

# Thursday Evening Poster Sessions, November 16, 2006

## Applied Surface Science

### Room 3rd Floor Lobby - Session AS-ThP

#### Aspects of Applied Surface Science Poster Session

**AS-ThP1 TOF-SIMS Analysis of pH Dependent Structure of Protein-A Immobilized on ITO Coated Substrate, N. Kato, M. Higuchi, Seikei University, Japan; S. Aoyagi, Shimane University, Japan; M. Kudo, Seikei University, Japan**

It is known that the environmental conditions, such as pH and temperature, control the reactivity of the protein immobilized on the biosensor surface. For example, at pH < 3.0, protein-A which is used as antigen for immunosensor can not bind to immunoglobulin-G (IgG). In contrast, for pH = 7.0, protein-A can bind to IgG. To explain this difference on reactivity, it is important to examine the structural change of protein-A caused by varying pH condition. Time-of-flight secondary ion mass spectrometry (TOF-SIMS) is one of the most useful techniques for the investigation of biomaterial surfaces because of its ability to provide detailed molecular information on material surfaces. However the TOF-SIMS spectra of protein samples are very complex with multiple fragments resulting from each of the 20 amino acids. It was shown that information theory can select the appropriate peaks of secondary ions characterizing samples out of numerous candidate peaks in the TOF-SIMS spectra with the calculation of mutual information. In this study, the structural change of protein-A caused by varying pH condition was analyzed by TOF-SIMS with the information theory and principal component analysis (PCA). PCA of the TOF-SIMS spectra from protein-A immobilized on ITO coated glass showed explicit distinction between the chemical structures at pH=7.4 and pH=3.0. The calculation of mutual information for TOF-SIMS spectral data at the two pH conditions provided specific peaks related to protein-A at each pH condition. From comparison between the variation of the specific peaks at each pH condition and the amino acid sequences of Protein-A, the structural change of protein-A caused by varying the pH condition will be discussed. @FootnoteText@ @footnote 1@S. Aoyagi, M. Hayama, U. Hasegawa, K. Sakai, M. Tozu, T. Hoshi, M. Kudo, J. Surf. Sci. Nanotech. 1, 67 (2003).

**AS-ThP2 ToF-SIMS as a Reliable Tool for Cyanobacterial Toxic Molecules Research, C. Bittencourt, H. Sarmento, J.-P. Descy, J.-J. Pireaux, L. Houssiau, University of Namur, Belgium**

In a previous work@footnote 1@ we have demonstrated that ToF-SIMS (Time-of-Flight Secondary Ion Mass Spectrometry) is a reliable tool to probe bixin, a natural carotenoid used as food colorant, present in bixa orellana seeds. In this work, we have applied the technique to the analysis of cyanobacterial toxic molecules. Toxin production by cyanobacteria is a prominent research topic due to the increasing occurrence of these organisms following eutrophication and global warming as well as due to its association with human diseases such as amyotrophic lateral sclerosis/Parkinsonism dementia complex (ALS/PDC). Among several toxins that threaten the current life microcystins and  $\beta$ -N-methylamino-L-alanine (BMAA) come into view as important cases of studies due to their proximity to human life. To assess the specific hazards of cyanobacterial toxic molecules it is necessary to understand their chemical and physical properties. We show that ToF-SIMS can be used as an important complementary tool in the characterization of cyanobacterial toxic molecules. Standards were studied in order to obtain reference spectra. We found that the parent molecules are readily detected by means of (M) and (M+1) molecular ions. The spectra recorded on the BMAA exhibit high intensity peak m/z 118, which can be related to the parent molecule along with mass ions fragments which can be understood from the molecular structure. Similar results were found for Microcystin-LR; the parent molecule at m/z 995.56 and its related fragments. The sensibility of the ToF-SIMS to analyze cyanotoxins shows that this technique is a potential tool for its analysis. @FootnoteText@@footnote 1@L. Houssiau, M. Felicissimo, C. Bittencourt and J.J. Pireaux, Appl. Surf. Sci. 231-232 (2004) 416.

**AS-ThP3 High Resolution Mass Spectrometric Analysis of Non-Dehydrated Biological Samples, H.F. Arlinghaus, J. M@um o@ller, C. Kriegeskotte, D. Lipinsky, Universit@um a@t M@um u@nster, Germany**

ToF-SIMS and laser-SNMS are increasingly important tools for analyzing the elemental and molecular distribution in biological samples. However, in-vivo analyses of tissues or cell cultures are impossible because the sample must accommodate the vacuum conditions of the instrument. Thus, fixing the sample in its vital state, such as freezing, is essential. Sample preparation by cryofractioning or cryosectioning techniques followed by

freeze-drying has been successfully used. However, these techniques exhibit several limitations. In order to overcome these limitations, a combination of a ToF-SIMS/laser-SNMS instrument and an in-vacuum cryosectioning instrument was developed for directly preparing and analyzing frozen non-dehydrated samples. In our presentation, we will discuss various sample preparation techniques for analyzing cell cultures and tissue samples and the possibility of obtaining 3D molecular images of frozen biological samples. Particularly, we will show that the analysis of frozen non-dehydrated samples with an in-vacuum preparation technique for exposing the interesting layers of the sample and creating pristine surfaces offers several advantages in comparison to techniques using freeze-dried samples. However, the analysis of cold samples may lead to problems with especially H@sub 2@O adsorption onto the cold surfaces. This is avoided by using a special temperature treatment. Our analysis showed that increasing the temperature to around -110 °C removes the adsorbed water from the top surface. At this temperature freeze-drying effects are not significant enough to influence the measurements during normal analysis times.

**AS-ThP4 Conformational Susceptibilities of Peptides at Interfaces, W.K. Browne, R.L. York, O. Mermut, P.L. Geissler, G.A. Somorjai, University of California at Berkeley**

We have used a combination of surface-specific experimental techniques and molecular simulations to examine the adsorption of short chain polypeptides at hydrophilic and hydrophobic interfaces. Sum frequency generation (SFG), a non linear optical spectroscopy, in concert with Monte Carlo simulations provide insight into the effect of adsorption on polypeptide conformation. Since hydrophobic phenomena are known to have a large effect on any peptide system, our simulations include an explicit coarse-grained solvent. Particularly, the structural features of polylysine at the hydrophobic and hydrophilic interface have been examined. In addition, key forces in the adsorptive behavior of poly-lysine are isolated. Using the data from computer simulations and SFG spectra, the structural characteristics of short chain polypeptides at hydrophilic and hydrophobic interfaces will be presented.

