI-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 parasitic resistance become very important for a high performance operation. Resistance at extension egde and contact resistance at silicide-Si interface are dominant factors. The traditional approach is to use a higher RTA temperature and a shorter RTA time. The ultimate RTA is laser annealing. We will demonstrate the laser annealing process with an ultra-low contact resistance of 4 x 10-8 Ω-cm^2 and shallow extension simultaneously. By integrating the above technologies, in addition to ultra-thin gate insulators and gate-depletion free electrodes, we can establish front-end process for sub-0.1 μm generations.

9:30 AM *J1.3
ADVANCED ION IMPLANTATION TECHNOLOGY FOR HIGH PERFORMANCE TRANSISTORS. Kyoichi Suguro, Atsushi Murakoshi, Toshihiko Iinuma, Haruko Akutsu, Takeshi Shibata, Atsushi Yagishita, Kazuyoshi Sugihara, and Katsuya Okumura, Process & Manufacturing Engineering Center, Semiconductor Company, Toshiba Corporation, Yokohama, JAPAN.

Defect control in shallow source and drain and precise dose control in channel are important issues in high performance transistors of 0.1-0.13 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 defects around deep junctions by small thermal budget annealing. Therefore, the annihilation of defects by annealing with small thermal budget is a key issue for 0.1-0.13 micron regime. We have developed a process module combined with cryo-implantation and rapid thermal annealing in order to annihilate defects in source and drain regions. [1] 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, chip size implantation technology without photoresist mask was developed. [2] 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 experimental results are reviewed and the some applications are presented. REFERENCES: [1] A. Murakoshi et al., MRS 2000 spring meeting abstract B3.8 p.53. [2] T. Shibata et al., IEDM 2000 Late News to be presented.

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

10:30 AM *J2.1
STATISTICAL CHARACTERISATION OF MOSFET MATCHED PAIRS: A POWERFUL TECHNIQUE FOR STUDYING MICROSCOPIC TRANSISTOR PROPERTY FLUCTUATIONS. Hans P. Tuinhout, Jurriaan Schmitz, Frans P. Widdershoven, Andre H. Montree, Peter A. Stolk, Philips Research Laboratories, Eindhoven, THE NETHERLANDS.

As transistor minimum dimensions continue to shrink, microscopic device property fluctuations are becoming significant contributors to the overall process/device performance spread in advanced analogue as well as digital CMOS circuits. Recent research has demonstrated that random local phenomena such as dopant fluctuations and gate poly-silicon grain boundary related effects can dominate MOSFET threshold voltage spread. Due to their inherent independence of global process spread, pairs of closely spaced identical transistor(matched pairs) 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 characterisation techniques will briefly be reviewed. Subsequently, our paper will discuss several examples where evidence of excessive MOSFET threshold voltage fluctuation observations could be traced back to physical device construction irregularities. In this way we obtained new insights about the impact of effects like dopant fluctuations, grain boundary diffusion and poly-silicon gate activation on CMOS transistor matching. More in particular we revealed the impact of fluctuation of gate depletion and boron penetration by investigating their relation with the activation RTA as well as poly-silicon morphology. Furthermore we 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 Decaborane implantation. Transistor matching characterisation studies are necessary to provide the required information on device performance spreads that electronic circuit designers have to take into account for performance and yield optimisation. But moreover, these studies provide unique insights into microscopic device properties that, due to their statistical nature, cannot be obtained through other physical characterisation techniques such as TEM, SEM, SIMS, etc.

11:00 AM J2.2
SSRM AND SCM OBSERVATION OF MODIFIED LATERAL DIFFUSION OF AS, BF2 AND SB INDUCED BY NITRIDE SPACERS. P. Eyben, N. Duhayon, C. Stuer, I. De Wolf, R. Rooyackers, T. Clarysse, W. Vandervorst and G. Badenes, IMEC vzw, Leuven, BELGIUM.

Initial studies (using Scanning Spreading Resistance Microscopy) on the lateral diffusion of B and As have shown an important influence of the thickness of oxy/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 SSRM-data. In fact both techniques show a similar increase in lateral diffusion with increasing spacer thickness ($\sim$0.2 nm/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 CBED 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 final) stress is not really jusitified. 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

stress, interstitials, hydrogen incorporation, TED,..) we have expanded the experimental matrix with a vacancy diffuser such as Sb and simulated the potential H-incorporation during 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; R.J. Phaneuf, Dept. of MS&E, 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 oxide-passivated Si pn junctions can be imaged by Scanning Tunneling Microscopy (STM), mainly due to tip-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-gap-sample metal insulator semiconductor (MIS) junction. [1] M.L. Hildner, R.J. Phaneuf, and E.D. Williams, Appl. Phys. Lett. 72, 3314 (1998).

11:30 AM J2.4
DEMONSTRATION OF THE STATE-OF-THE-ART OF FORMATION AND CHARACTERIZATION OF ULTRA-SHALLOW JUNCTIONS. P. Borden[b], J. Madsen[b] and L. Bechtler[b], A. Al-Bayati[a], C. Lazik[a], S. Tandon[a], P. Carey[a], and A. Mayur[a]. [a]Applied Materials, Santa Clara, CA. [b]Boxer Cross Inc, Menlo Park, CA.

The 2003 source/drain doping requirements in the International Technology Roadmap for Semiconductors (ITRS) are 24-40 nm depth, 240-675 Ω/□ 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 required levels of 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[1].
This paper will start with a discussion of the fabrication and characterization of advanced layers formed with low energy (LE) implants and spike anneals[2]. Using careful process optimization, it is shown that this process module can meet or exceed the ITRS requirements. This indicates the LE implant/spike RTA option 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%, indicating 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 alternative doping methods such as Laser Thermal Annealing (LTA). The paper will close with a comparison of the current state of the art of the implant/anneal and LTA doping solutions and the application of the CI method to characterization and process optimization of LTA layers[3].
1. P. Borden, "Junction depth measurement using Carrier Illumination," 2000 International Conference on Characterization and Metrology for ULSI, Gaithersburg MD, June 26-29, 2000.
2. A. Al-Bayati, M. Foad, A. Mayur, S. Tandon, D. Wagner, R. Murto, C. Ferguson, L. Larson, T.S. Wang and A. Cullis, "Exploring the Limits of Pre-Amorphization Implants on Controlling Channeling and Diffusion of Low Energy B Implants and Ultra Shallow Junction Formation," XIII International Conference on Ion Implantation Technology IIT-2000, Alpbach Austria, Sept. 17-22, 2000.
3. D. Sing, P. Borden, L. Bechtler, R. Murto, and S. Talwar "Boxer Cross Measurements of Laser Annealed Shallow Junctions," XIII International Conference on Ion Implantation Technology IIT-2000, Alpbach Austria, Sept. 17-22, 2000.

11:45 AM J2.5
SPV MONITORING OF NEAR SURFACE DOPING - ROLE OF BORON-HYDROGEN INTERACTION; BORON PASSIVATION AND REACTIVATION. D. Marinskiy, J. Lagowski, Semiconductor Diagnostics, Inc, Tampa, FL.

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, and 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, V_{sb}, and the semiconductor capacitance of the surface depletion layer, C_D, allows calculating the concentration of boron atoms in submicron distance from the Si surface or Si/SiO_2 interface. The technique was proven very successful in monitoring low dose implant 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 behavior in wafers 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 acceptors 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
Chairs: Lourdes Pelaz and Peter A. Stolk
Tuesday Afternoon, April 17, 2001
Golden Gate A2 (Marriott)

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

The phenomenon of sputtering of the target during ion implantation been known about and studied for several decades. Only recently, however, with the advent of ultra-low sub-keV energy dopant implantation, has this phenomenon become relevant to front-end semiconductor processing. At ultra-low implant energies (sub-keV for B, and sub-2 keV for As) a significant fraction of the intended dose can be lost due to self-sputtering of the dopant during the implantation process itself. Such an effect when combined with the difficulty of achieving large beam currents at ultra-low energies can become a decisive factor in the choice of dopant implant energies. This paper reviews several recent measurements of the dopant-self sputtering effect from implantation of boron, boron diflouride, decaborane and arsenic silicon and/or 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 sputtering yield of these various dopant species from silicon and silicon dioxide. The experimentally observed sputtering yields are an order of magnitude larger than what is predicted by theory.

2:00 PM J3.2
POINT-DEFECT PROPERTIES OF INDIUM IN SILICON AND SILICON DIOXIDE. V.C. Venezia, H.-J.L. Gossmann, and D.C. Jacobson, Bell Laboratories, Lucent Technologies, Murray Hill, NJ; K.K. Bourdelle, Jennifer Mckinley, Fred Stevie, Bell Laboratories, Lucent Technologies, Orlando, FL; Aditya Agarwal, Greg Luckman and Peter Frisella, Axcelis Technologies, Beverly, MA.

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 SiO_2, i.e. diffusion, segregation, and solubility. We used In implanted with an energy of 210 keV into bare Si or Si covered with 90 and 500nm of SiO_2 to doses of 10^{12} to 10^{15} cm^{-2}. This placed the In profile either fully into SiO_2, on the Si/SiO_2 interface, or in the Si bulk. In was also incorporated into Si 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 we find that In diffuses almost as fast as B, and exhibits OED and TED. In 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. In segregates strongly from Si to 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 In depth profiles of high dose implants.

2:15 PM J3.3
SELF-DIFFUSION IN EXTRINSIC SILICON USING ISOTOPICALLY ENRICHED ^{30}SILICON LAYER. Yukio Nakabayashi, Hirman I. Osman, Toru Segawa, Kazumasa Saito, Satoru Matsumoto, Keio Univ, Dept of Electronics and Electrical Engineering, Yokohama, JAPAN; Junichi Murota, Tohoku Univ, Res Inst of Electrical Communication, Sendai, JAPAN; Kazumi Wada, Massachusetts Institute of Technology, Dept of MS&E, Cambridge, MA; Takao Abe, Sin-Etsu Handooutai, 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 stringently 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 ^{31}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 as a tracer. Recently, Si isotope heterostructures have been used in order to investigate the silicon self-diffusion. It consists of pure ^{28}Si epitaxial layer on natural Si. However, there is no report on self-diffusion using ^{30}Si 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 isotopically 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 B, As or Sb ([B] = 2×10^{19} cm^{-3}, [As] = 3×10^{19} cm^{-3}, [Sb] = 1×10^{18} cm^{-3}) and the other is lightly doped with B ([B] = 1×10^{16} cm^{-3}). These samples were annealed simultaneously in a resistance heating furnace in pure Ar (99.999%) ambient 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 diffusivity was extracted by numerical fitting process by solving Fick's equation. Since B concentration of lightly B-doped sample ([B] = 1×10^{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 intrinsic Si, the ^{30}Si diffusion in heavily B-doped Si is found to be enhanced and its enhancement ratio is about twice. On the other hand, in heavily As or Sb-doped Si, the diffusion profiles are hardly different from the profile of intrinsic Si. Doping effect on ^{28}Si self-diffusion is similar to that of ^{30}Si. For both intrinsic and extrinsic silicon, the ^{28}Si self-diffusion coefficients are larger than those of ^{30}Si. The average ratio of ^{30}Si to ^{28}Si is 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 J3.4
A NEW MODEL FOR BORON DIFFUSION RETARDATION IN SiGe-STRAINED LAYERS ACCOUNTING FOR THE MECHANISM OF BORON TRAPPING/DETRAPPING BY Ge ATOMS. Victor Kol'dyaev, PDF/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 phenomenological approach to simulate the B diffusion retardation effect in such layers was proposed by N. Cowern in 1994. This model describes the B diffusion from SiGe-layers. However, this approach fails when describing the B diffusion into the SiGe. The Cowern's model predicts the continuous B concentration at the interface of Si-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 therefore there must be the same flux of Boron through the interface. Our experimental study of the B diffusion into the SiGe layer from the Si one shows a segregation process of B into SiGe-layer is happening indicating that a 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 quantitatively the electric field can provide only a twice as high the diffusivity 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 excellent agreement between the experiment and the simulation. Microscopic theory of the capturing which has been developed has allowed us to decompose the total B diffusion retardation in SiGe-layer into two components: about 45% of the total diffusivity reduction is due to the strain and about 55% is due to Boron capturing resulting in an effectively less value of the total diffusivity. 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 J3.5
SHALLOW P-TYPE JUNCTIONS FOR SUB-100-NM CMOS. Veerle Meyssen, Philips Research Eindhoven, THE NETHERLANDS; Peter Stolk, Philips Research Leuven, BELGIUM; Jeroen van Zijl, Philips Research, Eindhoven, THE NETHERLANDS; Jurgen van Berkum, Willem van de Wijgert, Philips CFT, Eindhoven, THE NETHERLANDS.

