Thursday Morning, October 5, 2000

Manufacturing Science and Technology
Room 304 - Session MS-ThM

Advanced Modeling and Control for IC Manufacturing

Moderator: S.S. Shankar, Intel Corporation

8:20am **MS-ThM1 Simulation of Transient Enhanced Diffusion of B in Si***,* ***G.S. Hwang****, W.A. Goddard III,* California Institute of Technology

Ever shrinking 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 (TED) of dopants and (ii) the dynamics of defect/dopant clustering during implantation and postimplantation annealing. We present a systematic approach to address such issues in which we combine (i) kinetic Monte Carlo (kMC) mesoscale simulations capable of describing the length and time scales of TED with (ii) quantum mechanics [density functional theory (DFT)] calculations of the fundamental atomic level processes and (iii) experimental validation. In recent years much effort has been devoted to understanding the TED of B in Si; however, most studies have been performed using moderate energy (~40 keV) Si@super +@ implants into MBE-grown B-doped layers. The dominant mechanisms of the B TED based on this previous work may not be dominant for the low energy (10@super 20@ cm@super -3@) inherent to ultrashallow junction fabrication. In this talk, we will present (i) new mechanisms of B clustering and (ii) strain-induced defect-defect and defect-dopant interactions, and discuss how crucial it is to have such detailed information for accurately predicting the doping profiles in ultrashallow junction processing. We will also address several unresolved issues in the low-energy and high-concentration regime: (i) the validity of '+1' model, (ii) the surface proximity effect, and (iii) the role of defect/dopant clustering in determining junction profiles.

8:40am **MS-ThM2 New Physics for Models of Transient Enhanced Diffusion***, M.Y.L. Jung,* ***E.G. Seebauer****,* University of Illinois, Urbana-Champaign

As device dimensions continue to shrink, the constraints on processing imposed by Mother Nature become ever more stringent. The optimization of chemical kinetics and mass transport is therefore playing an increasingly important role in defining and widening process windows. Here we discuss TCAD modeling of transient-enhanced diffusion (TED) after ion implantation during ultrashallow junction formation by rapid thermal annealing. TED has long been modeled using a large set of reaction-diffusion equations for the dopant, point defects, and extended defects. However, current commercial and public-domain SUPREM-based software mishandles several important aspects of the reaction-diffusion network. For example, many of the diffusivities are inappropriately parameterized. Also, the software lacks a self-consistent, time-dependent treatment of Poisson's equation and therefore miscalculates the electric-field-driven drift of charged defects. There are further problems: even the best TED models neglect important effects of the nearby free surface and of intense illumination. For example, there is no incorporation of near-surface band bending, of changes in charged defect concentration during illumination, or of enhancement of point defect motion though local energy dumping by e-h recombination. This talk outlines how such effects can be incorporated and discusses conditions under which they are likely to be important.

9:00am **MS-ThM3 Fast-Ramp Annealing for Reducing Implant-Induced Transient Enhanced Diffusion***,* ***M.Y.L. Jung****, R. Gunawan, R.D. Braatz, E.G. Seebauer,* University of Illinois, Urbana-Champaign

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/s or more. This procedure supposedly optimizes junction depth and sheet resistance by reducing transient-enhanced diffusion (TED) of the dopant. However, the theoretical justification for using such fast ramps has been weak. Since the design and use of fast-ramp annealing tools will require substantial investments by equipment manufacturers and IC manufacturers alike, it is important to confirm by TCAD modeling the existence and potential magnitude of such effects. TED has long been modeled using a large set of reaction-diffusion equations for the dopant, point defects, and extended defects. However, current commercial and public-domain SUPREM-based software mishandles or ignores several important aspects of the reaction-diffusion network. We briefly discuss how we have fixed these problems, focusing in particular how proper incorporation of surface oxidation or nitridation kinetics closely couples the gas ambient in the annealer to dopant motion down near the junction within the Si bulk. We then show how variations in heating and cooling rates can be used to favor or disfavor important reaction-diffusion pathways within the overall system of effects that governs TED. In particular, we point out how the widely-used contant-temperature annealing step near 500 C for pyrometer calibration actually influences subsequent profile evolution in a profound way.

