Wednesday Morning, October 27, 1999

Applied Surface Science Division
Room 6A - Session AS-WeM

Gaede-Langmuir Award Address and Quantitative Surface Analysis

Moderator: P.M.A. Sherwood, Kansas State University

8:20am **AS-WeM1 Monte Carlo Simulations for Tilted Electron Multipliers@footnote 1@**, ***Y.S. Choi***, *S.G. Yu, J.M. Kim,* Samsung Advanced Institute of Technology, Korea

Microchannel electron multipliers are simulated using the Monte Carlo method. Gains of secondary electrons are calculated for different structures of the electron multiplier. For a tilted cylindrical channel of the electron multiplier the gain has a maximum at a tilt angle. The maximum gain is about a thousand times larger than that of the not-tilted channel. An explanation is suggested for the improvement of gain in the tilted channel. @FootnoteText@ @footnote 1@This work was supported by the Korean Ministry of Science and Technology through the Creative Research Initiative program.

8:40am **AS-WeM2 Gaede-Langmuir Award Address: Early Development of Auger and ESCA Instrumention**, ***P.W. Palmberg***, Physical Electronics **INVITED**

The role of the author in the early development of practical Auger and ESCA instrumentation is reviewed. The significance of these early 1970's developments to the surface science community and industrial users is discussed. The authors contributions to both instrument and application development are outlined.

9:40am **AS-WeM5 Consistent, Combined Quantitative AES and XPS Digital Data Bases - Convergence of Theory and Experiment**, ***M.P. Seah***, *I.S. Gilmore, S.J. Spencer,* National Physical Laboratory, United Kingdom

AES and XPS have more aspects in common than they have in distinction. Therefore, tests of aspects for one spectroscopy, applicable to the other, should be validated for both. Digital databases for elemental spectra for both AES and XPS have thus been measured using an electron spectrometer that has fully calibrated intensity and energy axes. This provides true spectra to give absolute Auger electron yields and relative photoelectron yields. The AES database is measured for both 5 and 10 keV electron beam energies, whereas the XPS database is measured for both Al and Mg unmonochromated X-rays at the magic angle. The combination of these databases allows a refinement of the theories to obtain an overall convergence between theory and experiment. Improvements have been obtained by identifying three classes of parameter to consider: (i) parameters for both AES and XPS, such as electron transport, the methodology of evaluation of peak areas and the spectrometer response function, (ii) parameters for AES only, such as the electron ionisation cross section, backscattering and specific electron backgrounds and (iii) parameters for XPS only, such as the photon-ionisation cross section. Using this approach, improvements to the theories of all three classes of parameter and their method of use have been established. The formalism for quantitative analysis in AES and XPS, using relative sensitivity factors, has been revised to develop an accurate matrix-less formalism that is very simple for use by the analyst. This formalism has the same accuracy as the full matrix formalism but its simplicity permits ready extension to systems beyond binary. Details of these and recent advances, particularly with improvements in the background subtraction for the peak area measurement, lead to excellent convergence between theory and the data. This will be discussed, together with outstanding issues for general quantitative analysis with AES and XPS.

10:00am **AS-WeM6 Relationships between Parameters Describing Inelastic Electron Scattering in Solids**, *A. Jablonski,* Polish Academy of Sciences; ***C.J. Powell***, National Institute of Standards and Technology

The terms inelastic mean free path (IMFP), effective attenuation length (EAL), and mean escape depth (MED) are frequently used to specify the surface sensitivity of AES and XPS and also for quantitative applications. These terms are different conceptually because of the effects of elastic-electron scattering, and generally have different numerical values. In addition, EAL and MED values depend on the instrumental configuration. We apply an analytical formalism developed from a solution of the kinetic Boltzmann equation within the transport approximation@footnote 1@ to demonstrate the relationships between the IMFP, EAL, and MED for selected elemental solids and for common measurement conditions. It is shown that EAL and MED values can be derived from an analytical representation of the emission depth distribution function and values of the IMFP and the transport mean free path.@footnote 2@ Examples are given to show the magnitude of elastic-scattering effects on MED values for angle-resolved XPS and AES. If XPS or AES data are acquired for emission angles between zero and 60°, the ratio of the MED to that found with elastic scattering neglected is approximately constant (to within 10 %), and this ratio can be used to determine an average value for the EAL. This EAL value can then be used to establish the depth scale in the data analysis. For emission angles greater than 60°, conventional data analysis (in which elastic-scattering effects are neglected) becomes unreliable. Finally, we show ratios of the EAL to the IMFP for XPS from the Au 4s subshell with Mg K@alpha@ x rays as a function of emission angle and depth; this ratio has a weak dependence on emission angle from zero to 40° but a more pronounced dependence for larger emission angles. @FootnoteText@ @footnote 1@I. S. Tilinin, A. Jablonski, J. Zemek and S. Hucek, J. Electron Spectrosc. 87, 127 (1997). @footnote 2@A. Jablonski and C. J. Powell, J. Electron Spectrosc. (in press).