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-100-nm 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 were obtained with sheet 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 (featuring gate lengths down to 50 nm), allowing an electrical assessment of the junction performance in terms of series resistance, underdiffusion, overlay capacitance and parasitic leakage.

3:30 PM J3.6
THE ROLE OF ION MASS ON END-OF-RANGE DAMAGE IN SHALLOW PREAMORPHIZING SILICON. Mark H. Clark, University of Florida, Dept of MS&E, Gainesville, FL; Kevin S. Jones, University of Florida, Dept of MS&E, Gainesville, FL; Tony E. Hanes, Oak Ridge National Laboratory, Oak Ridge, TN; Charles J. Barbour, Sandia National Laboratories, Albuquerque, NM; Ebrahim Andideh, Intel Corporation, Portland, OR.

Preamorphization is commonly used in the shallow junction formation of silicon CMOS devices. The purpose of this experiment was to study the effect of the preamorphizing species' mass on the interstitial 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 Å deep) were amorphized using implants of 17 keV $^{28}Si^+$, 32 keV $^{73}Ge^+$, 40 keV $^{119}Sn^+$ or 45 keV $^{207}Pb^+$ resulting in similar amorphous layer depths. All species were implanted at a dose of 5x10^{14}/cm^2. Cross-sectional transmission electron microscopy (XTEM) and Spectroscopic Ellipsometry were used to measure amorphous layer depths (approximately 400 Å). Post-implantation anneals were performed at 750°C for times ranging from 15 to 240 minutes. Plan-view transmission electron microscopy (PTEM) was used to observe and quantify the defect evolution path upon annealing. Secondary ion mass spectrometry (SIMS) was used to monitor the transient enhanced diffusion (TED) of the buried boron marker layer caused by the end of range damage of the amorphizing implants. Base upon the SIMS results the Florida object oriented process simulator (FLOOPS) calculated the resulting diffusion enhancements. Results show that increasing the ion mass over a significant range (28 to 207 AMU) can result in reduced interstitial injection and TED.

3:45 PM J3.7
USE OF ISOTOPICALLY PURE SILICON MATERIAL TO ESTIMATE SILICON DIFFUSIVITY IN SILICON DIOXIDE. D. Tsoukalas, C. Tsamis and P. Normand, Institute of Microelectronics, NCSR 'Demokritos', Aghia Paraskevi, GREECE.

The recombination properties of silicon atoms generated in the bulk of the material and arriving at the Si/SiO_2 is of importance for better understanding interface phenomena in silicon processing. Along these lines we have performed a series of experiments to measure the diffusivity of Si in the oxide. Early direct experiments on the diffusion of Si in silicon dioxide have been performed by Brebec et al. [Acta Metallurgica 28, 327, (1980)]. Other indirect measurements by Celler

at al [APL 54, 1427 (1989)] report much higher diffusivity values. In this work we report measurement of the silicon diffusion coefficient in silicon dioxide films using isotopically enriched ^{28}Si silicon dioxide layers that enable relatively low ^{30}Si concentration measurements to be performed using Secondary Ion Mass Spectrometry. Two types of experiments are made. ^{30}Si atoms are introduced in excess in a stoichiometric isotopically pure silicon dioxide layer either by ion 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 simualtions with the experimental 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 Si isotopes in their natural abundance on top of an isotopically pure SiO_2 layer. ^{30}Si atoms are generated in the crystalline silicon by oxidation and then diffuse in the oxide layer. Their profile in the isotopically pure oxide is then monitored by SIMS. These experiments are representative of any physical situation where excess silicon atoms are introduced into silicon dioxide layers. The diffusivity measured is three orders of magnitude higher than reported direct measured values with an estimated activation energy of 5eV. Possible mechanisms for the diffusion of silicon in the oxide will be discussed.

4:00 PM J3.8
THE EFFECT OF TRIPLE WELL IMPLANT DOSE ON PERFORMANCE OF NMOS TRANSISTORS.
Konstantin K. Bourdelle, Samir Chaudhry, 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 flash memories (higher density and faster devices). In a triple well technology an addition of one moderate dose high energy phosphorus implant allows the creation of a separate p-tub which is junction isolated from the substrate. In this work we study the dependence of NMOS device performance and leakage current in diode 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 a 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 threading dislocations. This interpretation is supported by the defect etch and transmission electron microscopy measurements

4:15 PM J3.9
PHOSPHORUS INTRINSIC DIFFUSION IN PURE EPITAXIAL SILICON.
Jens S. Christensen, Andrej Yu. Kuznetsov, Henry H. Radamson, 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 (LPCVD) were used to study phosphorus diffusion in silicon. The sample was 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 Arrhenuis dependence with the activation energy E_a = 2.74±0.07 eV and the prefactor (8±5)E-4 cm^2/s. The activation energy and the prefactor differ considerably from the previously reported and widely accepted literature values (3.66 eV and 3.84 cm^2/s respectively). Phosphorus diffusion in silicon was studied extensively during the 70-80's, and is commonly believed to be well understood. Most of the studies have been, however, performed in bulk Czochralski (Cz) grown silicon with high contamination of competing traps for silicon self-interstitials, which is considered as the main vehicle mediating phosphorus diffusion. In contrast, LPCVD epitaxially grown silicon contains substantially smaller concentrations of such impurities, in particular 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 J3.10
DIFFUSION OF NITROGEN IMPLANTED INTO SILICON AT AMORPHIZING DOSES.
Lahir Shaik Adam, Lance Robertson, Mark E. Law, 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 non-amorphizing doses. Those studies showed that nitrogen diffuses rapidly towards the surface at 750°C. The present study looks at the diffusion behavior of nitrogen implants at amorphizing doses of $5*10^{14}$ N_2^+ and $2*10^{15}$ N_2^+/cm^2 at 40 keV. XTEM reveals that the highest dose forms a continuous amorphous layer to a depth of about 800Å while the lower dose forms a buried amorphous layer between 100Å and 600Å from the surface. After implantation, the samples were furnace annealed at 750°C for times from 12 min to 4 hours in an inert ambient. This should form end of range (EOR) or Type II defects for the higher dose and Type IV defects (where the amorphous interfaces meet) 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 $2*10^{15}$ N_2^+/cm^2, the nitrogen segregates towards the EOR defects (at about 800-900Å) up to the longest anneal time. However, in the case of the lower dose of $5*10^{14}$ N_2^+/cm^2, while the profile shrinks with time, the peaks are pinned at about 500Å. This is in contrast to the non-amorphizing case where the peaks shift towards the surface with time. Further, while 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. While the trend in the extent of 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. Defect evolution at these doses for the various times would be presented and correlated to 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 J4: POSTER SESSION
Chairs: Jinning Liu and Wolfgang Skorupa
Tuesday Evening, April 17, 2001
8:00 PM
Salon 1-7 (Marriott)

J4.1
EFFECTS OF MULTIPLE NONMELT LASER PULSES ON BORON IMPLANTED IN SILICON.
Susan Earles, Mark Law, Kevin Jones, Univ of Florida, SWAMP Center; Somit Talwar, Verdant, San Jose, CA; Sean Corcoran, Intel, Portland, OR.

The effects of multiple nonmelt laser pulses on boron implanted silicon has been studied. The energy of the implanted boron varied from 3keV down to 250eV at implant doses from 1e15 ions/cm^2 to 3e15 ions/cm^2. The samples recieved one to 1000 laser pulses at a constant energy low enough not to melt the silicon. Furnace anneals and RTA followed by Hall Effect, Four-point probe, SIMS, and Plan-v iew TEM were then done to study the activation, diffusion, and microstucture of the boron implanted silicon. SIMS results indicate that the samples processed with a laser anneal prior to the RTA diffuse less than the sample recieving just the RTA. 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 ION IMPLANTED BORON IN SILICON.
K.A. Gable, L.S. Robertson, K.S. Jones, Univ of Florida, Dept of MS&E, Gainesville, FL.

The interaction between boron and silicon interstitials caused by ion implant damage is a physical process which hinders the formation of ultra-shallow, low resistivity junctions. The possibility of mitigating the interaction between boron and silicon interstitials by co-implanting chlorine with ion implanted boron in silicon 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 $1x10^{15}/cm^2$. The Si^+ implants produced a 2800Å deep amorphous layer, which was then implanted with 8 keV $1x10^{15}/cm^2$ B^+ and Cl^+ ions with energies ranging from 30 to 90 keV and doses ranging from 5 $x10^{14}$ 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 impurity implant. Post-implantation anneals were performed in a tube furnace 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 co-implantation resulted in an improvement in the boron junction characteristics. Detailed chemical and microstructural analysis will be presented to explain the observed phenomenon.

J4.3
VACANCIES AND OXYGEN BEHAVIOR IN HIGHLY CARBON DOPED SILICON. P. Lavéant, P. Werner, U. Gösele, G. Gerth, Max-Planck-Institut für Mikrostrukturphysik, Halle, GERMANY.

Carbon and oxygen are the two major electrically inactive impurities of Si and have been studied separatly for 20 years. High carbon concentrations in silicon gained some interests recently due to the beneficial role of carbon in suppressing transient enhaunced diffusion. Carbon, when incorporated well above its solubility in silicon ($5 \times 10^{17}\ cm^{-3}$ at melt temperature) changes the silicon point defect equilibrium. Self-interstitials are consumed in the carbon diffusion process leading to their undersaturation whereas vacancies become oversaturated. After annealing, it appears also that the oxygen concentration increases localy in carbon rich areas. We try to explain this carbon oxygen affinity in taking silicon vacancies into account. Molecular beam epitaxy (MBE) growth of carbon-rich samples on oxygen-rich or poor substrates and annealing of these structures were performed. Simulation of the interaction of vacancies with carbon and oxygen will be shown. The precipitation of carbon will also be discussed.