**AS-ThP5 Investigation of the Use of IR Ellipsometry for the Detection of Biological Molecules, S. Sarkar, University of Nebraska, Sweden**

FTIR spectroscopy has been in wide spread use for the detection and identification of the definitive 'fingerprints' of molecules for some time now. Most applications of FTIR spectroscopy have been limited to utilizing and interpreting mostly transmitted and reflected intensities either in terms of relative intensities or as circular dichroism changes. Thin films formed by biological molecules have thus been investigated and limited use of ellipsometric analysis made. The limited use mainly attributable to the limitations of the method as well as the esoteric theory and modeling required in interpreting the results. In our current work, we investigate the use of an attenuated total internal set up to perform IR ellipsometry on a few model biological molecules and present preliminary data obtained there off. Molecules of interest were chiefly human albumin, immunoglobulin and fibrinogen.

**AS-ThP6 Surface Potential Imaging of Self-Organized DNAs acquired by Kelvin Probe Microscopy, T. Ishizaki, N. Saito, O. Takai, Nagoya University, Japan**

Bioelectronics has been known as a frontier in electronics since biomolecules have attractive functions, which may not be artificially created. Generally, biomolecules work in self-organized units. Novel devices with complex or fuzzy functions would be fabricated when biomolecule is mounted on electronic devices. At first, the basic characteristics of biomolecules on various surfaces must be evaluated toward such technical innovations. There are some reports on the self-organized structures and mechanical properties of biomolecules with atomic force microscopy (AFM) and scanning tunneling microscopy (STM). However, the electric properties have not yet been evaluated by 2-dimensional images, since it is difficult to acquire such images. Kelvin probe force microscope (KPFM) is a powerful tool for measuring microscopic surface potential. In this study, we aim to acquire surface potential images of self-organized DNAs. The DNA sample used in this research was poly(dA-dT)@sub n@poly(dA-dT). The DNA was dissolved in ultrapure water (18.2 M@) or 0.1 mM MgCl2. The solutions of 10 Åµl were dropped onto Si(111) substrate, amino-terminated Si(111) substrate or HOPG. The sample solution was allowed to remain on the substrates for 1min and it was then blown off with air. The surface potential images of the samples were acquired by Kelvin probe force microscopy (KPFM). We first observed that the network structure of DNA was formed. The mean height of DNA was 1.2 nm, indicating that the

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clusters mainly comprised a single layer of DNA molecule. This may be due to an attractive electrostatic force between the substrates and the phosphate group of DNA. The clear surface potential images of self-organized DNA on Si and HOPG were acquired under the condition of an a.c. voltage of 2 V and a frequency of 23 kHz. The surface potential of DNA was c.a. 10 mV higher than that of Si substrate, while it was c.a. 20 mV lower than that of HOPG.

## **AS-ThP7 Surface Potential Measurement of Human Hair using Kelvin Probe Microscopy, R. Lodge, B. Bhushan, The Ohio State University**

Surface charge of human hair has a significant effect on manageability, feel, and appearance. For this reason, controlling charge buildup to improve these factors is an important issue in the commercial hair care industry. In this study the surface potential of human hair is measured using the Kelvin Probe method with an atomic force microscope (AFM). Charge is induced triboelectrically by rubbing lightly with a silicon AFM tip. The potential is then measured with a conductive tip over an area containing the charged surface. Caucasian virgin (undamaged), chemically damaged, and mechanically damaged hair samples are studied to determine the effect of damaging treatments on surface charge properties. Virgin samples of African and Asian subjects were measured to determine if ethnicity dependence exists. Samples treated with commercial conditioner as well as those treated with an amino silicone conditioner are also studied to determine the effect of conditioner treatment. Similarly, the effect of surrounding environment is studied by varying the relative humidity and temperature of the sample during both charging and surface potential measurement. The contrast in electrical properties between cuticle scale edges and cuticle surface is also presented. Electrical, chemical, and mechanical mechanisms for the given results are discussed and recommendations given.

## **AS-ThP8 Fabrication of Nanoscale Craters In PMMA Due to Exposure to Condensing Solvent Vapor, C.M. Bates, S.C. Langford, J.T. Dickinson, Washington State University**

When cooler surfaces are exposed to hot vapors, nucleation of tiny droplets can occur. We exploit this condensation to explore the consequences of exposure of poly(methyl methacrylate) films to formic acid vapor. After rapid evaporation of these droplets we observe the surface with atomic force microscopy. The surface is dramatically modified by the formation of nanometer scale craters. Careful image analysis suggests that the mechanism is a combination of two processes: (a) dissolution and transport of polymer to the rim of the crater, similar to the formation of coffee stain patterns described by Deegan, and (b) densification of the polymer during resolidification. Such features could be useful for modifying the surface properties of the polymer, serve as molecular reservoirs, and possibly modify the mechanical properties of the surface.

## **AS-ThP9 Surface Characterization for MEH-PPV of Difference Molecular Weight Analyzed by XPS and SPM, N. Keiichi, I. Yoshitoki, O. Toshiyuki, JEOL Ltd., Japan**

It is well known that x-ray photoelectron spectroscopy (XPS) is a meaningful analytical technique for the chemical characterization of polymer compounds. In particular, surface segregation occurs by a change of molecular weight in polymer. Recently, the development of organic EL materials advances, and the characteristic of these materials are analyzed by various analysis instruments. Usually, structural analysis of organic EL materials is investigated by GC-MS and NMR. On other hand, XPS is used for surface chemical composition analysis mainly. However, organic EL materials are different in a characteristic by a difference of molecular weight. In particular, EL luminous efficacy of high polymer materials shows molecular weight dependence. In this work, we examined the chemical bonding state and structure of different molecular weight organic EL material. We have investigated MEH-PPV [poly(2-methoxy,5-(2-ethyl-hexyloxy)-p-phenylenevinylene)] of different molecular weight. This MEH-PPV die formation with THF solvent on ITO film. X-ray photoelectron spectrometer used for this experiment is JPS-9200 (JEOL.Ltd.), and the measurement condition is as follows. X-ray used this measurement is AlK $\alpha$  monochromatic x-ray, and energy resolution for each elements is 0.65 eV. The surface was observed with SPM (JSPM-5400, JEOL Ltd.). The next results were provided from XPS measurement. It was observed that the amount of C-O group decreased with increase of molecular weight, and CH peak intensity and FWHM of CH peak increased. After decrease of surface segregation, as for the increase of CH peak intensity and FWHM, recombination of hole and electron occurs in CH intramolecule.

