Thursday Afternoon, November 6, 2003

Applied Surface Science
Room 324/325 - Session AS-ThA

Electron and Photon Spectroscopies
Moderator: R. Haasch, University of Illinois, Urbana-Champaign

2:00pm AS-ThA1 Spin Polarization Modulation through Circular Polarized Light Modulation, *S. Balaz, L.G. Rosa, H.K. Jeong, P.A. Dowben,* University of Nebraska, Lincoln

Spin-polarized electron sources have important applications in electron spectroscopies. Such electron spectroscopies can provide considerable insight into the spin- polarized electronic structure of magnetic materials. A variation to the spin polarized electron gun, based on photoemission from a GaAs cathode,@footnote 1@ has been designed for spin polarized inverse photoemission and spin polarized electron scattering.@foonote 2,3@ The goal is to improve the emitted electron spin polarization by improving the control of the incident circularly polarized light, and then modulating the light polarization on the photocathode to modulate the spin polarized photocurrent. A solid state laser, of 780 nm wave length, in combination with a retarder was used to generate the circularly polarized light. Scheme for electron spin polarization modulations, through modulating the applied voltage to a liquid crystal retarder, we show that polarization can be modulated as well. Inclusion of such a spin polarized electron gun as part of spin-polarized inverse photoemission and spin-polarized electron energy loss spectroscopies is discussed. @FootnoteText@ @footnote 1@D.T. Pierce, and F. Meier, Phys. Rev. B 13, 5484 (1976) @footnote 2@F. Ciccacci, E. Vescovo, G. Chiaia, S. De Rossi, and M. Tosca, Rev. Sci. Instrum. 63, 3333 (1992) @footnote 3@Takashi Komesu, C. Waldfried, Hae-Kyung Jeong, D.P. Pappas, T. Rammer, M.E. Johnston, T.J. Gay and P.A. Dowben, in: Laser Diodes and LEDs in Industrial, Measurement, Imaging and Sensor Applications II: Testing, Packaging, and Reliability of Semiconductor Lasers V, Edited by Geoffry T. Burnham, Xiaoguang He, Kurt J. Linden and S.C. Wang, Proceedings of the SPIE 3945, 6 (2000) .

2:20pm AS-ThA2 A PRBS-modulated TOF-HREELS Spectrometer with High Throughput and Multiplex Advantage, *B.G. Frederick, Z. Yang, P. Kleban,* University of Maine

We present an analysis of the factors that control the resolution, dynamic range, throughput-, and multiplex advantage of a novel time-of-flight (ToF) pseudo-random binary sequence (PRBS) modulated high resolution electron energy loss spectrometer (HREELS). We describe probability based spectral estimation methods for signal recovery that achieve a throughput advantage of 100-1000, a factor of 8-16 resolution enhancement, and account for the Poisson noise distribution in the measured data. The multiplex advantage achieved depends upon a number of factors, but significantly improves upon the multiplex disadvantage expected with the conventional cross-correlation or Hadamard transform methods when the detector signal is shot-noise limited. We describe how the optical properties of the chopper affect the PRBS modulated data within a theoretical framework and utilize trajectory calculations over an analytical potential to compare with data measured on azimuthally oriented polytetrafluoroethylene (PTFE, or Teflon) films.

2:40pm AS-ThA3 Ab initio Modeling of the Vibrational Spectrum of Adsorbed Cyclopentadienyl Anion, *C.M. Woodbridge, D. Kemp,* Hillsdale College; *D.L. Pugmire,* Los Alamos National Laboratory; *M.A. Langell,* University of Nebraska, Lincoln

Ab initio methods have been used to model the vibrational spectrum of cyclopentadienyl (Cp), a fragment obtained from the decomposition of metallocenes, adsorbed on various substrates. In the present work, the adsorbate-substrate system was modeled using a single atom as the substrate. Vibrational frequencies, bond lengths, and bonding energies for complexes of the form [Mn@super+@Cp@super-@]@supern-1@ where M=Ag, Ni, and Si have been computed. The complexes were constructed to model two different orientations of the adsorbed Cp ring: one where the plane of the Cp ring is parallel to the surface normal and the other where the plane is perpendicular to the surface normal. The computed vibrational frequencies have been compared to vibrational losses observed in HREEL spectra of Cp, produced from the decomposition of nickelocene, adsorbed the Ag(100), Ni(100), and Si(111)-7x7 substrates. Despite the relative simplicity of the model, the calculated vibrational frequencies are in good agreement with the HREEL spectra.