J4.4
MODELING OF THREADING DISLOCATION LOOPS NUCLEATION AND EVOLUTION IN MeV BORON IMPLANTED SILICON. I. Avci , M.E. Law, Swamp Center, Department of Electrical and Computer Engineering, University of Florida, Gainesville, FL; C. Jasper; H.A. Rueda; R. Thoma, Motorola, Predictive Engineering Laboratory, Mesa, AZ.

High energy boron implantation into silicon generates severe lattice defects in the region near the projected range. These defects can be dislocation loops, {311}s 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 condition 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 this study, a statistical point defect based model for the nucleation and evolution of TDLs is developed in Florida Object Oriented Process Simulator (FLOOPS). Modeling results are in agreement with the experimental results. The model assumes that all the nucleated loops come from {311} unfaulting and the loop density and average loop radius follow a log normal distribution. Ostwald ripening becomes dominant when excess interstitial density drops to the values close to equilibrium interstitial concentration. Loops whose radius close to the their distance from the surface are considered as TDLs.

J4.5
CHARACTERIZATION OF DAMAGE INDUCED BY CLUSTER ION IMPLANTATION. Takaaki Aoki, Jiro Matsuo, Gikan H. Takaoka, Ion Beam Engineering Experimental 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, decaborane ($B_{10}H_{14}$), 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 B 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 was as same as those by B monomer ion with same energy per atom. However, in the point of the damage formation mechanisms, there are huge difference between cluster and monomer. For both cases of the impact of B monomer and cluster, the maximum number of displaced Si atoms induced by one B atom was almost the same at 0.1ps after the impact. However, the damage recovery process is different, depending on cluster size. Damage induced by B_{10} recovers more slowly than those by B_1 ions. Compared to the B_1 ion impact, there were several times larger number of displaced Si atoms by B_{10} cluster ion impact after 8ps. These displaced Si atoms by B_{10} 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 annihilation.

J4.6
ATOMISTIC MODELING OF CARBON-BORON INTERACTIONS IN Si. Chun-Li Liu, L.J. Borucki, X.-Y. Liu, and W. Windl, Advanced Systems Research Lab, Motorola, Mesa, AZ.

Ab initio 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 $< 100 >$ C-B split interstitial is relatively stable compared with the $< 110 >$ 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 $\sim$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 initio results and in reasonable agreement with experiment. Implications of these results on understanding of the effect of C on B diffusion in Si will be briefly discussed.

J4.7
COMPUTER SIMULATION OF DECABORANE IMPLANTATION INTO SILICON, ANNEALING AND RE-CRYSTALLIZATION OF SILICON. Zinetulla Insepov, Isao Yamada, 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 re-crystallazation have been developed. The B and Si atomic positions for irradiation with many Decaborane ions, with energy up to a few keV per B atom, and, for comparison, with monomer B ions were obtained by MD simulation. 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 a 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 details at various temperature and pressure regimes. According to our 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.

J4.8
EFFECT OF THE Ge PREAMORPHISATION DOSE ON THE THERMAL EVOLUTION OF END OF RANGE DEFECTS. Benjamin Colombeau, Gérard Ben Assayag, Alain Claverie, CEMES/CNRS, Toulouse, FRANCE; Jean Christophe Marrot, Fuccio Cristiano, LAAS/CNRS, Toulouse, FRANCE.

To realise ultrashallow junctions compatible with advanced CMOS technology, it is now admitted that preamorphisation of the wafer prior to low energy dopant implantation has several advantages. After annealing of such preamorphised implants, End of Range (EOR) defects are formed below the a/c interface. As these defects strongly influence dopant diffusion, it is necessary to know how process parameters such as the preamorphisation ion dose affect their thermal evolution. In this paper, we study the effect of the Ge^+ preamorphisation 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 interstitial atoms (Si_{int}s) found below the a/c interface on the kinetics of EOR defects. Amorphisations 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 time-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_b) of Si_{int}s bound to the EOR defects is a monotonically increasing function of the Ge ion dose. Furthermore, we found that N_b is directly proportional to the number of Si atoms in excess to the vacancies found below the a/c 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 preamorphisation ion dose has no effect on the defect mean size. This invariance of the mean size of precipitates with respect to the initial supersaturation introduced in the matrix is an expected characteristics of a conservative Ostwald ripening mechanism.

J4.9
MONTE-CARLO SIMULATIONS OF THE CLUSTERING OF CARBON IN SILICON AND ITS INFLUENCE ON CARBON DIFFUSION AND SELF-INTERSTITIAL TRAP ROLE.
Ruth Pinacho, Pedro Castrillo, Martín Jaraíz, Juan Barbolla, Dto. Electricidad y Electrónica, Univ Valladolid, SPAIN; Hans-Joachim L. Gossmann, George H. Gilmer, Janet L. Benton, Bell Laboratories, Lucent Technologies, Murray Hill, NJ; Peter Werner, MPI of Microstructure Physics, Halle, GERMANY.

Carbon in silicon appears in high concentrations, ranging from 10^{16} to 10^{18} cm^{-3},well above its solubility at the usual annealing temperatures. Carbon diffusion in Si is therefore intimately linked to C clustering and precipitation. Only simulation tools that take both phenomena into account will be able to model experiments accurately. Such a tool is the Monte-Carlo atomistic simulator DADOS. Through the use of DADOS it has been shown earlier that the formation of carbon/Si self-interstitial clusters with a low content of Si interstitials accounts for the faster diffusion of C compared with that predicted by the kick-out mechanism alone. In this work, we show that, at higher temperatures, the Carbon/Si self-interstitial clusters are bigger and have a higher C content. This fact results in an immobilized fraction of C in the high concentration regions, in good agreement with the experimental results of C diffusion in doping-superlattice C structures grown by MBE. Furthermore, under conditions of thermal generation of intrinsic point defects, the low temperature dependence of Si interstitial under-saturation in the C rich-regions can be well reproduced. Finally, we will show that this model is also consistent with recent experiments of formation of the C_2 cluster detected by infrared absorption spectroscopy at room temperature.

J4.10
KINETICS OF STACKING FAULT ANNIHILATION IN BORON IMPLANTED SILICON.
D. Luebbert, J. Arthur, J.R. Patel, SSRL/SLAC, Stanford University Stanford, CA; (JRP) ALS/LBL, Berkeley, CA; M. Sztucki, T.H. Metzger, ESRF, Grenoble, FRANCE.

In a grazing incidence x-ray diffuse scattering study of ion implantation damage in silicon we have found a clear signature of stacking faults generated during anneals in the temperature range 900 - 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 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 averagesize of the faults at first increases, peaks and then decreases again with the decrease in intensity. Previous estimates of integrated intensity andhalf width based on radial x-ray scans suggested a dislocation based annihilation mechanism for the stacking faults. Recent more accurate transverse x-ray scans of integrated intensity and halfwidth would indicate that a point defect diffusionmechanism is involved. Kinetics of the growth and shrinkage of the faults will be discussed based on these findings.

J4.11
DIFFUSION IN SILICON AND THE PREDICTIVE POWER OF AB-INITIO CALCULATIONS II.
Wolfgang Windl, Xiang-Yang Liu, Roland Stumpf and Michael P. Masquelier, Computational Materials Group, Motorola, Inc, Austin, TX, and Los Alamos, NM; Blas P. Uberuaga and Hannes 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 will cover work performed within 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 contradictory experimental diffusivities and their use in process simulations.

J4.12
ULTRA-SHALLOW Sb-DOPED LAYER FORMATION IN SILICON(001) BY ARGON RECOIL IMPLANTATION.
Kurt E. Daley, David T. Vonk and Robert J. Culbertson, 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 Sb film. The deposition is followed by high energy positive argon ion irradiation. In the last step, the structure undergoes a final chemical stripping of the residual Sb film. MeV Ion Beam Analysis shows that the Sb concentration increases linearly with argon ion dose. High resolution 200 keV Medium Energy Ion Scattering (MEIS) makes it possible to measure the projected range with good accuracy, 3.0 ± 0.2 nm. The doped layer width is found to be less than 2.8 nm. The final Sb concentration is found to be weakly dependent on the initial Sb layer thickness. T. Michael was supported by National Foundation grant DMR-9988056 for Research Experience Undergraduates (REU) while working on this project.

J4.13
A MOLECULAR DYNAMICS STUDY OF DAMAGE IN A VICINAL (100) SILICON SURFACE. EFFECTS OF LOW-ENERGY IMPLANTS OF ARGON AND BORON.
A.M. Mazzone, CNR, 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 monoatomic 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 epitaxis. No 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 a kinetic energy in the range from 5eV 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.

J4.14
EVOLUTION OF DEFECTS INDUCED BY HIGH ENERGY He IMPLANTATION IN SILICON CONTAMINATED BY VARIOUS IMPURITIES.
Rachid El Bouayadi, Gabrielle Regula, Bernard Pichaud, Maryse Lancin, UIII, TECSEN, Marseille, FRANCE; Christiane Dubois, LMP, Villeurbanne, FRANCE; Esidor Ntsoenzok, CERI-CNRS, Orleans, FRANCE.

Homogeneously contaminated silicon samples were implanted with helium ions at 1.6 MeV at a fluence of 5 1016 cm-2. Both Ni and Pt were used as impurities. Since Ni is a fast diffuser and Pt an hybrid one, differences in their gettering behavior could lead to speculations 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 both to grow cavities and drag impurities to them. After the annealing , the width of the damaged zone shrinks down from 0.5 μm to 0.2 μm and consists essentially in cavities 10 to 100 nm in size. These cavities are faceted mainly along {111}, but also along {110} and {100} planes as provided by high resolution electron microscopy. Secondary ion mass spectroscopy (SIMS) profiles on the samples exhibit a shouldered shape with a maximum at the projected range. These measurements demonstrate that cavities are very efficient sinks for any impurities regardless their nature. Nevertheless, the width of the SIMS peak was found to be about five times larger than that of the cavity chain for all impurities used. The broadening and the shouldering of the gettering band have also been reported by RBS measurements. That demonstrates that MeV helium implantation induces not only well known and expected cavities 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 cavities and the diffusion of impurity take place during the same annealing.

J4.15
MOLECULAR DYNAMICS SIMULATION OF RADIATION-ENHANCED MIGRATION OF POINT DEFECTS AND

IMPURITIES AND THEIR INTERACTIONS IN SILICON. Z.M. Khakimov, F.T. Umarova, N.T. Sulaymonov, Sh. Makhkamov, N.A. Tursunov, Institute of Nuclear Physics of Uzbek Academy of Sciences, Tashkent, UZBEKISTAN.