## **AS-ThP10 Application of a Recent Algorithm to Patterned Polymer Overlayers, S. Hajati, S. Tougaard, University of Southern Denmark; J.J. Coultas, C. Blomfield, Kratos Analytical Ltd, UK**

Initial studies have shown the potential of a recent algorithm<sup>1</sup> for the processing of XPS image data.<sup>2</sup> The algorithm lends itself to automated data processing, essential for the practical analysis of XPS images. Application of the algorithm determines both the total amount of atoms within the outmost 3 inelastic mean free paths and an estimation of their depth distribution. In this work we extend the application of the algorithm to a series of samples with overlayers of known thicknesses to produce a more accurate indication of the depth distribution. The resultant images show both the amount and depth distribution of each element. We also look at ways of streamlining the data acquisition to develop this in to a practical technique for producing thickness maps. <sup>1</sup>S. Tougaard, J. Vac. Sci. Technol. A21, 1081 (2003) <sup>2</sup>S. Hajati, S. Coultas, C. Blomfield, S. Tougaard, Surf. Sci. (2006).

## **AS-ThP12 Applications of ToF-SIMS in a Research and Development Laboratory, V.S. Smentkowski, S.G. Ostrowski, GE-GRC-N**

Time of flight secondary ion mass spectrometry (ToF-SIMS) has a number of desirable characteristics for surface analysis in a research and development laboratory. In this presentation, we show the benefits of ToF-SIMS analysis via real industrial examples. We will show that ToF-SIMS is able to detect and image species that are below the detection limit for other analytical instruments. We will also show that depth profiles measured on ToF-SIMS instruments are comparable to depth profiles measured on dynamic SIMS instruments. One advantage of performing depth profiles using ToF-SIMS instrumentation is that an entire mass spectrum is saved at each depth and the analyst can perform retrospective analysis and/or multivariate statistical analysis of the entire measured depth profile data set in order to understand the material. In a research and development laboratory, the analyst does not always know a-priori which species should be monitored; we will show that advanced multivariate statistical analysis tools are useful for a complete analysis of the measured data.

## **AS-ThP15 Doping Area Analysis using Atomic Force Microscopy in Si Devices, K.-W. Kim, E.-J. An, K.-Y. Choi, S.-Y. Lee, Hynix Semiconductor Inc., Korea**

In the fabrication of nano-scale silicon devices, accurate doping area characterization is one of the important fields to be solved. Characterization methods such as scanning capacitance microscopy (SCM) and scanning spreading resistance microscopy (SSRM) have provided two-dimensional profiling of the carrier distribution in semiconductors. In this study, the possibility and the effectiveness of applying the atomic force microscopy (AFM)-imaging combined with delineation method are discussed for two-dimensional dopant profiling. Shallow junctions were fabricated in p-type silicon wafers by the implantation of As ions ( $\sim 10^{15}/\text{cm}^2$ ) at an energy of 55keV. Also selective etching was successfully performed using the chemical etching solutions of HF:HNO<sub>3</sub>:CH<sub>3</sub>COOH mixture. We found that different etching rates of the doped regions resulted in a surface topography, height difference and surface roughness. The reason for the visibility of dopant distribution is the relatively strong changes of the etching rate and the stained surface roughness in dependence on the doping concentration. We focused on evaluating an adequate roughness, etch line profile and the junction depth position in the junction area. The resulting dopant profile shapes and junction depth resembled the ones as measured by secondary ion mass spectroscopy (1-D), transmission electron microscopy combined with delineation and SCM (2-D). The spatial resolution of the chemical delineation was extremely good (better than 10nm) due to the capabilities of the AFM-microscope. Especially, dopant depth profiles of arsenic showed the similar values of junction depth ( $\sim 200\text{nm}$ ) at the above methods for a medium dose range. Further investigations are required that the accuracy of the measurement is determined by the repeatability of the etching procedure and the dopant concentration is related to the delineated surface roughness quantitatively.

## **AS-ThP16 Stress in FIB Exposed Si, K.M. Archuleta, D.P. Adams, M.J. Vasile, Sandia National Labs; J.E. Fulghum, University of New Mexico; P.G. Kotula, Sandia National Labs**

Focused Ion Beam (FIB) systems are increasingly utilized for the milling of micro-tools and building of architectures on the nano-scale. It is thus critical to understand the impact of FIB milling on the properties of relevant materials. In this study, high energy (30 keV) focused gallium ion beams are

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used to expose silicon samples. The samples are then removed and analyzed using ex-situ techniques. Compressive stress due to FIB shaping of silicon is investigated through atomic force microscopy (AFM), optical interferometry, tunneling electron microscopy (TEM) and x-ray photoelectron spectroscopy (XPS) measurements.

**AS-ThP17 Quantification of Fe-Ni Alloy Films by XPS, AES and SIMS.** *K.J. Kim*, Korea Research Institute of Standards and Science, Republic of Korea; *D.W. Moon*, Korea Research Institute of Standards and Science, Korea; *C.J. Park*, *H.J. Song*, Korea Research Institute of Standards and Science; *D. Simons*, *G. Gillen*, National Institute of Standards and Technology; *H. Jin*, *H.J. Kang*, Chungbuk National University, Korea

Although XPS and AES are commonly used for the quantitative surface analysis of multi-component materials, quantitative analysis of alloy and compound materials is still difficult because of both the matrix effect occurring in quantification and the surface composition change by ion beam sputtering. Therefore, we need reference materials to ensure reliable analysis. It is more desirable that reference materials should minimize both the matrix effect and the surface composition change during ion sputtering for surface cleaning. Quantification of Fe-Ni alloy thin films was suggested as a new subject for a pilot study in the surface analysis working group of CCQM. Fe-Ni alloy thin films have been developed as the certified reference materials (CRM) for quantitative surface analysis by XPS and AES. Fe-Ni alloy films (Fe28 at%-Ni 72 at%, Fe51 at%-Ni 49 at%, Fe78 at%-Ni 22 at%) were grown on Si (100) wafers by ion beam sputter deposition. The relative compositions of the alloy films were controlled using in-situ XPS analysis. The nominal compositions of the CRMs were certified by inductively coupled plasma-mass spectrometry with the isotope dilution method. SIMS depth profiling using a C<sub>60</sub><sup>+</sup> ion source showed uniform depth distributions of relative compositions. The Fe concentrations of the three specimens selected from the center, medium and edge of the 6 inch wafer showed a good agreement within the relative standard deviation of 0.05 %. In this study, some preliminary results for the CCQM pilot study will be presented. The quantification of Fe-Ni alloy films was performed by XPS, AES and SIMS. Sputtering of Fe-Ni alloy films with 0.5 - 5 keV Ar ions showed no severe modification in surface compositions. For nominal surface composition and measured composition, the calibration curves of the alloy compositions by XPS, AES and SIMS showed almost identical slopes within the range of 1.01 - 1.03.