9:20am **MS-ThM4 Dynamic Simulation: Guiding Manufacturing from Process Mechanisms to Factory Operations***,* ***G.W. Rubloff,*** University of Maryland **INVITED**

Dynamics plays a critical role in the behavior and performance of semiconductor manufacturing from the unit process level to full factory operations, yet major gaps exist in our ability to simulate the consequences of this dynamics. At the process level, process models can provide a reasonable description of steady-state process behavior, but the realities of semiconductor equipment dictate that both total process times and thermal histories depend on the dynamics of the equipment and control systems, as well as on the raw process itself. We have developed physically-based dynamic simulation strategies which accurately reflect time-dependent behavior of equipment, process, sensor, and control systems, and we have used them to understand and optimize equipment systems and process recipes. Another dimension of dynamics appears in the behavior of cluster tools, where the tool architecture, process module populations, and scheduling algorithms add further dynamics to tool behavior. We have integrated reduced-order process models, reflecting dynamic unit process simulations, with discrete event simulations of cluster tool performance to enable co-optimization of process recipes, cluster tool configurations, and their scheduling algorithms. Finally, we have incorporated these integrated models into factory-level operational models to facilitate the evaluation of factory-level performance as a function of process, equipment, and logistics choices. These simulation strategies seem attractive in terms of their ability to represent dynamics, from continuous parameter dynamic recipes at the unit process level, to discrete-event dynamics associated with scheduling and throughput at the factory level.

10:00am **MS-ThM6 Integrated Metrology with Run to Run Control***,* ***P.R. Solomon****, P.A. Rosenthal, S. Bosch-Charpenay, J. Xu, W. Zhang,* On-Line Technologies, Inc. **INVITED**

The semiconductor industry is moving to adopt copper/low-k interconnect technology, smaller critical dimensions and 300 mm wafers. Many of these changes require tightening of the process specifications. Introducing these changes while maintaining product quality and reducing costs is a formidable challenge. Especially important are low-k dielectrics, chemically amplified resist, FSG and BPSG films that require control of their chemical composition as well as thickness. Integrated metrology with run-to-run control can facilitate the introduction of these new technologies because of its ability to improve process control while at the same time reducing manufacturing costs. Such benefits can be achieved for most current process steps as well. This paper will review some early success stories for Epi silicon and CMP processes. The integrated metrology for Epi employs an FTIR based film thickness monitor with model based analysis, integrated onto the cooldown chamber of the cluster tool for 100 % multi-point measurement and control. The FTIR is also applicable to the monitoring of thin film chemical composition. While FTIR has been widely used in R&D environments, its application to mainstream production metrology and process monitoring on product wafers has historically been limited by: 1) the optical complexity of film stacks used in production, 2) sample-dependent backside reflection artifacts caused by substrates which are transparent in the infrared, and 3) the lack of robust models of the chemically variable optical constants of modern IC materials. These limitations have been eliminated in a series of recent FTIR technology advances. The paper considers these recent advances, how the technology is integrated with the processing tools, the operation of the system, the improvement in the product and the cost of ownership. The paper will also examine the metrology available for integration and the future course for making such technology widely available, including standards for integration and methods for delivering the technology.

10:40am **MS-ThM8 W CVD Thickness Metrology and Run-to-Run Control using Mass Spectrometry*, Y. Xu*,** *T. Gougousi, R. Sreenivasan, G.W. Rubloff, J.N. Kidder, E. Zafiriou,* University of Maryland

For a H2/WF6 CVD process for selective W deposition in an Ulvac cluster tool, mass spectrometry has been used to observe HF product generation and H2 depletion. HF signal was proportional to the deposited W thickness to about 7%, providing an in-situ thickness metrology as a candidate to drive run-to-run thickness control. To assess this possibility, a systematic temperature drift of -50C per wafer was introduced, which in the absence of control would cause the film thickness to decrease by 40-50% over a ten wafer lot. Using a robust control algorithm to maintain a constant integrated HF mass spec signal by adjusting the nominal deposition time, the effect of the temperature drift on deposited film thickness was largely compensated, and the W film thickness was maintained within 10% of the target value. The metrology accuracy was limited by the low (about 3%) reactant conversion rate of the process, coupled with significant background signals. Since blanket W CVD processes as employed in manufacturing achieve much higher conversion efficiencies (40-50%), we anticipate considerable improvement in the efficacy of metrology and control in these situations. Our results, and their projection to realistic manufacturing scenarios, present an encouraging opportunity to use in-situ chemical sensing for process metrology and control.