Excess charge carriers produced by the electron and gamma-ray irradiation can influence upon relative stability of configurations of defects and impurities, as well as their migration and interactions, which gives unique opportunity for modification of semiconductor materials properties in the atomistic level. However, microscopic picture and mechanisms of such influence is not quite understood yet. There are several atomistic calculations with a static minimization of potential energy surfaces in silicon devoted to this subject, but molecular dynamics simulations almost have not been used for studying dynamics of point defects and impurities and impurity-defect interactions with accounting for charge state effects. In this work the self-consistent tight-binding molecular dynamics simulations were performed to reveal peculiarities of state and motion of vacancy, Si self-intersitial, and carbon, as well as reactions between them due to excess charge carriers, implementing new efficient algorithm for integration of equations of motion. The obtained results were used, in particular, to explain the experimental data on the formation rate of main radiation defects (divacancy, A-center, etc) on the intensity of electron irradiation.

J4.16
ACCURATE MODELING OF RESIDUAL RECOIL-MIXING DURING SIMS MEASUREMENTS. Ming Hong Yang, Robert Odom, Charles Evans Associates, Sunnyvale, CA.

Secondary ion mass spectrometry (SIMS) is an effective and powerful analytical technique, widely used in accurately determining dopant distributions (depth profiles). However, primary ion beam induced mass transport (ion mixing), especially the residual effect during SIMS profile measurements, greatly limits the accuracy at nanometer depth resolutions by displacing and broadening the measured depth profile. In this paper, we present a simple deconvolution algorithm based on the general characteristics of the experimentally observed SIMS response function to reduce this broadening effect, thereby providing more accurate depth profiles. The results for several specific applications of this approach are presented and its strengths and limitations are discussed.

J4.17
APPLICATIONS OF AFM/SCM IN IMAGING IMPLANT STRUCTURES OF SUBMICRON DEVICES WITH FIB ASSISTANCE. Kuo-Jen Chao, Jeffrey R. Kingsley, Hoainam Ho, Ian Ward, Charles Evans & Associates, Sunnyvale, CA.

As the minimum feature size of the semiconductor devices continues shrinking, it has been very difficult to identify such small features optically. Therefore, marks, which are optically visible and close to the features of interest, have to be made. In this work, we use FIB to make small marks near the features of interest and then polish the sample to expose the cross-section of the specified device features for AFM/SCM study. It would be better if the FIB marks are as close to the area of interest as possible. Nevertheless, there are dead layers near the FIB marks. So if the implant structures are to be studied, then the near-by FIB marks may influence the results. A set of FIB marks created by different conditions are studied by AFM/SCM to determine the dead layers. Implant structures of submicron device features specified by FIB marks are investigated by AFM/SCM. In addition, applications of AFM/SCM in process control and failure analysis will be discussed and presented.

J4.18
AB INITIO STUDY OF SELF-INTERSTITIAL CLUSTERS. Maxim Chichkine, Merlyne De Souza, 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 9 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 localised orbitals corresponding to these levels. The energetics of the investigated models shows the non-monotonic dependence of the binding energy with cluster size.

J4.19
MODELING OF BORON IMPLANTATION WITH DECABORANE IONS. Zinetulla Insepov, Lab of Adv Sci & Technology, Himeji Inst of Technology, JAPAN; Marek Sosnowski, NJIT; Isao 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 decaborane 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 ten times higher energy since their kinetic energy is partitioned among the constituent atoms. Moreover, there is only one charge unit for ten B atoms. While there is a growing interest in decaborane implantation and more experimental results are being reported, the understanding of the fundamental processes associated with implantation of these ions is still lacking. We have applied the computational methods, involving Molecular Dynamics Simulation and Monte Carlo, to the study of decaborane ion implantation in Si. These methods were used previously to investigate the effects of larger clusters of argon on a variety of materials. Of particular interest in the case of decaborane ions were implantation range, damage and amorphization, and sputtering. Comparison with available experimental data is reported.

J4.20
PHOTOLUMINESCENCE STUDY OF DEFECTS INDUCED BY $B_{10}H_{14}$ IONS. Noriaki Toyoda, Massachusetts Institute of Technology, Cambridge, MA.

$B_{10}H_{14}$ ion implantation is one of the candidates for the ultra shallow junction formation below 50nm. 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 $B_{10}H_{14}$ (decabane) was studied with photoluminescence measurements. In the PL spectra, we focused on the W-line (1018meV). From the recent first-principle calculations, the W-line is originated from interstitial Si aggregates. This W-line is observed as-implanted Si with $B_{10}H_{14}$ ion implantation over the implant energy 10keV, and 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 (<5keV) $B_{10}H_{14}$ 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, Rudyanto Gunawan, Richard D. Braatz, Edmund G. Seebauer, Dept of Chemical Engineering, Univ of Illinois C-U, 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 heretofore neglected phenomenon of surface Fermi level pinning. We find that such pinning greatly reduces dose loss, induces pileup of electrically-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 interstitials of all types. The mechanism is that pinning sets up an electric field in the space charge region that opposes the diffusive motion of charged interstitials toward the surface. Analogous effects should occur for n-type dopants like As; the sense of the electric field should be all that changes. Pinning should occur on an oxided surface just after implant, and possibly during the slow oxide growth that sometimes occurs during RTA. Pinning also occurs on the clean Si surface - a fact that should help solve the dose loss problem that will appear as device scaling forces elimination of sacrificial oxide. However, quantitative modeling of the various pinning phenomena require the measurement of healing kinetics for pinning on an oxided surface, and the desorption kinetics of native oxide.

J4.22
Abstract Withdrawn.

SESSION J5: DOPANT DEFECT CLUSTERING
Chairs: Kevin S. Jones and Jiro Matsuo
Wednesday Morning, April 18, 2001
Golden Gate A2 (Marriott)

8:30 AM *J5.1
DAMAGE EVOUTION IN ION IMPLANTED c-Si. Sebania Libertino, Salvatore Coffa, Antonino La Magna, Corrado Spinella, CNR-IMETEM, Catania, ITALY.

An increasing interest is nowadays devoted to the comprehension and modeling of damage related phenomena in c-Si. The continuos shrinking of electronic devices has evidenced that dopant diffusion and activation are controlled by its interactions with defects, mainly generated during the dopant implantation. 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 compared the experimental results of the electrical, optical and structural characterization of the residual damage with kinetic lattice Monte Carlo (KLMC) simulations. Experimental data were taken as a function of the implantation and annealing conditions. Mainly Si and B were implanted on epitaxial and Czochralski n-type and p-type Si with energies of 0.04-1.2 MeV and doses of $1x10^{9}$-$1x10^{14}cm^{-2}$. Samples were characterized from the as implanted state up to annealing temperatures of 900°C for times in the range 5s-30h. Low temperature (300-500°C) annealing causes the formation of I-type point-like defects. Simulations at this stage indicate that small clusters, containing only few interstitials in a over-coordination state, are formed. Annealing at intermediate temperatures (550-650°C) produces the formation of I-clusters, which are experimentally detected observing the effects of their induced strain on the electrical, optical and structural properties. The two broad features centered at ~1300 and 1400nm observed in photoluminescence and the highly strained regions revealed by transmission electron microscopy are fully consistent with the features and the evolution of large I agglomerates derived by KLMC simulations. High annealing temperatures cause the transition from I-clusters to {311} defects. It takes places only if the I supersaturation exceeds a certain value, corresponding to implantation doses $\geq 1x10^{13}Si/cm^{2}$ in pure Si. Moreover, {311} form only after annealing $\geq$ 650°C, thus showing the existence of a temperature threshold. In fact, even for $5x10^{13}$ Si/cm^{2} implantation, we did not observe {311} after annealing at 600°C for times up to 30h. These results, combined with simulations suggest the presence of a strong structural rearrangement during the transition. The comparison of experiments and simulations provides a unique scenario for the defect evolution in ion implanted c-Si.

9:00 AM J5.2
EFFECT OF ARSENIC ON EXTENDED DEFECT EVOLUTION IN SILICON. R. Brindos, P.H. Keys, K.S. Jones, Univ. of Florida, Dept of Materials Science and Engineering, Gainesville, FL; M.E. Law, Univ. of Florida, Dept of Electrical and Computer Engineering, Gainesville, FL.

In previous studies, the effect of arsenic on {311} nucleation and dissolution was studied at 750°C using wells of As doped Si and subsequent non-amorphizing Si implants. It was determined that the arsenic was competing with {311} defects for excess interstitials from the Si implant and acting to decrease the number of interstitials in {311} defects by the formation of arsenic-interstitial clusters (AsIC's). In a follow up experiment, the interstitial flux released from the arsenic implanted region was studied using boron marker layer experiments and it was determined that the arsenic is reducing the injection of interstitials, consistent with AsIC formation. The goal of the present research was to study AsIC formation and dissolution over a range of temperatures from 650°C to 800°C. This made it possible to determine the energetics of the arsenic-interstitial interaction. Quantitative plan-view TEM was used to obtain the density of {311} defects and the total number of trapped interstitials within the {311}'s after multiple temperature annealing cycles. The use of a system of annealing times and temperatures allows for dissolution curves for the {311} defects as a function of arsenic background concentration and temperature to be determined. From these dissolution curves, the dissolution rate constant and activation energy for the dissolution of {311} defects was obtained for this system. These experimental results were compared with {311} models developed in FLOOPS (Florida's Object Oriented Process Simulator) to solve for the arsenic-interstitial binding energy. Using a simple arsenic diffusion pair model and an arsenic-interstitial binding energy in the AsIC of -0.95eV, a good fit to the experimental data at 750°C was attained. Additional fits at other temperatures were compared to experimental data and these results will be discussed. The effect of the arsenic-interstitial binding energy on the formation of {311} defects is presented and discussed.

9:15 AM J5.3
LATTICE SITE LOCATION OF ULTRA-SHALLOW IMPLANTED B IN Si USING ION BEAM ANALYSIS. Hajime Kobayashi, Ichiro Nomachi and Susumu Kusanagi, Sony Corporation, Technical Support Center, Yokohama, JAPAN; Fumitaka Nishiyama, Hiroshima University, Department of Applied Physics and Chemistry, Higashi-Hiroshima, JAPAN.

In the development of MOS LSI, electrical activation of impurities is the key issue in ultra-shallow junction formation. The lattice site location of impurities plays an important role in the electrical activation. We have investigated the lattice site location of B in Si using ion channeling in combination with nuclear reaction analysis (NRA). Boron implanted Si at an energy of 10 keV with a dose of $5x10^{14}$ cm^{-2} (low dose) or $5x10^{15}$ cm^{-2} (high dose) were annealed at 1000°C for 10 seconds (RTA) or at 800°C for 10 minutes (FA). The activation ratio of these samples were estimated from the B atomic concentration and the hole concentration obtained by secondary ion mass spectrometry (SIMS) and spreading resistance profiling (SRP), respectively. Channeling analysis suggests that approximately 20% of B atoms are in substitutional sites even in the as-implanted sample, whereas 60% of B atoms are in substitutional sites in the low dose RTA sample while only 30% of B atoms are in substitutional sites in the high dose RTA sample. Substitutionality of B in the FA samples is only 10% in the low dose sample and almost zero in the high dose sample. We found a strong correlation between the substitutionality of B and the activation ratio. We also studied the ion implantation damage of Si crystals using ion channeling combined with Rutherford backscattering spectrometry (RBS), and found that the crystalline quality of Si was not fully recovered in the high dose samples even after RTA. The deactivation mechanism of B in the high dose samples will be discussed from these data.