**AS-ThP18 Epitaxial Growth of NbN and MgO Films for Superconducting Single Photon Detectors and Josephson Junction Qubits.** *J.S. Kline*, *S. Oh*, *R.H. Hadfield*, *A. Lita*, *S.W. Nam*, *D.P. Pappas*, National Institute of Standards and Technology

The growth of ultrathin epitaxial aluminum oxide tunnel barriers on Re has been proven to reduce the number of spurious resonators in Josephson phase qubits when compared to qubits fabricated with amorphous tunnel barriers. Other epitaxial tunnel barrier materials such as MgO may also improve device performance. The superconductor NbN is latticed matched to MgO and was studied in this work. The NbN/MgO material system is also well suited for superconducting single photon detectors and NbN thin films were grown for this purpose. Niobium nitride films were deposited on MgO substrates by UHV reactive sputtering in an argon/nitrogen gas mixture. Magnesium oxide tunnel barriers were deposited by RF sputtering and also by reactive evaporation of magnesium in a controlled oxygen background. To achieve epitaxy, the substrate was held at elevated temperature during the deposition. Surface science tools such as Auger electron spectroscopy, scanning tunneling microscopy, and reflection high energy electron diffraction were used for in-situ analysis of the grown films.

**AS-ThP19 Large-Area Pulsed-Laser-Deposition of Dielectric and Ferroelectric Thin Films.** *S. Sakai*, *M. Takahashi*, *K. Motohashi*, *Y. Yamaguchi*, *N. Yui*, *T. Kobayashi*, National Institute of Advanced Industrial Science and Technology, Japan

Pulsed laser deposition (PLD) is a successful method for obtaining high quality films of various kinds of materials, and has an advantage of clean deposition without impurities of undesired element (e.g., carbon) in the films. However, the PLD method tends to show poor uniformity of film thickness mainly due to small laser-ablation plume, thus PLD has not been regarded as a good method for large-area thin-film depositions. In order to improve the thickness uniformity, we recently developed the PLD technology using a prototype machine of VPLD-8000 (Vacuum Products Co Ltd) and succeeded in depositing large-area films of high-k dielectric HfO<sub>2</sub> and ferroelectric SrBi<sub>2</sub>Ta<sub>2</sub>O<sub>9</sub> (SBT) on Si wafers. In this work, we demonstrate good thickness uniformity of 8 and 6inch HfO<sub>2</sub> and 4inch SBT films. The HfO<sub>2</sub> was deposited at

room temperature in 13Pa N<sub>2</sub>. The SBT was deposited at 400°C in 13Pa O<sub>2</sub>. Standard deviations of the thicknesses all over the 42nm-thick 8inch HfO<sub>2</sub>, 6nm-thick 6inch HfO<sub>2</sub>, and 94nm-thick 4inch SBT were 1.3%, 1.6%, and 1.2%, respectively. Cross-sectional TEM showed that an interfacial layer between HfO<sub>2</sub> and Si was thinner than 1nm in the 6nm-thick 6inch HfO<sub>2</sub>. Standard deviation of accumulation-mode capacitances was 1.9% for Pt/HfO<sub>2</sub>/Si MIS diodes, which were fabricated by evaporating Pt top electrodes on a diametrical line of the 6nm-thick 6inch HfO<sub>2</sub> and annealing at 700°C in N<sub>2</sub> for 10 min. In our PLD technique, KrF laser beam is aligned parallel to a face-down substrate surface, and a 3x12cm<sup>2</sup> ceramic target is set to be inclined to the substrate surface by 30°. Since the substrate does not block off the incident laser beam, available Si wafer size is easily extendable to 300mm in diameter. Therefore, our developed PLD technique meets industrial needs of high and uniform qualities over large area of high-k dielectric and/or ferroelectric thin films for LSIs.

**AS-ThP20 Ordered Au(111) Surfaces Grown on Si(111).** *K. Pedersen*, *A. Silva*, Aalborg University, Denmark; *P. Morgen*, University of Southern Denmark, Denmark; *Z.S. Li*, University of Aarhus, Denmark

Gold surfaces are the primary choice as substrate in studies of organic structures on surfaces since they are stable in various biochemical environments and allow attachment of biomolecules through thiol groups. Typically, surfaces of bulk Au crystals or thin films on Mica are used. However, formation of well-ordered thin Au films on Si would be a step in the direction of direct integration of biosensors on wafers containing Si electronics. Deposition of Au directly on Si leads to formation of a disordered surface layer containing a mixture of Si and Au that floats on top of the Au layer even for relatively thick Au films. In the present work the properties of thin Au films grown on top of a thin (7 layers) Cu film as a buffer between the Si substrate and the Au overlayer are described on the basis of photoemission spectroscopy and AFM. Previous investigations have shown that the Cu buffer layer improves the growth of Ag and Al relative to direct growth on clean Si(111)7x7. For both Ag and Al the Cu buffer layer leads to improved sharpness of quantum well (QW) peaks and surface states. The present experiments demonstrate that also in the case of Au deposition a thin Cu layer improves the film properties. A sharp Au(111) LEED pattern is observed even for films that are only a few layers thick. The Shockley surface state characteristic of Au(111) surfaces appears at a binding energy of 0.5 eV. Furthermore, structures appear that disperses toward the sp-band edge 1.1 eV below the Fermi level as the film thickness grows. This is characteristic of QW levels. The energy window for observing QW effects is narrow in Au compared to for instance Ag and Al where the sp bands extend over ~4 eV. In Au the window from the sp-band edge to the onset of the d-bands is less than 1 eV. The appearance of QW levels indicates flat domains on the atomic monolayer level. This is supported by AFM and STM investigations performed ex situ on the samples investigated by photoemission.