3:00pm AS-ThA4 Photon Angle Dependence of Plasmon Loss Measured by the Double Angular Photoelectron Integrated Analyzer System, *A. Tanaka,* ULVAC-PHI, Inc., Japan; *H. Yoshikawa,* NIMS, Japan; *M. Kimura,* SPring-8 Service, Japan; *S. Fukushima,* NIMS, Japan

Plasmon loss peaks associated with photoelectron peaks from the silicon specimen is measured. The analyzer and the specimen are tilted simultaneously with maintaining the emission angle constant. This tilting effectively changes the incident angle of photons to the specimen. The angle of photon incidence was ranged from 35 to 90 degree. It caused a change of relative intensity of 1st plasmon loss peaks to the original photoelectron peaks. Photon energy was chosen to match the Si 1s photoelectron energy at the Si 2s energy excited by Mg K@alpha@ x-ray. Ellipsoidal andulation is applied for the synchrotron radiation to simulate the x-ray used for X-ray photoelectron spectroscopy. 3 loss peaks generated by Si 1s, Si 2s and Si 2p are compared. The plasmon loss ratios to mother peaks approximately 10% reduced according to the angle of incidence for all of these spectra, and reduced more at the total reflection conditions. Only for total reflection conditions, this result shows the limitation of excitation range close to the surface, as the energy loss zone becomes smaller comparable with electron inelastic mean free paths. However, this phonomenon is different from surface effect as the emission angle was kept constant at 0±2° and acceptance angle of the analyzer smaller than 10°. When we require precise quantification, we have to consider energy loss process generated in deeper range, too.

3:20pm AS-ThA5 Photon, Electron, and Ion Spectroscopies Applied to Thin Strained Si Films, *S. Zollner, R. Liu, M. Canonico, M. Kottke, Q. Xie, S. Lu, M. Sadaka, T. White, A. Barr, B.-Y. Nguyen, S. Thomas,* Motorola; *C.S. Cook,* Arizona State University; *A. Volinsky,* Motorola **INVITED**

Applied thin-film spectroscopies can be classified by the primary (incident) and secondary (scattered, specularly reflected, diffracted) particle (photon, electron, ion) and by the energy loss (elastic, inelastic) of the interaction. The term spectroscopy implies that the energy of the primary and/or secondary particle is well-known, measured, or varied. We describe applications of various thin-film spectroscopies to thin (15-20 nm) Si layers under tensile biaxial stress, grown pseudomorphically on thick relaxed Si@sub 1-x@Ge@sub x@ buffer layers. Such Si layers have higher electron and hole mobilities than regular bulk Si and are therefore considered for next-generation CMOS technologies. Particular emphasis is placed on the physical mechanism of each spectroscopy technique, the results obtained (thickness, composition, stress), and the potential shortcomings. Specifically, we use UV Raman spectroscopy (325 nm laser excitation) to determine the strain in the Si layer from the frequency shift of the Si-Si lattice vibration. The contributions of the tensile hydrostatic strain and the compressive shear strain to the E1 peak shift (near 3.4 eV) cancel almost exactly, therefore ellipsometry cannot be used to determine strain. However, the piezo-optical effects are significant enough to make ellipsometry unreliable for the determination of the Si thickness or the Ge content of the alloy buffer. Piezo-optical effects are not an issue for x-ray reflectivity, since the dielectric constant of most materials is very close to unity for Cu K@sub alpha@ radiation, but surface roughness can be a problem. We also discuss results from secondary ion mass spectrometry and Auger electron spectrometry to determine composition of the layers.