9:30 AM J5.4
DIRECT OBSERVATION OF BORON AND ARSENIC IN LOW ENERGY ION IMPLANTED SILICON. E.J.H. Collart, A.M. Murrell, Applied Materials, Transistor and Capacitor Group, Foundry Lane, Horsham, W-Sussex, UNITED KINGDOM; T.-S. Wang, A.G. Cullis, Dept. of Electronic & Electrical Engineering, University of Sheffield, Sheffield, UNITED KINGDOM; M.G Dowsett, J. Bellingham, Dept. of Physics, University of Warwick, Coventry, UNITED KINGDOM.

The International Technology Roadmap for Semiconductors (ITRS) has established junction depth, dopant activation and lateral abruptness as bottlenecks for next-generation CMOS technology. In order to achieve the necessary low Rs a high dopant activation and mobility are needed. The clustering of the implant damage and the implanted species reduces both the activation and the mobility. A quantitative understanding of the dopant clustering behaviour is needed, but not yet available. B and As cluster size and evolution during rapid thermal annealing (RTA) has so far only been inferred from indirect evidence and from modeling. A more direct measurement of cluster size and content is crucial. (100) Si wafers were implanted with 1 keV B at doses between 1×10^{15} cm^{-2} and 1×10^{16} cm^{-2} and 1 keV and 5 keV As at 1×10^{15} cm^{-2} and 5×10^{15} cm^{-2}. The wafers were then annealed in pure N_2 ambient for B and a 10 % O_2 ambient for As. Anneal conditions were 10 s between 700°C and 1100°C or spike annealed at 1050°C. Secondary ion mass spectroscopy (SIMS) was used to determine the chemical profile. Electrical activation was measured with a four point probe technique. The electrically active profile was determined with spreading resistance probing on some of the samples. Energy filtered transmission electron microscopy (EFTEM) and X-ray energy-dispersive spectrometry (XEDS) have been employed to obtain elemental maps of B and As, allowing, for the first time, for a direct observation of dopants and dopant clusters in Si. The evolution of the B and As clusters will be discussed in terms of the changes in the SIMS and SRP profiles. Depth profiles were extracted from the EFTEM and XEDS maps and will be compared with SIMS depth profiles, in particular the surface peak.

9:45 AM J5.5
DOPANT-DEFECT CLUSTERING IN PHOSPHORUS IMPLANTED SILICON: EXPERIMENTATION AND MODELING. P.H. Keys, K.S. Jones, MS&E Dept. Univ. of Florida; M.E. Law, Electrical and Computer Engineering Dept., Univ of Florida, FL; M. Puga-Lambers, MICROFABRITECH, Univ. of Florida, FL; S.M. Cea, Intel Corporation, Hillsboro, OR.

Given the appropriate ion implant and anneal conditions, stable Phosphorus Interstitial Clusters (PICs) can nucleate. An experimental study is conducted to demonstrate this phenomena for subamorphizing $1x10^{14}$ cm^{-2} phosphorus implants with energies ranging from 10 - 100 keV and anneal temperatures between 650 - 800°C. In this work PICs form at phosphorus concentrations below the solid solubility limit due to high interstitial supersaturations. The critical concentration for clustering (approximately $1x10^{19}$ cm^{-3} at 750°C) is shown to be strongly temperature dependent and in close agreement with the kink concentration of phosphorus diffusion. For the given implant dose, clustering is more apparent in lower energy implants because of the increased peak concentration of the as-implanted phosphorus profile. These clusters are shown to influence dopant activation, dose loss, transient enhanced diffusion (TED), and secondary defect morphology. The presence of PICs is evidenced by a reduction of {311} defects observable in plan-view TEM and the appearance of an electrically inactive, non-diffusive portion of the phosphorus profile measured by SRP. Critical PIC dissolution energetics are extracted through gaussian deconvolution of the chemical profile detected by SIMS. A continuum-based diffusion

model is developed in the Florida Object Oriented Process Simulator (FLOOPS) using the single set of extracted parameters. The nucleation of defects is controlled by the diffusion limited competition for excess interstitials between PICs and {311} clusters. Once formed, the release of interstitials influencing TED is driven by cluster dissolution. Modeling results show a strong correlation to those experimentally observed over a wide temporal and thermal 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 J5.6
A NEW KINETIC MODEL FOR THE NUCLEATION AND GROWTH OF SELF-INTERSTITIAL CLUSTERS IN SILICON. Christophe Ortiz, PHASE/CNRS Laboratory, Strasbourg, FRANCE and ECTM Laboratory, Delft 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), {113} 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 emission of interstitials to and from clusters of different sizes (up to a few hundred atoms) and includes the interstitial recombination at the surface. On one hand 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 free physical parameters, our model accounts for main experimental results on TED found in the literature. Physical parameters such as the interstitial diffusion coefficient and solid solubility will be fitted on published experimental results.

10:45 AM J5.7
EFFECTS OF CLUSTERING AND PRECIPITATION ON THE INTERSTITIAL CONCENTRATION IN HIGH-DOSE As^+-IMPLANTED SILICON. Michelle Griglione, 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 Rendon, Motorola Corporation, Phoenix, AZ; Bob Murto, Sematech International, Austin, TX; Edwin Arvelo, Marty Dignard, Varian Semiconductor Equipment, Gloucester, MA.

Arsenic is the most common n-type 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, monoclinic SiAs precipitation then occurs. This investigation isolates 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 $2x10^{14}$, $7x10^{14}$, $2x10^{15}$, and $4x10^{15}$ cm^{-2}. The Ge implants result in EOR damage for all doses. The As implants result in EOR damage as well as clustering ($2x10^{14}$ and $7x10^{14}$ cm^{-2}) or precipitation ($2x10^{15}$ and $4x10^{15}$ cm^{-2}) after a 1050°C RTA spike anneal. Change in the interstitial concentration as a result of EOR damage and As clustering or precipitation (As implants) was observed as an enhancement 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 dose regimes. SIMS analysis was performed to quantify the movement of the B marker layer, and PTEM was performed to verify the extent of EOR damage from implants.

11:00 AM J5.8
DETERMINING THE RATIO OF THE PRECIPITATED VERSUS SUBSTITUTED ARSENIC BY XAFS AND SIMS IN HEAVY DOSE ARSENIC IMPLANTS IN SILICON. M.A. Sahiner, S.W. Novak, Evans East, East Windsor, NJ; J. Woicik, NIST, Gaithersburg, MD; J. Liu, Varian Semiconductor Equipment Associates, Gloucester, MA; V. Krishnamoorty, Department of MS&E, 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 monoclinic SiAs causing electrical deactivation of the dopant. Information on the local structure around the As atom, and the As concentration depth profiles is important for the implantation and annealing process in order to reduce the precipitated As and maximize the electrically activated As. In this study, 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 $1 \times 10^{15}/cm^2$ to $1 \times 10^{18}/cm^2$. The samples were subjected to different thermal annealing conditions. We used secondary ion mass spectrometry (SIMS) and UT-MARLOWE simulations to determine the region where the As-concentration is above the solid 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 precipitates as monoclinic SiAs, the nearest-neighbor distances and coordination numbers are $\sim$2.37 $\AA$ and $\sim$3, as opposed to $\sim$2.40 $\AA$ and $\sim$4 when As is substitutional. 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 were determined.

11:15 AM J5.9
PARALLEL REPLICA SIMULATIONS FOR GROWTH MODELING OF Si-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-interstitial clusters containing n = 4-8 interstitials. Mobile interstitials released from stable extended {311} defects are linked to transient enhanced diffusion (TED) of boron in ion-implanted samples. Boron TED observed without visible extended defects is attributed to small interstitial defects that can provide mobile interstitials at low temperature.[1] Furthermore, small interstitial clusters can provide growth nuclei for extended defects. Our previous calculations[2] established that compact interstitial clusters are favorable for n = 2-4, while elongated clusters are energetically favorable for larger clusters. We perform extensive atomistic simulations using Modified Embedded Atom Method (MEAM),[3] tight-binding (TB) and *ab initio* Hamiltonians to determine the interstitial-binding energies and capture radii for small clusters. For each cluster, we performed parallel replica simulations[4] 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 structure. Interstitial diffusion in the presence of the clusters and interstitial-cluster diffusion are investigated by parallel replica method[4] using MEAM and TB potentials.

11:30 AM J5.10
MODELING OF ANNEALING OF HIGH CONCENTRATION AS PROFILES. Pavel Fastenko, 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-resistant junctions requires implantation of high doses of As at low energy. At present, simulation models are not capable of accurate predicting junction depth and resistivity of high concentration arsenic profiles. The standard approach for simulating As anneal would consider amorphization of surface layer and include {311} /loop 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 is critical for accurate modeling of As implants. High arsenic concentration accelerates generation of Frenkel 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 deactivation of laser annealed samples and non-linear dependence 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_nV clusters. We also take into account the effect of As concentration on 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 MS&E, Gainesville, FL; Daniel F. Downey, Varian Semiconductor Equipment Associates, Gloucester, MA.

Preamorphization is commonly used in the formation of ultra-shallow 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-to-medium energy 5-30 keV germanium implants on silicon. The implant doses were 5 x 10^{14}, 1 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 keV to 5 keV, an alternate path of excess interstitials evolution may exist. For higher implant energies, the interstitials evolve from clusters to {311}'s 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}'s forming. These results imply there is another alternative to {311} dissolution during TED for these ultra-low energy implants. The energetics of the dissolution process for small dislocation loops will be discussed.

SESSION J6: DOPANT IMPURITY EFFECTS
Chairs: Mark E. Law and Erik J.H. Collart
Wednesday Afternoon, 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.A. Gable, K.S. Jones, M.E. Law, SWAMP Center, University of Florida, Gainesville, FL; D.F. Downey, Varian Semiconductor Equipment Associates, Gloucester, MA; M.J. Rendon, 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 ultra-shallow junctions. An alternative approach to achieve ultra-shallow low-resistivity junctions by co-implanting fluorine with boron has shown promise 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 n-type Czochralski wafer was achieved using a 70 keV 1x10^{15}/cm^2 Si^+. The Si^+ implant produced a 1500$\AA$ deep amorphous layer, which was then implanted with B^+ ions with energies ranging from 500 eV to 1.1 keV and doses ranging from 1x10^{15}/$cm^2$to 4x10^{15}/cm^2. The wafers were subsequently implanted with F^+ ions with energies ranging from 3 to 36 keV and doses ranging from 1x10^{15}/$cm^2$to 8x10^{15}/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 a tube furnace 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. The addition of fluorine reduces the boron diffusion enhancement by 50x, increases the boron activation by 3x, and increases the boron concentration gradient in the tail of the profile by 6x. 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 phenomenon.

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 Mehta, Varian Semiconductor Equipment Associations, 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 phenomenon of Fluorine related Boron diffusion. We observed 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 5e15 at./cm^2. The Si PAI was 10 and 20 keV with a dose of 5e14 at./cm^2. The Boron implants were 250 eV to 1 keV with a dose of 1e15 at./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. V.C. Venezia, H.-J.L. Gossmann, H.-H. Vuong, A.T. Fiory, and C.S. Rafferty, 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 B in Si by monitoring substrates. 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 Si-self ion implants or Cl ion implants. We find that although the initial 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 float zone silicon.