**AS-ThP21 Aluminum Induced Crystallization (AIC) of Amorphous Silicon.** *H.M. Meyer*, Oak Ridge National Laboratory; *K. Sharif*, *H. Naseem*, *H.H. Abu-Safe*, *W.D. Brown*, University of Arkansas

A process for producing epitaxial Si thin films using the method of aluminum induced crystallization (AIC) of amorphous silicon (a-Si) was investigated. AIC holds promise for producing polycrystalline Si (p-Si) on inexpensive glass and plastic substrates. TEM and Auger analysis have shown that these efforts were successful. Initial results from Auger depth profiles showed that while we achieved a good measure of the composition versus depth, reproducing the data was difficult, even from a small area on the same sample. The complexity of these systems was revealed by interrupting the depth profiles and mapping the lateral distribution of Si, Al, and O. These 2-D maps readily showed that the distribution was more complex than anticipated. A second set of samples, prepared to bracket the optimum AIC anneal time for a given temperature, was analyzed by Auger microanalysis to further explore the nature of the Al/Si intermixing. All of the samples for this group were prepared by depositing a 300 nm Al layer onto the Si wafer, followed by a 300 nm layer of a-Si. This poster will present results for samples annealed at 525°C for times ranging from 0 min to 120 min. Auger elemental maps of a cross-section for a sample no annealing showed individual layers, with a-Si on top. Depth profiles for annealed samples clearly show changes occurring on the surface after 10 min of annealing and that further annealing drives the AIC process. Research sponsored by the Assistant Secretary for Energy Efficiency and Renewable Energy, Office of FreedomCAR and Vehicle Technologies, as part of the High Temperature Materials Laboratory User Program, Oak

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## AS-ThP22 MD/MC Simulations of Reactive Sputtering Deposition of Amorphous SiO<sub>2</sub>, M. Taguchi, S. Hamaguchi, Osaka University, Japan

Silicon Dioxide (SiO<sub>2</sub>) thin film deposition processes were studied with the use of classical Molecular Dynamics (MD) simulations combined with Monte Carlo (MC) simulations. The effects of the incident energy and angle of deposition species on film properties and high energetic argon ions during reactive sputtering deposition processes for amorphous SiO<sub>2</sub> are examined. From the simulation results, it has been confirmed that some properties of the deposited film strongly depend on the incident energy and angle of Si atoms sputtered from the target. For example, the film density is shown to become lower at lower Si incident energy and larger Si incident angles. The stoichiometry of the film expressed by the ratio of the number of O atoms to that of Si atoms contained in the film has been also shown to increase as the Si incident energy decreases and Si incident angle increases. In other words, as the vertical momentum of Si atoms becomes small, the film becomes more oxygen rich and porous. Possible physical mechanisms causing these effects are also discussed from the viewpoint of motion of incident Si atoms interacting with the surface atoms. It is also confirmed that additional injections of highly energetic argon ions further press the SiO<sub>2</sub> thin films to make them denser. If the argon incident kinetic energy is sufficiently high, however, etching of the deposited films also takes place.

## AS-ThP23 Development of Closed Field Reactive Magnetron Sputtering for Multilayer Optical Coating, J.M. Walls, D.R. Gibson, E.M. Waddell, Applied Multilayers Ltd, UK

Closed Field reactive magnetron sputtering has been used for many years to produce state-of-the-art tribological and wear resistant coatings. In this paper, we report on its recent development and application to multilayer optical coatings. Optical coatings require precise control of the stoichiometry of dielectric metal oxides and layer thickness control within sub-nanometre tolerance. The process operates with metal targets and although the targets are partially oxidised the deposition rates are close to the metal mode. This requires the use of pulsed dc power and a new hysteresis control strategy based on monitoring target Voltage. Thickness control is achieved using time only. In addition, the process incorporates shutters to allow target pre-conditioning and fine interface control. In addition to describing the new process, this paper will discuss the optical properties of a range of optical materials including dielectrics such as SiO<sub>2</sub>, Nb<sub>2</sub>O<sub>5</sub>, TiO<sub>2</sub>, ZrO<sub>2</sub> and Al<sub>2</sub>O<sub>3</sub> together with important transparent conducting oxides such as indium tin oxide (ITO). The Closed Field technique produces reactive plasma conditions that combine low energy (5mA.cm<sup>-2</sup>) to provide ideal conditions for thin film growth with the further advantage that the vacuum hardware is relatively simple and there is no requirement for an auxiliary ion or plasma source. The process produces non-absorbing, dense, spectrally stable coatings that are also exceptionally smooth (rms roughness typically

## AS-ThP24 Advanced Process Modelling of the Rotating Magnetron, O. Kappertz, T. Kubart, T. Nyberg, S. Berg, Uppsala University, Sweden

Thin films of transition metal oxides and nitrides find numerous applications in modern technology, for example as antireflective or protective coatings in architectural glazings. Frequently such films are deposited by direct current reactive magnetron sputtering, and for large area coatings rotatable magnetron systems are commonly used. The rotation of a cylindrical target around a fixed magnet system leads to a uniform target erosion, and thereby more efficient material utilization and extended target lifetime. In such a setup a fixed point at the target surface is periodically exposed to sputter erosion, while for the rest of the period compound is formed at the target surface due to its exposure to the reactive gas. Recently a simplified analytical model has been proposed, which describes how several parameters, like the speed of the target rotation, size of the sputter zone and the current density, influence the compositional balance between compound formation and removal. In this report, the model is extended by including a full numerical simulation of the dynamical balance between sputter erosion and compound formation by both chemisorption and ion implantation. The influence of the target rotation on processing characteristics is discussed and compared to experimental observations.

## AS-ThP26 Decomposition of Titanium Deuteride Films Protected by Ultra-Thin Pd Layers; Thermal Desorption Kinetics Studies Combined with Microstructure Analysis of Bimetallic Films, W. Lisowski, Polish Academy of Sciences, Poland; E.G. Keim, University of Twente, The Netherlands, Netherlands; A.H.J. van den Berg, M.A. Smithers, University of Twente, The Netherlands; Z. Kaszukur, Polish Academy of Sciences, Poland