10:20am **AS-WeM7 Straightforward Methods for Accurate Estimation of Attenuation Length and Similar Quantities in XPS and AES**, ***P.J. Cumpson***, National Physical Laboratory, UK; *M.P. Seah, I.S. Gilmore,* National Physical Laboratory, UK, United Kingdom

The surface-sensitivity of X-ray Photoelectron Spectroscopy (XPS) and Auger Electron Spectroscopy (AES) is due to strong inelastic scattering of electrons. Elastic scattering also takes place, and modifies@footnote 1@ the absolute intensities, the sensitivity factors, the intensities from layers, and (in the case of XPS) the asymmetry parameter @beta@, all of which feed-in to quantitative analysis of spectra. The modification is a multiplicative factor of between 3% and 30% depending on the kinetic energy and material. The behaviour of the asymmetry parameter is particularly important for those using monochromated XPS instruments. Elastic scattering affects these quantities in a straightforward way. This leads to some simple recommendations on analysis geometry, and estimation of Attenuation Lengths to optimise the accuracy of quantifications without increasing complexity. One can measure surface composition and layer thicknesses to known, acceptable accuracy,@footnote 2@ provided one can estimate the Attenuation Length of signal electrons in the sample being analysed. In particular, Attenuation Lengths for organic materials are important in defining polymer, lubricant or contamination surface layers by Angle-Resolved XPS. We therefore pay particular attention to how to estimate Attenuation Length values for an arbitrary organic material. These estimates are in excellent agreement with Monte Carlo calculations. @FootnoteText@ @footnote 1@ A Jablonski, Surf. Sci. 364 (1996) 380. @footnote 2@ P J Cumpson and M P Seah, Surf. Interface Anal. 25 (1997) 430.

10:40am **AS-WeM8 Quantitative Auger Spectroscopy: Applications to Process Development and Qualification of Tungsten Silicide Films**, ***C.T. Dziobkowski***, *S.C. Ramac,* IBM Corp., E. Fishkill; *E.D. Adams,* IBM Corp., Burlington

Tungsten silicide films are widely used in gate conductors for DRAM gate structures for complementary metal-oxide-silicon (CMOS) integrated circuits. Careful characterization of these films with Rutherford backscattering spectrometry (RBS) and Auger electron spectroscopy (AES), the two most commonly used techniques, helps define and control a practical tungsten silicide process. The correct choice of analytical parameters is essential in obtaining accurate and reproducible compositional analysis. The enhanced depth resolution of Auger spectroscopy is especially critical in viewing the region of the interface between the tungsten silicide and polysilicon. Currently, an intrinsic polysilicon cap is used between the doped polysilicon and the CVD deposited tungsten silicide to prevent an unwanted secondary reaction between phosphorus and tungsten hexafluoride which leads to a tungsten enriched interface. This enriched tungsten interface can result in abnormal oxidation, stress and loss of adhesion between the intrinsic polysilicon and tungsten silicide. AES and RBS analytical techniques have been applied to examining the control of this interface to allow extension of CVD tungsten silicide to the thinner gate polysilicon needed for advanced technologies. Examples will be given of the effects of varied gate cap thickness of both amorphous and intrinsic polycrystalline silicon on the tungsten silicide / polysilicon interface using these analytical techniques. The interface composition is known to have a profound effect on the performance of these devices.