2:15 PM J6.4
DIFFUSION AND DEFECT STRUCTURE IN NITROGEN IMPLANTED SILICON. Omer Dokumaci, R. Kaplan, M. Khare, P. Ronsheim, A. Domenicucci and R. Fleming, IBM SRDC, Hopewell Junction, NY; L.S. Adam and M.E. Law, University of Florida, Gainesville, FL.

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 oxidation greatly affects the oxidation rate and oxide reliability. 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 2e14 to 2e15 cm^{-2}. The samples were annealed with an RTA system from 750C to 900C. The nitrogen profiles were obtained by SIMS. Cross section TEM was done on selected samples. For lower doses, most of the nitrogen diffuses 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 bugdet. 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 2e15 cm^{-2} dose creates a continous amorphous layer from the surface. Even after a 750C anneal, there is residual amorphous Si at the surface which has not been recrystalized. 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/crystal interface. After the 900C anneal, the silicon has fully recrystalized 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 INDIUM ELECTRICAL ACTIVITIES IN SILICON IN THE PRESENCE OF NITROGEN. Vladimir Zubkov, Sheldon Aronowitz, Helmut Puchner, LSI Logic, Santa Clara, CA; Juan Senosiain, 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 activity is lowered by at least 20% . The ab initio code, VASP, was applied to exploration of the B - N and In - N interactions effect on acceptors activities. Si64 supercells were mainly employed. Forma tion energy, Ef, of a negatively charged supercell and a band gap from calculations with one k point were chosen as indices of acceptor activity. For qualtitative study of long 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 that 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 drastically lowered Ef and increased gap values, ie., suppressed electrical activity. It also lead to formation of N-X chemical bonds in some cases (X= B,In). Calculated Ef, gap, and electron affinities values indicate tha the X-N systems exhibit reduced electrical activity when the X-N are adjacent but also when they are separated by four and more bonds. These results correlate with decreased in electrical activities 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.

2:45 PM J6.6
Abstract Withdrawn.

3:30 PM J6.7
SILICON INTERSTITIAL DRIVEN LOSS OF SUBSTITUTIONAL CARBON FROM SiGeC STRUCTURES. M.S. Carroll and J.C. Sturm, Dept. of Electrical Engineering, Princeton University, Princeton NJ; E. Napolitani, D. de Salvador and A. Drigo, INFM and Dept. of Physics, University of Padova, Padova, ITALY; J. Stangl and G. Bauer, Institute for Semiconductor Physics, Johannes Kepler University Linz, Linz, AUSTRIA; D. Tweet, SHARP Laboratories of America, Inc., Camas, WA.

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 effected by the excess interstitials is not known and furthermore excess 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 interstitials injected by oxidation. Single crystal, 25 nm thick, $Si_{0.7765}Ge_{0.22}C_{0.0035}$ epitaxial layers were grown on Czchrolaski silicon substrates and capped by silicon layers of 40, 300, and 700 nm by rapid thermal chemical vapor deposition at temperatures of 550-750°C. The samples were subsequently annealed in either nitrogen or oxygen ambients at 750°C or 850°C for times of 30-960 minutes. Carbon concentrations before and after annealing are measured by secondary ion mass spectrometry 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 interstitial injection case nearly all the carbon in the as-grown SiGeC layer leaves the sample by diffusion through the thin silicon cap out the surface. No sign of any immobile carbon spikes, to SIMS detection limits, are observed in this extreme case demonstrating that diffusion is the dominant interstitial-carbon reaction in this annealing regime. Furthermore, because the interstitial injection during oxidation in these conditions is now known [3], the number of carbon that leave the SiGeC layer can be correlated with the number of injected interstitials. This work was supported by ARO and DARPA. [1] P.A. Stolk, H.-J. Gossmann, D.J. Eaglesham, D.C. Jacobson, J.M. Poate, and H.S. Luftmann, Appl. Phys. Lett. 66, 568 (1995) [2] W.J. Taylor, T.Y. Tan, U. Goesele, Appl. Phys. Lett. 62, 3336 (1993) [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 J6.8
DIFFUSION AND CLUSTERING OF SUPERSATURATED C IN SiGeC LAYERS. D. De Salvador, E. Napolitani, A. Coati, M. Berti, A.V. Drigo, INFM and Dept. of Physics, 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-interstitials and supersaturated carbon are rather complex and not yet well understood, involving self-interstitial driven C diffusion and/or clustering or precipitation. In this work we investigated the diffusion and clustering of supersaturated substitutional carbon 200 nm thick $Si_{0.926}Ge_{0.07}C_{0.004}$ layers buried under silicon cap layers of 40 nm. The samples are annealed in nitrogen or oxygen ambient at 850C for times between 2-10 hours. Total and substitutional carbon concentration profiles are measured by secondary ion mass spectrometry (SIMS), x-ray diffraction (XRD), Rutherford and resonant backscattering spectrometry in random and channeling geometry (RBS/rBS-channeling). 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 layer, or be trapped by other C atoms forming clusters. In the early stage of the annealing, carbon escape by diffusion across the layer/cap interface dominates. This phenomenon saturates after 4 hours, because the interstitial injection during oxidation also promotes the formation and growth of precipitates. The latter prevents further loss of C, which instead in our samples diffuses and accumulates inside the layer at about 40 nm below the cap/layer interface. However, the precipitate density profile extends also deeper in the layer. Accordingly, 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 C profile doesnt 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 J6.9
BORON SEGREGATION AND ELECTRICAL PROPERTIES IN POLYCRYSTALLINE SiGeC. E.J. Stewart and J.C. Sturm, Center for Photonics and Optoelectronic Materials, Department of Electrical Engineering, Princeton University, Princeton, NJ.

Previously, it has been reported that PMOS capacitors with heavily boron-doped polycrystalline SiGeC gates are less susceptible to boron penetration than those with Si gates (1). Boron appears to accumulate in the SiGeC layers during anneals, reducing boron outdiffusion from the gate despite high boron levels at the gate-oxide interface. In this abstract, we report clear evidence of strong boron segregation to polycrystalline SiGeC layers from Si or SiGe layers, and present electrical data indicating that the boron in these layers remains active. Polycrystalline layers were deposited by RTCVD at ~575°C and 700°C using SiH_4, GeH_4, $SiCH_6$, and B_2H_6 as silicon, germanium, carbon, and boron sources, respectively. All layers were in-situ doped and grown on 200 nm oxides. To study segregation, a two layer structure was grown consisting of ~100 nm p^- (~10^{18} cm^{-3}) poly SiGeC (Ge=25%, C=1.6%) next to ~300 nm of p^+ (~10^{20} cm^{-3}) poly Si. This sample was annealed in N_2 at 800°C for long times to allow the boron to move from the heavily doped Si to the lightly doped SiGeC layer. Single layer samples of p^+ (~10^{20} cm^{-3}) poly Si, SiGe, and SiGeC 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 clearly segregated to the poly SiGeC 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 SiGeC layer's conductivity remains roughly constant during the anneal. In the two layer sample, the boron that has segregated to the SiGeC layer appears active, but less so than in the single layer SiGeC sample. Segregation has also been observed in single crystal SiGeC. The driving force for segregation is under further study; however, it appears that at least a significant amount of the boron is not forming inactive carbon-related defect complexes. (1) C.L. Chang and J.C. Sturm, Applied Physics Letters, 74 (17), 2501 (1999).

4:15 PM J6.10
A COMPREHENSIVE MODEL FOR CARBON SUPPRESSION OF BORON TRANSIENT ENHANCED DIFFUSION. Julie L. Ngau, Peter B. Griffin, 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 $Si_{1-x-y}Ge_xC_y$ and $Si_{1-y}C_y$ where $x = 9.6\%$ and $y = 0.018 - 0.037\%$ was studied for 10 s to 60 min, 750°C anneals. The combination of having low C concentrations, which reduce B TED without 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 C-rich Si is caused by

the non-equilibrium Si point defect concentrations, specifically the undersaturation of Si self-interstitials, that result from the coupled out-diffusion of carbon interstitials via the kick-out and Frank-Turnbull reactions. Attempts to model our data with these two reactions revealed that the time evolved diffusion behavior of B was not accurately simulated and that an additional carbon reaction was necessary. In this work, we incorporate a carbon interstitial, carbon substitutional (C_iC_s) pairing reaction into a comprehensive model that includes the C kick-out reaction, C Frank-Turnbull reaction, {311} defects, and boron interstitial clusters (BICs) and demonstrate that this model successfully simulates C suppression of B TED at 750°C for anneal times ranging from 10 s to 60 min.

4:30 PM J6.11
A QUANTITATIVE MODEL OF THE ELECTRICAL ACTIVITY OF METAL SILICIDE PRECIPITATES IN SILICON BASED ON THE SCHOTTKY EFFECT. T.Y. Tan and P.S. Plekhanov, Department of Mechanical Engineering and Materials Science, Duke University, Durham, NC.

Metal silicide precipitates in Si are experimentally known to be prominent carrier recombination/generation centers, and in the past there was no quantitative model. Presently, we have worked out the first phase of such a quantitative model in which the carrier recombination properties are addressed. This model is based on the Schottky nature of the precipitate-Si system. In this model, carrier diffusion as well as carrier drift in the Si space charge region are accounted for, and carrier recombination is attributed to the thermionic emission mechanism of charge transport across the Schottky junction. It is shown that the minority carrier capture cross-section of the precipitate can be as large as the total capture cross-section of its constituent metal atoms dissolved in the Si matrix. Under weak carrier generation conditions, the supply of minority carriers was found to be the limiting factor of the recombination process. The plausibility of the model is demonstrated by a comparison of calculated and available experimental results.

SESSION J7: LASER ANNEALING
Chair: Majeed Foad
Thursday Morning, April 19, 2001
Golden Gate A2 (Marriott)

8:30 AM *J7.1
IMPACT OF PRE-AMORPHIZATION IMPLANTS ON LASER ANNEALED JUNCTIONS. Somit Talwar, Yun Wang, Verdant Technologies, San Jose, CA; Mike Thompson, Cornell University, Department of Material Science, Ithaca, NY; Kevin Jones, University of Florida, SWAMP Center, Gainesville, FL.

Abrupt, shallow and highly activated junctions will be required for the sub 100 nm technology nodes 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 concurrently demonstrated all the desired junction characteristics for at least the 70 nm node. The LTP junction demonstrations have been made on blanket silicon 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, defect density etc. by changing the melt/recrystalization dynamics. The changes introduced by the amorphization and absorber layer steps in the melt and recrystalization dynamics have been studied using time resolved reflectometry and transient conductance measurements. The resulting modifications in the defect density, and dopant activation, deactivation and diffusion behavior have also been investigated using a combination of SIMS, TEM, four point probe and hall mobility analysis. 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 SILICON. E. Kuryliw, K.S. Jones, Univ of Florida, Dept of MS&E, Gainesville, FL; Somit 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 anneals are inevitable, 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 $1x10^{15}/cm^2$ Si^+ implant was done followed by a 1 keV $4x10^{14}/cm^2$ B^+ implant. The surface was then laser melted at laser powers between 0.625 and 0.825 J/cm^2 using a 308 nm excimer-laser. Transmission electron microscopy was used to analyze the defect formation after LTP. It was found that increasing laser power reduces 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 1000°C. For powers in the LTP processing 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 powers 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 the presence of a supersaturation of quenched in interstitials located within the regrown melt region. This possibility is investigated and discussed.