11:00am **MS-ThM9 Feedback Control of Morphology During III-V Semiconductor Growth by Molecular Beam Epitaxy@footnote 1@*, R.L. Kosut*,** *J.L. Ebert, S. Ghosal,* SC Solutions*; R. Caflisch,* University of California, Los Angeles*; M. Gyure, J.J. Zinck,* HRL Laboratories

This paper addresses the modeling and control of epitaxial growth of III-V semiconductor material by Molecular Beam Epitaxy. In layer-by-layer growth mode, oscillations and envelope decay in the specular intensity of the reflection high energy electron diffraction (RHEED) pattern have been correlated to the instantaneous density of steps on the surface. This allows for the possibility of in situ monitoring and control of surface morphology during growth. A control algorithm and strategy was first developed using a KMC simulation model of III-V growth together with dynamic thermal models of the effusion cells and cracker valves. The strategy discovered from the simulations was to control growth layer-to-layer which turns out to have two important features: (1) it is very robust to chamber variations and uncertainties, and (2) the resulting form of the system is well modeled as a discrete-time system where sample times are replaced by layer number. There is a vast body of control theory which can be applied to such systems. The control was implemented on the MBE system to control RHEED oscillations and decay rates in real-time during III-V growth in HRL Laboratories MBE chamber. The RHEED signals were used to estimate oscillation period which was compared to a reference and the error was used in a control algorithm to adjust, in real-time, the set-point temperature of the III material effusion cell. The RHEED signals were also used to estimate oscillation decay and then used to adjust the V material cracker valve opening. Simulations compared well with experimental data in both open and closed loop. Investigations are currently under way to use a photoemission (PE) sensor in place of the RHEED sensor. Hopefully results will be available at the time of the AVS conference. @FootnoteText@ @footnote 1@ Research supported by DARPA, Applied Computation & Mathematics Program.

11:20am **MS-ThM10 Data Requirements and Communication Issues for Advanced Process Control*, R.J.M. Markle,*** *E.C.J. Coss, Jr,* AMD **INVITED**

Data streams and communication issues are the most critical areas for successful Advanced Process Control (APC) programs. These areas are vital for both APC run-to-run controllers and Fault Detection and Classification (FDC) systems used for high volume manufacturing applications in the semiconductor industry. All APC systems rely on data streams to make their process changes, to keep the process on target and in control, and to otherwise signal a need for engineering involvement to make similar corrective actions. The access to, communication of, and reliability and integrity of these data streams are essential to all APC programs. APC run-to-run controllers use the data to make changes in the process. FDC systems focus on predicting pending equipment- or process- related problems or detecting them quickly when they occur. The inability to access the needed data stream can prohibit the use of APC run-to-run controllers or FDC systems on critical process operations. Worse yet, the use of unreliable or corrupted data can cause undesirable consequences. In order to better capitalize on the improvements demonstrated with APC run-to-run controllers and FDC systems, end users have often had to create their own communication and data processing methods. The first decade of the 21st century will place increased demands on process and metrology equipment manufacturers, APC software and hardware suppliers, and APC programmers. Improvements in these areas through the use of industry standards and best known methods could greatly accelerate the APC field. Wafer-to-wafer and within wafer process control could be essential for 300 millimeter wafer and large flat panel processing will need these improvements. We will discuss examples that Advanced Micro Devices (AMD) experienced in Fab25 within the past year. The case studies relate to complex but necessary methods to get the data we need for a FDC system and the role of metrology data on APC run-to-run controllers. Data and communication requirements for the next three to five years will also be discussed. The increased demands on current process and metrology systems will increase as we begin to use new and alternative technologies to support more advanced APC strategies.

Author Index

Bold page numbers indicate presenter