11:00am **AS-WeM9 Naphthalocyanine Molecules onto Si(111)7x7 and Si(100)2x1: Modes of Adsorption and Effects of Oxygen Doping Investigated with XPS**, *L. Ottaviano,* INFM, Italy; ***L. Lozzi,*** *A. Montefusco, S. Santucci,* University of L'Aquila and INFM, Italy

We have deposited in ultra high vacuum various thickness of metal free naphthalocyanine (H@sub 2@NPc) onto Si(111)7x7 and Si(100)2x1 and studied in situ the interfaces by means of standard monochromatized X-ray Photoelectron Spectroscopy.@footnote 1@,@footnote 2@ By comparing the core level N1s and C1s spectra obtained for the pure molecule with those typical of the interface at submonolayer and intermediate level of deposition we derived information on the ways of adsorption of the isolated molecules onto the substrates used. In particular NPc adsorbs planarly to the Si(111)7x7 substrate showing strong chemisorption effects involving all the atoms of the molecule. On the other hand, the chemisorption involves only two C atoms when using the Si(100)2x1 substrate. In this case the NPc molecules are likely to be adsorbed in a out of planar mode. In a dedicated series of experiments, the interfaces have been doped with oxygen. An integer ratio of the estimated oxygen atoms per Naphthalocyanine (NPc) molecule in the quantitative XPS elemental analysis of the spectra gives evidence for a preferential adsorption of oxygen in molecular form onto NPc. A careful analysis of the spectra indicates that oxygen mainly interacts with the inner porphyrin structure of the molecule. @FootnoteText@ @footnote 1@ L. Ottaviano, L. Lozzi, and S. Santucci, Surf. Sci. (in press). @footnote 2@ L. Ottaviano, L. Lozzi, A. Montefusco, and S. Santucci, Surf. Sci. (submitted).

11:20am **AS-WeM10 Technique for Production of Calibrated Metal Hydride Films**, ***R.A. Langley***, *J.F. Browning, S.D. Balsley, J.C. Banks, B.L. Doyle, W.R. Wampler,* Sandia National Laboratories

A technique has been developed for producing calibrated metal hydride films for use in the measurement of high-energy (5-15 MeV) particle reaction cross sections for hydrogen and helium isotopes on hydrogen isotopes. Absolute concentrations of various hydrogen isotopes in the film is expected to be determined to better than ± 2% leading to the capacity of accurately measuring various reaction cross sections. Hydrogen isotope concentrations from near 100% to 5% can be made accurately and reproducibly. This is accomplished with the use of high accuracy pressure measurements coupled with high accuracy mass spectrometric measurements of each constituent partial pressure of the gas mixture during loading of the metal occluder films. Various techniques are used to verify the amount of metal present as well as the amount of hydrogen isotopes: high energy ion scattering analysis, PV measurements before, during and after loading, and thermal desorption/mass spectrometry measurements. The most appropriate metal to use for the occluder film appears to be titanium but other occluder metals are also being considered. Calibrated gas ratio samples, previously prepared, are used for the loading gas. Deviations from this calibrated gas ratio are measured using mass spectrometry during and after the loading process. These techniques will be discussed and results presented.

11:40am **AS-WeM11 The Role of SIMS for Interface Control in the MBE Growth of InGaSb/InAS Strained Layer Superlattices**, ***J.S. Solomon***, *M.L. Seaford, D.H. Tomich, K.G. Eyink,* Air Force Research Laboratory

Secondary ion mass spectrometry (SIMS) was used to evaluate beam flux control used for the molecular beam epitaxial (MBE) growth of an indium gallium antimonide/indium arsenide (InGaSb/InAs) strained layer superlattice. Two methods of control were compared: (1) a computer controlled mechanical shutter and (2) a computer controlled system consisting of both a mechanical shutter and a servo operated valve. The issue is the unintentional incorporation of arsenic in the InGaSb layer due to inadequacies of beam flux control mechanisms, such as shutters, to completely shield sources that are part of a cyclic growth process. Test structures of GaAs and GaSb were used in the study with the former used to evaluated antimony control and the latter used to evaluate arsenic control. SIMS results showed arsenic levels as high as 2-4% in GaSb layers when only a mechanical shutter was used. Neither arsenic nor antimony were detected in their respective test structures when growth was controlled with the combination of mechanical shutter and valve. SIMS results correlated with arsenic and antimony levels determined by high resolution x-ray diffraction (HRXRD) analysis of the same test structures. Finally, HRXRD showed improved interface integrity in the SLS structures grown using the combination of mechanical shutter and vale to control arsenic and antimony beam fluxes.

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