9:15 AM J7.3
ULTRASHALLOW, LOW RESISTIVITY JUNCTIONS IN MOS DEVICES. Yayoi Takamura, Sameer Jain, Peter Griffin, J.D. Plummer, Stanford University, Center for Integrated Systems, Stanford, CA.

As semiconductor device dimensions continue to decrease, the main challenges in the area of junction formation include decreasing the junction depth while simultaneously increasing the dopant concentration. The current technique of ion implantation followed by rapid thermal annealing (RTA) is limited by the solid solubility of the dopants in silicon. Laser annealing is being investigated as a possible alternative to RTA. Laser annealed samples have uniform, box-shaped profiles, with dopant concentrations that can exceed equilibrium solubility limits. Unfortunately, these super-saturated dopant concentrations exist in a metastable state and deactivate upon further thermal processing. In this work, we have begun a comprehensive study of the deactivation kinetics of common dopants (As, P, B, and Sb) across a range of concentrations and annealing conditions. The different dopants exhibited different deactivation behavior, however, in each case, the deactivation rate was greater for the more highly doped samples, resulting in lower sheet resistance for the lower doped samples. In the case of the Sb and B doped samples, the dopant remains fully active until 700-800C, while the As and P doped samples deactivate at temperatures as low as 500C. A simple single cluster model is proposed to explain the deactivation behavior. We are also investigating ways to maintain these metastably doped layers with the goal of meeting the International Technology Roadmap for Semiconductors (ITRS) requirements for ultrashallow junctions.

9:30 AM J7.4
LASER THERMAL INDUCED CRYSTALLIZATION AND 20 NM DEVICE STRUCTURES. Shenzhi Yang, Michael O. Thompson, Cornell Univ, Dept of Materials Science and Engineering, Ithaca, NY.

Laser thermal processing is emerging as a primary processing technique to allow scaling of conventional CMOS below the 100 nm node. Much of the current understanding of LTP is, however, based on blanket irradiations of bare Si surfaces absent of any complex circuit features or films. Insertion of LTP will, in contrast, likely require an isolation layer and a metal absorber layer to manage thermal and optical inhomogenities on patterned wafers. In this work, we have experimentally investigated the quantitative melt and solidification dynamics of both crystal silicon and very thin amorphous layers (~20 nm) capped by an oxide and metal layer irradiated by a 30 ns 308 nm excimer laser. The dynamics of the process were followed using transient conductance and reflectance in real time, and ex-situ sheet resistance measurements. The application of transient conductance measurement (TCM) was validated with both reflectance and sheet resistance results for silicon-on-insulator (SOI) substrate. Numerical simulation of the process has been refined to properly simulate the behavior under these more realistic irradiation conditions. Transient superheating of the amorphous silicon(above its reduced melting temperature) within the confined oxide layer, and changes to the explosive crystallization dynamics, have been investigated. In addition, the effect of impurities at concentrations near the metastable limit (i.e., 3% boron) has also been studied. These processes directly impact the window available for controlled growth of shallow junctions.

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

10:15 AM *J8.1
IMPLANT DOSE AND SPIKE ANNEAL TEMPERATURE RELATIONSHIPS FOR SHALLOW EXTENSION JUNCTIONS.

K.K. Bourdelle, A.T. Fiory, H.-J.L. Gossmann, Bell Laboratories, Lucent Technologies; S.P. McCoy, Vortek Industries.

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 are 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 incandescent lamp (Heatpulse) or arc lamp (Vortek) heating methods, the latter allowing higher spiking temperature and dopant solubility at equivalent thermal budget. For targeted sheet resistance and junction depth, spiking temperature trends lower with implant dose, concomitant with decreasing fraction of activated dopant.

10:45 AM J8.2
BORON DIFFUSION IN SILICON AND SILICON GERMANIUM UNDER THE INFLUENCE OF POINT DEFECT INJECTION BY RAPID THERMAL ANNEAL. Aihua Dan, Arthur F.W. Willoughby, Janet M. Bonar, School of Engineering Sciences, University of Southampton, Southampton, UNITED KINGDOM; Nicholas E.B. Cowern, Philips Research Labs, Eindhoven, THE NETHERLANDS; Barry M. McGregor, Department 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 coated samples in oxygen) with injection diffusion (RTA oxidation of bare 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 $Si_{0.9}Ge_{0.1}$. The diffusion profiles for as-grown and annealed samples were measured on Secondary Ion Mass Spectrometry (SIMS). Diffusivities for B in Si and $Si_{0.9}Ge_{0.1}$ were obtained using computer simulations of the measured boron profiles for annealed samples. Boron diffusion in Si and $Si_{0.9}Ge_{0.1}$ was found enhanced by interstitial injection. The enhancement from the interstitial injection of the measured B diffusivity in $Si_{0.9}Ge_{0.1}$ is similar to that in Si. These results confirm that B diffusion in $Si_{0.9}Ge_{0.1}$ is involved by an interstitially mediated mechanism and slower than in Si. The effect of the diffusion time on the boron diffusion in Si and $Si_{0.9}Ge_{0.1}$ has also been investigated. The diffusivity versus diffusion time of B in Si and $Si_{0.9}Ge_{0.1}$ 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 J8.3
INFLUENCE OF LOW THERMAL BUDGET PRE-ANNEALS ON THE HIGH TEMPERATURE REDISTRIBUTION OF LOW ENERGY BORON IMPLANTS IN SILICON. F. Boucard, PHASE / CNRS, Strasbourg, FRANCE, and SILVACO France, Gieres, FRANCE; M. Schott, D. Mathiot, PHASE / CNRS; P. Rivallin, P. Holliger, LETI, Grenoble, FRANCE; and E. Guichard, SILVACO 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 sub-micron devices. It is also known that this TED is linked to the fate (elimination and agglomeration) of the ion 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 aspect 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 temperature. Thus it can be thought that low thermal budget pre-anneals, by affecting the initial self-interstitials distribution, could affect B redistribution during subsequent high temperature RTA. The purpose of this contribution is to present the experimental evidence that such low thermal pre-anneals do indeed affects 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)

11:15 AM J8.4
REVERSE DIODE LEAKAGE IN SPIKE-ANNEALED ULTRA-SHALLOW JUNCTIONS. Tao Feng, University of Florida, Gainesville, FL; Hans-Joachim L. Gossmann, Bell Laboratories, Lucent Technologies, Murray Hill, NJ; Aditya Agarwal, Peter Frisella and Leonard M. Rubin, Axcelis Technologies, Beverly, MA.

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 may lead to excessive junction leakage current, I_{lkg}. We have investigated diode leakage in junctions produced by ion-implantation of B with energies of 0.5 - 2 keV and doses of 2×10^{14} - 2×10^{15} cm^{-2} into n-type wells of $\sim 1 \times 10^{18}$ cm^{-3}, after rapid-thermal anneals (RTA) in lamp-based and hot-wall furnaces. Junctions are as shallow as 30 nm and were directly probed to avoid complications arising from metalization. The leakage current, I_{lkg}, was found to be independent of the implant dose at any reverse voltage (-1 and -5 V). This implies that the electrically active defects are sufficiently far removed and on the surface-side of the junction. In both systems, a spike anneal (no intentional dwell time at peak-temperature) resulted in higher I_{lkg} than a soak anneal (dwell time of several seconds at peak-temperature). However, for the same spike annealing recipe, the hot-wall RTA produces tighter distributions than the lamp-based RTA. The width of the distribution is a measure of the temperature uniformity across the wafer. Best leakage currents are of the order 1×10^{-6} A/cm^2. Simulations show that this rather large current can be accounted for by band-to-band tunneling and impact ionization. The shallowest junctions exhibit I_{lkg} $\sim 5 \times 10^{-4}$ A/cm^2. However, this contributes only $\sim$ 1 pA/μm to the transistor off-current in a fully scaled 100 nm technology, well below the specification of even the low power transistor (20 pA/μm).

11:30 AM J8.5
BORON SOLUBILITY LIMITS FOLLOWING LOW TEMPERATURE SOLID PHASE EPITAXIAL REGROWTH. C.D. Lindfors, K.S. Jones, Univ of Florida, Dept of Material Science and Engineering, Gainesville, FL; M.J. Rendon, Motorola Inc, Austin, TX.

Future advancements in microelectronics require shallow junction, high carrier concentration material. Alternative techniques for controlling transient enhanced diffusion (TED) are being explored for shallow junction formation. One such technique is implanting dopant into a preamorphized substrate and using low temperature solid phase epitaxial (SPE) regrowth so there is little or no motion of dopant atoms. Wafers were preamorphized with either silicon or germanium followed by 5 keV B^+ implants in the dose range of 5×10^{14} - 8×10^{15} cm^{-2}. Amorphous layers are regrown 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 lowest sheet resistances can be obtained. Finally, variable angle spectroscopic ellipsometry (VASE) is utilized to verify that the amorphous layers are regrowing. Results of the 500°C anneals from 30 to 45 minutes show that a minimum sheet resistance of about 140 Ω/square can be achieved for an implant dose of 2×10^{15} cm^{-2} of boron. In fact at all the various anneal times a minimum sheet resistance occurs for the 2×10^{15} cm^{-2} B^+ dose. Thin amorphous layers still exist after 30 and 35 minute anneals 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.

11:45 AM J8.6
RAMP-RATE EFFECTS IN TRANSIENT ENHANCED DIFFUSION: A QUASI-ANALYTICAL EXAMINATION. Michael Y.L. Jung, Edmund G. Seebauer, Univ of Illinois, C-U, Dept of Chemical Engineering, IL.