Thin titanium films can be applied as hydrogen storage material due to titanium hydride formation. Exposing hydrated Ti films to ambient conditions leads however, to a partial decomposition of titanium hydride. This can be prevented by covering such films by Pd. Here we present the results of TDMS, XRD, SEM, TEM and XPS, dealing with the question as to how TDMS controlled decomposition of titanium deuteride (TiD<sub>2</sub>) from films protected by Pd proceeds, and how TDMS heating affects the interface and bulk structure of such bimetallic films. TiD<sub>2</sub> films were prepared in UHV conditions at 300 K by exposing 100 nm thick Ti films to D<sub>2</sub>. The TiD<sub>2</sub> phase formation which results from this volumetrically controlled adsorption procedure, previously detected by ToF-SIMS, was now confirmed by XRD. The TiD<sub>2</sub> film was subsequently covered in-situ by a 6-20 nm thick Pd layer. Desorption of D<sub>2</sub> was monitored in situ by TDMS (see Ref. 4 for a description), all other analyses ex situ. It was found that a Pd layer, protecting the TiD<sub>2</sub> films, only slightly changes the thermal desorption kinetics of TiD<sub>2</sub> from the TiD<sub>2</sub> films. Thermal decomposition of TiD<sub>2</sub> is accompanied by a structural transformation of TiD<sub>2</sub> into an  $\alpha$ -Ti phase, resulting in less plastically deformed Pd/Ti films. However, we observed also TDMS heating induced intermixing of Pd and Ti phases within the Pd/Ti interface. Complex structures, including Moiré patterns, have been identified. W. Lisowski, A.H.J. van den Berg, M.A. Smithers (1998) Surf. Interface Anal. 26, 213 (1998). W. Lisowski, E.G. Keim, A.H.J. van den Berg, M.A. Smithers, Anal. Bioanal. Chem., in press. W. Lisowski, A.H.J. van den Berg, D. Leonard, H.J. Mathieu, Surf. Interface anal. 29, 292 (2000). W. Lisowski, E.G. Keim and M.A. Smithers, J. Vac. Sci. Technol. A21, 545 (2003).

## AS-ThP27 Photocatalytic Decomposition of CH<sub>3</sub>OH on TiO<sub>2</sub> Sputter Films Prepared by Changing Ar/O<sub>2</sub> Ratio and Working Gas Pressure, T. Takahashi, K. Prabakar, University of Toyama, Japan; T. Nakashima, Kashiwa Chuo High School, Japan; Y. Kubota, University of Yokohama City, Japan; A. Fujishima, Kanagawa Academy of Science and Technology, Japan

TiO<sub>2</sub> has attracted considerable attention as a photocatalyst with strong activity. We found that TiO<sub>2</sub> sputtered films prepared under heavy plasma exposure exhibited good photocatalytic decomposition of CH<sub>3</sub>OH. However, the TiO<sub>2</sub> films showed less than perfect transparency because of the slightly opaque surface. For practical use, transparency is desirable. In this study, to deposit transparent TiO<sub>2</sub> films, the substrates were placed at a position removed from the plasma. TiO<sub>2</sub> films were deposited on glass slide substrates. The ratio of Ar to O<sub>2</sub> (G<sub>Ar</sub>) were 9:1, 8:2, 7:3 and 6:4. The crystallographic and surface structures and optical properties of TiO<sub>2</sub> films deposited at working gas pressures (P<sub>subW</sub>) ranging from 0.2 to 0.8 Pa were investigated in detail. The decomposition of gaseous methyl alcohol was performed to investigate the dependence of the photocatalytic reactions on the structures and properties of the TiO<sub>2</sub> films. In all of the TiO<sub>2</sub> films, only the A(101) diffraction peak was observed from the x-ray patterns, where A indicates anatase TiO<sub>2</sub>. The crystallinity improved greatly with decreasing P<sub>subW</sub>. The transmittances of all of the TiO<sub>2</sub> films were constant at 80-90 % for wavelengths in the range of 900 nm to 380 nm. The as-deposited TiO<sub>2</sub> films successfully photocatalyzed the decomposition reaction of CH<sub>3</sub>OH to CO<sub>2</sub> and H<sub>2</sub>O, according to the infrared transmittance spectra. The decomposition rate using the TiO<sub>2</sub> films increased with increasing P<sub>subW</sub>. For the TiO<sub>2</sub> films deposited at a P<sub>subW</sub> value of 0.8 Pa and a G<sub>Ar</sub> value of 2.3, the CO<sub>2</sub> formation rates were about 2.2 times higher than those prepared at a G<sub>Ar</sub> value of 9 for a solar irradiation time of 130 min. In conclusion, the transparent TiO<sub>2</sub> films deposited in this study are quite photocatalytically active, supporting the decomposition of gaseous methyl alcohol.

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**AS-ThP28 A Short Review on the ESSCR Mechanism for Phosphor Degradation, H.C. Swart, J.J. Terblans, E. Coetsee, O.M. Ntwaeaborwa, M.S. Dhlamini, University of the Free State, South Africa; P.H. Holloway, University of Florida**

Standard cathodoluminescent phosphors normally lose brightness upon bombardment with electron beams. A combination of techniques such as XPS (X-ray photoelectron spectroscopy), AES (Auger electron spectroscopy) and CL (cathodoluminescence) was used to show that the main reason for the degradation in CL intensity is the formation of a non-luminescent dead layer on the surface due to a electron stimulated surface chemical reaction (ESSCR). The decrease in luminance was found to be a result of the growth of the dead layer. Different phosphors which include sulphide-based as well as oxide-based phosphors reacted similar under electron bombardment. When ZnS phosphor powder was exposed to the electron beam in a water-rich O@sub 2@ ambient, a chemically-limited ZnO layer was formed on the surface. A layer of ZnSO@sub 4@ was formed on the surface during the electron beam degradation of the ZnS phosphor powder in a dry O@sub 2@ ambient. The electron stimulated reaction led to the formation of a luminescent SiO@sub 2@ layer on the surface of the Y@sub 2@SiO@sub 5@:Ce phosphor powder. CeO@sub 2@ and CeH@sub 3@ were also detected on the surface. An increase in the CL intensity at a wavelength of 650 nm was measured during the formation of the luminescent SiO@sub 2@ layer. A less effective SiO@sub x@ (0<x<2) matrix layer was the main cause of degradation of the CL intensity of SiO@sub 2@:Ce,Tb nano-phosphor as well as SiO@sub 2@:PbS nano-phosphor.

**AS-ThP29 Synthesis and Characterization of Erbium Doped Metal Oxide Nanofibers for Applications in Thermophotovoltaics, E.T. Bender, R. Wang, M.T. Aljarrah, E.A. Evans, R.D. Ramsier, The University of Akron**

We report on the synthesis, characterization, and near-infrared emission of erbium doped metal oxide nanofibers, for applications in thermophotovoltaics (TPV). Erbium emits radiation selectively in the 6000 to 7000 wavenumber region, which can be converted into electricity by appropriately chosen photocells. Thus, TPV technology enables the direct conversion of thermal energy to electrical energy, with no moving parts. Erbium can be used as a coating on a solid substrate such as metal or ceramic. However, the greybody radiation from the substrate will reduce the overall efficiency of the TPV system, and can lead to excessive heating in the photocell. We overcome this problem by doping metal oxide nanofibers, typically titania, with erbium via an electrospinning process. These doped fibers are characterized with scanning electron microscopy (SEM), X-ray photoelectron spectroscopy (XPS), X-ray fluorescence (XRF) and Fourier transform infrared spectroscopy (FTIR). The structure of the doped nanofiber mats is ideally suited for direct heating in gas-flow applications, such as exhaust systems. Near-IR emission measurements are carried out using a quartz tube, with the self supporting nanofibers heated by the exhaust from a propane flame. We therefore demonstrate the ability of these nanofibers to function in TPV gas flow applications.