4:00pm AS-ThA7 Insights into the Physical and Electronic Structure of Surfaces from Reflection Anisotropy Spectroscopy, *P. Weightman,* University of Liverpool, UK **INVITED**

Reflection Anisotropy Spectroscopy (RAS) is a non destructive surface sensitive optical probe capable of operation within a wide range of environments. RAS achieves surface sensitivity by measuring the change in polarisation on reflection of normal incidence light from the surface of a cubic crystal. The technique has been shown to be a sensitive probe of molecular orientation on surfaces@footnote 1,2@ which is capable of monitoring growth at metal/liquid interfaces.@footnote 3,4@ Recent improvements in instrumentation@footnote 4@ have greatly increased the speed of response of RAS equipment so that it can be used to monitor growth at realistic growth rates and to provide information on the orientation and interaction between biological molecules at metal/liquid interfaces on a fast time scale. This talk will present recent results of studies of the physical and electronic structure of metal and semiconductor surfaces and of the RAS of DNA bases and DNA sequences adsorbed at the Au(110)/electrolyte interface. A brief description will be given of how the sensitivity, spectral range and in particular the timescale of RAS will be radically improved by the proposed UK Fourth Generation Light Source (4GLS). @FootnoteText@@footnote 1@J.R. Power, P. Weightman, S. Bose,

A.I. Shkrebtii and R. Del Sole, Phys. Rev. Lett. 80 3133-6 (1998).@footnote 2@B.G. Frederick, J.R. Power, R.J. Cole, C.C. Perry, Q. Chen, S.Haq, Th. Bertrams, N.V. Richardson and P. Weightman. Phys. Rev. Lett. 80 4490-3 (1998).@footnote 3@B. Sheriden, D.S. Martin, J.R. Power, S.D. Barrett, C.I. Smith, C.A. Lucas, R.J. Nichols and P. Weightman, Phys. Rev. Lett. 85 4618-21 (2000).@footnote 4@P. Harrison, T. Farrell, A. Maunder, C.I. Smith and P. Weightman, Meas. Sci. Technol. 12 2185-91 (2001).

4:40pm **AS-ThA9 Spectroscopic Ellispometry Analysis of Chemical Vapor Deposited Zirconia Thin Films**, *B.R. Rogers, Z. Song, R.D. Geil, D.W. Crunkleton,* Vanderbilt University

The integration of high-k dielectric materials into MOSFET fabrication processes will require a non-destructive, fast, and accurate method for film characterization and process control. Spectroscopic ellipsometry (SE) is an outstanding candidate for these applications. This study reports the results of a multi-sample, variable-angle SE (VASE) analysis to characterize zirconia thin films deposited on Si(100) by high vacuum chemical vapor deposition (HVCVD). We evaluated several optical models of the samples to determine which best described the experimental data. A two-layer model consisting of a Tauc-Lorentz layer on the top of a Lorentz interfacial layer resulted in the best fit. This model was used to extract the optical constants of both the zirconia and the interfacial layers. The extracted optical constants were then used as constants in additional models to optimize the analyses. Most of the models fit the data below 6.0 eV extremely well. However, significant differences in goodness of fit were seen between the models'predictions above 6.0 eV photon energies. We feel these differences are due to an increased sensitivity to the interfacial layers for photons above 6.0 eV. The influence of the quality of interfacial layers on the accuracy of extracted optical constants will be discussed. Supporting data from XPS, TEM, and time-of-flight medium energy backscattering analyses will also be presented.

5:00pm **AS-ThA10 Surface Vibrational Spectroscopy Beyond the Harmonic Approximation: On the Selection Rules of Binary Modes**, *P.E: Uvdal, M. Andersson,* Lund University, Sweden

Vibrational analysis of surface adsorbates involves in general the assignment of fundamental normal modes. Based on such assignment conclusions about chemical identity and geometry can be drawn. It is however well known from fundamental textbooks on molecular vibrations that if one goes beyond the harmonic approximation of the intramolecular bond potential overtone and combination modes are allowed. Binary modes, i.e. excitation of one vibration with two quanta or excitation of two vibrations with one quanta, will be the most intense even though higher excitations are allowed. The presence or absence of binary modes will contain information about bond anharmonicity and coupling between different modes. The selection rules, that is the absesence/presence of them will be descussed based on recent first principle calculations.@footnote 1@ @FootnoteText@ @footnote 1@M.P. Andersson and P. Uvdal, Phys. Rev. Lett. 90 (2003) 076103.

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