Some experimental evidence has accumulated in recent years to support the use of spike anneal temperature trajectories with very fast heating and cooling rates for making ultrashallow junctions by ion implantation. Improved device properties have been claimed using heating rates of 400°C or more. This procedure supposedly optimizes junction depth and sheet resistance by reducing transient-enhanced diffusion (TED) of the dopant. 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, obtain a clear picture for the occurrence and potential magnitude of such effects. 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 diffused profile according to $\beta^{-1/2}$ as long as TED runs out before the top of the spike. Improvement decreases

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 β depends sensitively on the temperature trajectory near the peak and the details of the clustering model used. The details 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)

1:30 PM *J9.1
MODELING OF DOPANT DIFFUSION AND ACTIVATION.
Mark E. Law, 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. The surface 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 complex surface reactions that can account for experimental results 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 J9.2
ATOMISTIC STUDY OF B-RELATED DEFECTS IN SILICON BY TIGHT-BINDING SIMULATIONS.
Paola Alippi, Luciano Colombo, Paolo Ruggerone INFM 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 diffusivity together with the formation of B-Si immobile clusters. Both features are believed to be driven by the excess Si self-interstitials 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 a single boron atom and a self-interstitial in a silicon matrix. DFTB results for equilibrium structures and formation energies of different defect 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 simulations at finite temperature which allowed to evaluate boron diffusivity in a temperature range between 900 K and 1500 K. Our simulations provide both a migration energy of about 0.7 eV and a full dynamical picture of B diffusion [4]. Finally, the investigation was extended to the analysis of the stability of boron-interstitial clusters, in the search for a growth pattern in either high or low Si-interstitial content conditions. We show the DFTB results for the binding energies of several B_nI_m complexes and discuss the competition between the formation of mixed and monoatomic clusters. This work was funded by INFM under project SIMS. [1] D. Porezag, Th. Frauenheim, Th. Koehler, G. Seifert, and R. Kaschner, Phys. Rev. B**51**, 12947 (1995). [2] P.M. Fahey, P.B. Griffin, T.D. Plummer, Rev. Mod. Phys. **61**, 289 (1989); A.D. Lilak, S.K. Earles, M.E. Law, and K.S. Jones, Appl. Phys. Lett.**74**, 2038 (1999). [3] B. Sadigh, T.J. Lenosky, S.K. Theiss, and M.-J. Caturla, Phys. Rev. Lett. **83**, 4341 (1999); W. Windl, M.M. Bunea, R. Stumpf, S.T. Dunham, and M.P. Masquelier, Phys. Rev. Lett. **83**, 4345 (1999). [4] P. Alippi, L. Colombo, A. Sieck, G. Seifert, and Th. Frauenheim, submitted for publication (2000).

2:15 PM J9.3
ATOMISTIC MODELING OF AMORPHIZATION IN Si.
Lourdes Pelaz, Luis A. Marques, University of Valladolid, SPAIN; George H. Gilmer, Bell Labs, Lucent Technologies, Murray Hill, NJ; Juan Barbolla, University of Valladolid, SPAIN.

The dimensional and electrical features of current Si devices require high dose and very low energy implants, which cause amorphization in the regions of high dopant concentration. The simulation of dopant diffusion and damage evolution is frequently done using the "1" model, but this approximation is not valid when a large fraction of the implanted ions are within the amorphous region. Monte Carlo and Molecular Dynamics simulations have been used to study the the amorphization and recrystallization processes and the interaction between dopants and defects for amorphizing implants. Molecular dynamics simulations are used to examine the extent of ion-induced amorphization and the mobility and recombination of defects, together with the recrystallization of amorphous pockets. For the Monte Carlo approach, we have modified the code DADOS in order to include the formation of amorphous regions, which allows accurate simulations of high implant doses. Amorphous regions are simulated as aggregates of point defects, with Frenkel-pair recombination rates reduced in regions of high point defect density. For the low implant temperatures, the damage is accumulated, with little diffusion of defects and dopants during the implant. When the dose exceeds the amorphization threshold and the amorphous layer extends to the surface, the transient diffusion of the dopant atoms is reduced. Most of the "1" interstitials in the amorphous layer are displaced to the free surface as this layer is recrystallized, and hence rendered ineffective for transient diffusion. Using this model, we discuss dopant diffusion accompanying amorphizing implants for a range of conditions. Good agreement with experiments is obtained.

2:30 PM J9.4
ATOMISTIC SIMULATIONS OF EXTRINSIC DEFECTS EVOLUTION AND TRANSIENT ENHANCED DIFFUSION IN SILICON.
Alain Claverie, Benjamin Colombeau, Gérard Ben Assayag, CEMES/CNRS, Toulouse, FRANCE; Fuccio Cristiano, LAAS/CNRS, Toulouse, FRANCE.

Transient Enhanced Diffusion (TED) of ion implanted dopants in silicon is driven by the thermal evolution of the various types of extrinsic defects formed during annealing. These defects evolve in size and type through the interchange of Si interstitial atoms (Si_{int}s). This competitive growth maintains in the region large supersaturations of Si_{int}s, in dynamical equilibrium with the extrinsic defects, which are at the origin of the TED process. The driving force for this evolution is the reduction of the formation energy of the defects as they grow in size or change their "crystallographical" structure. We have implemented an atomistic simulation tool based on the description of the diffusion process given above. Our model describes the concomitant evolution of the defects and of the Si_{int}s supersaturation in a variety of experimental conditions. It accounts for the capture and emission of Si_{int}s to and from extrinsic defects (defined by their formation energy) of sizes up to thousands of atoms and includes a loss term due to the interstitial flux to the surface. We have initially validated our model against some classical experiments concerning the TED of dopants in conjunction with the dissolution of {113} defects in Si^+ implanted wafers. We have subsequently applied our model to the case of B^+ implantation at both low and ultra low energy. In these energy regimes, the distance between the defect layer and the surface plays a crucial role in determining the TED decay time. The simulations show that defect dissolution occurs earlier and for smaller sizes 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 full understanding of the formation and the evolution of extrinsic defects, including their interaction with the surface, leads to a correct prediction of dopant enhanced diffusion in all experimental conditions.

2:45 PM J9.5
SIMULATION OF BORON-DOPANT PROFILE EVOLUTION DURING ULTRASHALLOW JUNCTION PROCESSING IN Si.
Gyeong S. Hwang, Eugene Heifets, Tahir Cagin, and William A. Goddard III, Materials and Process Simulation Center, Beckman Institute, California Institute of Technology, CA; Yuzuru Sato, Masayasu Miyata, and Masamitsu Uehara, Seiko Epson Corp., JAPAN.

An incessant 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 postimplantation 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 [density functional theory] simulation of the fundamental atomic-level processes, and (iii) experimental validation. We will present (i) new mechanisms of B diffusion, (ii) pathway of 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 ultrashallow junction processing: (i) the validity of '1' model, (ii) The surface proximity effect, and (iii) the role of defect/dopant clustering in determining junction profiles.

SESSION J10: GETTERING OF IMPURITIES
Chair: Alain Claverie
Thursday Afternoon, April 19, 2001
Golden Gate A2 (Marriott)

3:30 PM J10.1
INTERACTION OF TRANSITION METAL CONTAMINATION WITH ION-IMPLANTED B IN Si. Janet L. Benton, Thomas Boone, Dale C. Jacobson, Conor 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 diffusivities 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, 4d and 5d metals have a higher solubility for substitutional atoms over interstitial atoms in Si. Therefore, the interstitial and vacancy defects created by B ion-implantation control the diffusion of these elements. Gettering of this group of metals by high concentrations of B is not observed. In this work, Fe, Co, Cu, Mo, and Au are intentionally introduced into Si by ion-implantation and their interactions with ion-implanted B is monitored by SIMS, carrier recombination lifetime, and DLTS. Localization of Mo at ion-implantation induced damage is observed. SIMS profiles of shallow BF_2 implants 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 preferentially diffuse to 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 3d metals at implantation damage is limited by nucleation 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 coulomb attraction provided 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 that the final distribution of Co in Si reflects defect evolution during annealing. Thus, several gettering mechanisms operate during ULSI processing, influencing the diffusion of Co contamination during high temperature steps, and, consequently, controlling the effect of the metal on the electrical properties of the Si devices.

3:45 PM J10.2
METAL GETTERING IN THE Rp/2-REGION AND BEYOND Rp OF BURIED IMPLANTS IN SILICON: THE TWO SIDES OF THE SAME MEDAL? W. Skorupa, A. Peeva, Y. Gueorguiev and R. Kögler Forschungszentrum Rossendorf, Dresden, GERMANY.

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 to elucidate the formation kinetics and nature of the so called Rp/2 defects explored by decoration techniques using metal atoms. 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 temperature-time budget, we showed also, that it can also happen as a result of a low energy / light ion implant: Helium ions with 20 or 40 keV! This points to the fact that the Rp/2 effect is a common feature of ion implantation especially when the temperature-time budget decreases as proposed by the SIA roadmap for future technology schedules. Usually, its nature is discussed in the framework of excess vacancies as residuals of a local recombination between primarily ion-beam-induced vacancies and interstitials although annealing effects 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 will critically discuss these results putting also new pixels to the picture. All this demonstrates at least that the efforts of understanding ion implantation induced defect evolution do not come to end and never get boring!

4:00 PM J10.3
THE ROLE OF HIGH ENERGY CO-IMPLANTS IN LIMITING TRANSIENT ENHANCED DIFFUSION OF BORON IN SILICON AND SOI MATERIAL. Ahmed Nejim, Brian J. Sealy, Department of Electronic Engineering, University of Surrey, Surrey, UNITED KINGDOM; Changlong Liu, Institute of Modern Physics, Chinese Academy of Sciences, Lanzhou, CHINA; Elke Wendler, Friedrich-Schiller-Universitaet, Jena Institut fuer Festkoerperphysik, Jena, GERMANY; Graham Cooke, MATS, United Kingdom, Innovation House, Daten Park, Warrington, Cheshire, UNITED KINGDOM; Paul G. Coleman, Department of Physics, University of Bath, Claverdon, UNITED KINGDOM.

We investigate the role of high energy (0.5-1 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/cm^2 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 peak of the profile when all the boron is contained in the silicon overlayer. We will present accurate point defect profiles for the deep interstitials from Rutherford backscattering channelling (RBS-c) and Dechannelling In Crystals And Defect Analysis (DICADA) code and vacancy profiles from positron annihilation (PAS) analysis 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
BEHAVIOR OF VACANCY CLUSTERS GENERATED BY HIGH-ENERGY ION IMPLANTATION INTO SOI SUBSTRATES. R. Kalyanaraman[a,b], T.E.Haynes[a], H.-J.L.Gossmann[b], G.H.Gilmer[b], and C.S.Rafferty[b]. [a]Solid State Division, Oak Ridge National Laboratory, Oak Ridge, TN; [b]Bell Laboratories, Lucent Technologies, Murray Hill, NJ.

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 "0.5R_p." During any subsequent thermal treatments, both the interstitials from near R_p and the shallower vacancies evolve by ripening, recombining with each other, and annihilating at various sinks. While the energetics and kinetics 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 float-zone and epi-Si. In such substrates, the possibility of interference from interstitials near R_p remains as a complication. In this presentation, we report the results of similar new measurements in Si-on-insulator (SOI) substrates where the vacancy-rich region is isolated by the buried oxide from the deeper interstitials. Using isothermal and isochronal measurements, the kinetic and thermodynamic behavior of the vacancy clusters has been studied. 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/SiO_2 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.

4:30 PM J10.5
GROWTH MECHANISM OF CAVITIES IN MeV HELIUM IMPLANTED SILICON. Jérémie Grisolia, Alain Claverie, G. Ben Assayag, CEMES/CNRS, Toulouse, FRANCE; Sylvie Godey, Esidor Ntsoenzok, CERI/CNRS, Orléans, FRANCE; Freek Labhom, A. Van Veen, IRI, Delft Univ of Technology, Delft, THE NETHERLANDS.

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. Litterature is somehow 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 $5\times10^{16}/\mathrm{cm}^2$ i.e. at a depth of almost 6mm. After implantation samples were isochronnaly annealed for one hour at temperatures ranging from 400°C to 900°C under argon gas. NDP (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 ditributions, 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 independant on 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 interchanging the He atoms they contain. However, a more complex mechanism involving vacancy migration must be taken into account and will be discussed.