**AS-ThP30 Complimentary Information from Auger and EDS Analyses of Particles and Thin Films, S.A. Wight, NIST**

Auger electron spectroscopy (AES) and x-ray spectrometry are complementary: both are the result of a primary electron beam interacting inelastically with specimen atom core electrons. A core electron is ejected and as a higher level electron moves to fill the vacancy, the energy difference between these levels is released either with the ejection of another bound outer shell electron as an Auger electron with a characteristic kinetic energy or as a characteristic x-ray photon. Auger electrons and x-rays are produced throughout a sample volume defined by the beam energy and specimen composition, but the sampling depths are quite different. While x-rays can suffer absorption, those that escape retain their characteristic energy and therefore represent the entire range of generation, which may be micrometers. Because of the simultaneous nature of energy dispersive x-ray data collection, the entire spectrum can be collected at each pixel and post processed for composition. Auger electrons suffer inelastic scattering and so can only travel a small distance in the sample while retaining their characteristic energy. Only the Auger electrons that are created within a few nanometers of the surface have a sufficient mean free path to escape the specimen and be collected for analysis. Auger electrons are measured with a spectrometer that has a narrow energy bandpass and must be sequentially scanned to record the spectral energy range of interest. Auger spectroscopy provides elemental and chemical information because the atomic energy levels involved in Auger emission are also influenced by chemical bonding between atoms. The complementary nature of Auger and x-ray microanalysis with their

different sampling depths can be exploited to view the composition of the bulk and the surface of a specimen.

**AS-ThP31 Atom Probe Characterization of Thin Films, D.J. Larson, Imago Scientific Instruments Corp**

To accelerate research and development cycles for devices dependant on nanoscale materials,@footnote1@ it is important to correlate device microstructure with specific processing conditions and physical properties. In the magnetic storage and semiconductor industries, this is particularly important due to the ever-shrinking characteristic length scales on which devices are being fabricated. Atom probe tomography@footnote2,3@ has the capability to play an important role in this development due to its capability to provide quantitative 3-D atomic-scale imaging together with high analytical sensitivity. Local electrode atom probe (LEAP®) technology combines sub-nanometer spatial resolution with chemical composition at scales on the same order as device structures.@footnote 4@ In this presentation, applications of the LEAP microscope to a variety of nanomaterials systems used in the magnetic recording and semiconductor industries will be presented. These systems include 1) magnetoresistive spin valves and tunnel junctions@footnote 5,6@ which are two structures commonly used to form the "reader" portion of magnetic recording heads, 2) current-confined-path spin valve structures 3) perpendicular recording media in which oxygen is used to isolate magnetically the individual grains in Co-based alloys, 4) ultra shallow dopants implanted in silicon, and 5) silicon-germanium (SiGe) layered structures. @FootnoteText@ @footnote 1@ R. L. Comstock, J. Mat. Sci. Mat. Elec. 13(9) (2002) 509.@footnote 2@ A. Cerezo et al., Rev. Sci. Instrum. 69 (1998) 49@footnote 3@ M. K. Miller, Atom Probe Tomography, Kluwer Academic Publishers, New York, 2000.@footnote 4@ T. F. Kelly et al., Micro. Microanal. 10(3) (2004) 373.@footnote 5@ D. J. Larson, Thin Solid Films 505 (2006) 16.@footnote 6@ D. J. Larson et al., Acta Mater. 52(10) (2004) 2847.

**AS-ThP32 Relative Sputter Rates of Oxide Films: Constancy, Energy and Angle Dependence, A.S. Lea, M.H. Engelhard, D.R. Baer, T. Droubay, P. Nachimuthu, Pacific Northwest National Laboratory**

The increased use of oxide films for a variety of applications has produced a significant interest in knowing the relative rates that different oxides sputter. Because of the wide use of oxide films in our laboratory we have undertaken a series of measurements comparing the relative rates of sputtering of a variety of thin film oxides to a known thickness of SiO@sub 2@ on Si. We have found that these sputter rates differ by more than a factor of two. It is well established for pure materials that the sputter rates significantly change extensively as a function of energy and angle. In addition to the influence of damage that can also alter sputter rates, oxides may be susceptible to various stages of disorder and ion beam induced reduction that may lead to depth dependent changes in sputter rate. In this paper we report a series of measurements to determine the constancy of the oxide sputter rates and the dependence of the relative rates on angle and energy. We are using a number of different oxide films of known thickness, including @alpha@-Cr@sub 2@O@sub 3@, anatase, rutile, and zinc oxide. The oxides have been grown by MBE or PLD and measured by XRR. Time dependent sputter rates are being measured by EDS using a method described by Musket and Strausser.@footnote 1@ The energy and angle dependences are being made by argon ion sputtering in a Phi Quantum 2000 XPS system or a Phi 680 Auger Nanoprobe system that contains an EDS analyzer. @FootnoteText@ @footnote 1@ RG Musket and YE Strausser, Appl. Phys. Lett 37 (1980) 478-480.

**AS-ThP33 Transient Effects during Cs/Ga Dual Beam TOF-SIMS Profiling: Experiment and Simulation, R.G. Vitchev, J. Brison, L. Houssiau, Facultes Universitaires Notre-Dame de la Paix, Belgium**

Cs@super +@ sputtering beams are widely used in TOF-SIMS dual beam depth profiling. Loading the surface with Cs increases the negative ion yields and leads to formation of MCs@super +@ secondary ions (M stands for matrix). It was shown that the MCs@super +@ ions are suitable for quantitative analysis since they are relatively insensitive to matrix effects. Secondary ion yields change dramatically in the initial stage of the Cs bombardment due to the increase of the amount of implanted Cs in the surface until a steady-state is reached. This could be a problem if ultra-thin (nm) layers are analyzed. Having a better understanding of these transient phenomena is therefore crucial for such applications. In this work the secondary ion emission from Si H-terminated surface sputtered by Cs@super +@ ions (250 eV - 1 keV, 45°) and analyzed by 15 keV Ga@super +@ ions was studied. Xe@super +@ (350 eV) sputtering was used to determine the depth profile of the implanted Cs at steady-state. The steady-state Cs surface concentration was measured by XPS. A dynamic

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TRIM code was used to simulate the sputtering and composition change of the Si target under Cs bombardment and obtain the energy/velocity distribution of the atoms sputtered by the analyzing Ga beam. These results, combined with the electron tunnelling model for ion formation, were used to calculate the secondary ion yield at different Cs doses. The results were compared to those obtained experimentally.

## AS-ThP34 Preliminary Report of Evaluation of Automated Peak Detection Procedure in X-ray Photoelectron Spectra, M. Suzuki, ULVAC-PHI, Inc., Japan; S. Fukushima, S. Tanuma, NIMS, Japan

X-ray photoelectron spectra should be analyzed to detect peaks prior to elemental/chemical assignment and the peak detection routine has been discussed in ISO/TC201/SC3 activity. It is needed to estimate its effectiveness of the software as well as the uncertainties of the results and it has been investigated in VAMAS activity. Prior to the world-wide interlaboratory study, the preliminary investigation was performed to make artificial spectral data and analyze their efficiency using a peak detection software routine that included the three algorithms with (1) second derivative method, (2) peak-to-background method, and (3) background estimation method. Test spectra were composed from the actually measured Au, Ag, and Cu spectra and the artificially noise-superposed spectra were also composed. The number of the basic spectra is three for the mixing ratio of (Au, Ag, Cu) as (1, 1, 1), (1, 0.1, 0.01), and (1, 0.01, 0.001). The noise-superposed spectra have been prepared for each basic spectrum, considering the noise level and the randomization for each noise level. These basic and noise-superposed spectra were analyzed for peak detection using the software built according to the algorithms above mentioned. The number of detected peaks and the efficiency that is the relative number against the detection number by eyes have been compared for the three basic spectra. The quality of (1, 1, 1) is shown to be different from the other two spectra of (1, 0.1, 0.01), and (1, 0.01, 0.001). For the spectrum of (1, 1, 1) the second derivative method gave a large number of detected peaks than the others. On the other hand, for the spectra of (1, 0.1, 0.01), and (1, 0.01, 0.001) the background method gave a greater number of peaks than the other methods. The number of detected peaks for the noise-superposed spectra drastically decreased from those for the basic test spectra. Detailed results and investigations will be presented and discussed at the conference site.

## AS-ThP35 Calculations of Electron Inelastic Mean Free Paths In 12 Organic Compounds and 15 Inorganic Compounds Over the 50 - 30,000 eV Energy Range, S. Tanuma, National Institute for Materials Science (NIMS), Japan; C.J. Powell, D.R. Penn, National Institute of Standards and Technology

We have calculated electron inelastic mean free paths (IMFPs) for 50-30,000 eV electrons in 12 organic compounds (26-n-paraffin, adenine, beta-carotene, diphenyl-hexatriene, guanine, kapton, polyacetylene, poly(butene-1-sulfone), polyethylene, polymethylmethacrylate, polystyrene, and poly(2-vinylpyridine)) and 15 inorganic compounds (Al@sub 2@O@sub 3@, GaAs, GaP, H@sub 2@O, InAs, InP, InSb, KBr, KCl, LiF, MgO, NaCl, SiC, SiO@sub 2@, and ZnS) using their energy-loss functions and the Penn algorithm. The new IMFPs were calculated at equal energy intervals on a logarithmic scale corresponding to increments of 10 %. These IMFPs could be fitted to the modified Bethe equation for inelastic scattering of electrons in matter for energies from 50 eV to 30,000 eV. The average RMS deviations in these fits were 0.12 % for the 12 organic compounds and 0.62% for the 15 inorganic compounds. These RMS values are almost the same as those found in our fits of IMFPs calculated previously for the 50 - 2000 eV energy range. The new IMFPs were also compared with IMFPs from the TPP-2M equation; the average RMS deviations were 8.1 % for the 12 organic compounds and 18.2 % for the 15 inorganic compounds in the 50 eV to 30,000 eV energy range. These RMS value are almost the same as those found (8.5% for inorganic and 19.1% for inorganic compounds) in similar comparisons for the 50 - 2000 eV energy range. Relatively large RMS deviations were found for LiF (47 %), GaAs (37 %), and InAs (26 %). We conclude that the TPP-2M equation is useful for IMFP estimation in other compounds for energies up to 30,000 eV with an average uncertainty of about 18 %.

## AS-ThP36 Electron Energy Loss Function for Ultra-Thin HfO<sub>2</sub>, Al<sub>2</sub>O<sub>3</sub> and Hf-Al-O Dielectric Films on Si(100), H. Jin, S.K. Oh, H.J. Kang, Chungbuk National University, Korea; S. Tougaard, University of Southern Denmark

Due to the continuous decrease in device size toward atomic dimensions, Si devices are approaching fundamental limits. To avoid quantum tunneling, high-k (high dielectric constant) gate dielectric layer is required to replace SiO<sub>2</sub>. Hf-based transition metal dielectrics have received considerable attention. In particular, high-k alloys, such as aluminate or silicate are

proposed as promising gate dielectrics. Quantitative analysis of reflection electron-energy-loss spectra for ultrathin HfO<sub>2</sub>, Al<sub>2</sub>O<sub>3</sub> and Hf-Al-O dielectric thin films on Si(100) were carried out by using Tougaard Yubero QUEELS- $\hat{\mu}(k, \hat{\nu})$ -REELS package. For HfO<sub>2</sub>, the energy loss function shows peaks in the vicinity of 10, 17, 27, 37 and 47 eV. For Al<sub>2</sub>O<sub>3</sub>, a broad peak at 22 eV with a shoulder at 14 eV and a very mild shoulder at 32 eV were observed, while for the Al<sub>2</sub>O<sub>3</sub> doped HfO<sub>2</sub>, the peak position is similar to that of HfO<sub>2</sub>. This indicates that when Hf-Al-O film is used as a gate dielectric in CMOS transistor, its electronic structure is mainly determined by the d state of Hf. The results of a quantitative analysis successfully reproduced the trend that has been found in the experimental measurements. In addition, the inelastic mean free path (IMFP) was also calculated from the theoretical inelastic scattering cross-section. The IMFP at 300 eV was about 7.05, 9.62 and 8.48 Å. and that at 500 eV was 11.42, 15.40 and 13.64 Å. for HfO<sub>2</sub>, Al<sub>2</sub>O<sub>3</sub>, Hf-Al-O, respectively.

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