Strasbourg (France)

E-MRS 2005 Spring Meeting
May 31 – June 3, 2005

SYMPOSIUM P

Current trends in optical and X-ray metrology of advanced materials for nanoscale devices

Symposium Organizers :

Olivier Durand, Thales, Orsay, France

Mircea Modreanu, Tyndall National Institute, Cork, Ireland

Gerald E. Jellison, Oak Ridge National Laboratory, USA

Jean Massies, CRHEA/CNRS, Valbonne, France

Symposium Support

THALES
HINDS INSTRUMENTS, Inc., USA

Optical Metrology Innovations Ltd, Ireland
HORIBA Jobin Yvon, France

Papers to be published in APPLIED SURFACE SCIENCE

E-MRS 2005 Spring Meeting

SYMPOSIUM P

Tuesday, May 31, 2005 **Morning**
Mardi 31 mai 2005 Matin

8:30 **WELCOME**
by the Symposium Organizers

Session I : Applications : current trends in X-ray reflectometry
Session chairs : P. Mikulik, O. Durand

P-I.01 8:40 -Invited- ANALYSIS OF THIN FILMS BY X-RAY, OPTICAL REFLECTIVITY AND GRAZING INCIDENCE SMALL ANGLE X-RAY SCATTERING

Alain Gibaud(a), S. Dourdain(a) and G. Vignaud(b), (a)Université du Maine, Faculté des Sciences, LPEC UMR6087, 72085 Le Mans Cedex, France, (b)Université de Bretagne Sud, L2PIC, Rue St Maudé, 56321 L'Orient Cedex, France

It is well established that x-ray reflectivity is an invaluable tool to investigate the structure of thin films [1]. Indeed this technique provides under correct analysis, the electron density profile of thin films in the direction perpendicular to the substrate. The aim of this presentation will be to show how x-ray reflectivity data can be analyzed trough the matrix technique in order to obtain the electron density profile. As an example, the analysis of the x-ray reflectivity data of mesoporous silica thin films will be presented in details to show what kind of quantitative parameters can be accessed [2]. By combining x-ray and visible optical reflection, information about the index of refraction of thin films will be provided. Finally Grazing Incidence Small Angle X-ray Scattering (GISAXS) will be presented to show how the off-axis parameters can be ascertained [3].

1- A. Gibaud in "X-ray and neutron reflectivity : principles and applications" edited by J. Daillant and A. Gibaud, Springer, 87-115, (1999) 2- S. Dourdain et al. Submitted to Appl. Phys. Lett. 3- A. Gibaud, S. Dourdain, O. Gang and B. Ocko, Phys. Rev. B , B 70, 161403(R) (2004)

P-I.02 9:20 THIN MULTILAYERS CHARACTERISATION BY GRAZING X-RAY REFLECTOMETRY AND USE OF FOURIER TRANSFORM

F. Bridou(a), J. Gautier(a), F.Delmotte(a), M-F. Ravet(a), O. Durand(b), (a)Laboratoire Charles Fabry de l'Institut d'Optique, CNRS, Unité mixte de Recherche 85801, Bat 503, Centre Scientifique d'Orsay, 91403 Orsay Cedex, France, (b)Thales Research and Technology, Domaine de Corbeville, 91404 Orsay Cedex, France

Fourier transform method allows to obtain directly the values of distances between interfaces with a good approximation, depending on the maximum angular scan of the measure. It can also reveal some particularity of the multilayer**,** i.e. periodic multilayered structures with more than two layers per period. As an illustration of this characterization method, some exemples in XUV optical domain will be shown. This method can also be used for the characterization of many kind of multilayer stacks, in particular semi-conductor heterostrucures ones, under the condition that adjacent layers have sufficient contrast index at the wavelength of the X-ray source

P-I.03 9:40 ELECTRON DENSITY PROFILE AT THE INTERFACE OF SiO2/Si(001)

S. Banerjee(a), S. Ferrari(b), R. Piagge(c) and S. Spadoni(c), (a)Saha Institute of Nuclear Physics, 1/AF Bidhan Nagar, Calcutta 700064, India; (b)Lab. MDM—INFM via Olivetti 2, 20041 Agrate Brianza, Milano, Italy; (c)ST Microelectronics via Olivetti 2, 20041 Agrate Brianza, Milano Italy

We will present here a grazing incidence x-ray reflectivity (GIXR) study of ultra thin films of SiO2 on Si(001) substrate and its interfaces. We have analyzed the x-ray reflectivity data using recursive formalism based on matrix method and distorted wave Born approximation (DWBA). The matrix method gives non-unique solutions and hence non-unique electron density profiles (EDP), which can be overcome using the DWBA formalism. From the analysis of the reflectivity data we could obtain the EDP at the interface of SiO2/Si(001). The EDP obtained from the matrix method follows the DWBA scheme only when two transition layers are considered at the interface of SiO2/Si. The layer which is in proximity with the Si(001) substrate has a higher electron density value than that of Si substrate appearing as a maxima in the EDP. The layer which is in proximity with the dielectric SiO2 layer has an electron density value lower than the bulk SiO2 value and it appears as a minima in the EDP. When the thickness of the SiO2 layer is increased the lower density layer diminishes and the higher density layer persists. This interfacial layering will be discussed.

P-I.04 10:00

X-RAY METROLOGY FOR ADVANCED SILICON PROCESSES

C. Wyon(a), J.P. Gonchond(b), D. Delille(c), A. Michallet(b), J.C. Royer(a), F. Heider(d), L. Kwakman(c), S. Marthon(a), (a)CEA-LETI Grenoble, 17 rue des martyrs, 38054 Grenoble, France, (b)STMicroelectronics, 850 rue Jean Monnet, 38926 Crolles, France, (c)Philips Semiconductors, 860 rue Jean Monnet, 38926 Crolles, France, (d)Infineon, Siemensstrasse 2, 9500 Villach, Austria

Combined x-ray reflectivity (XRR) and x-ray fluorescence (XRF) were used to perform metrology of several advanced microelectronic processes on 200 and 300mm silicon wafers.

At the MOS transistor level XRR and XRF were used to control the thickness and the elemental composition of hafnium and tantalum based high κ materials, and to monitor the thickness and the germanium content of SiGe and strained Si epilayers. Thanks to the XRR accuracy for determining the layer density the elemental composition of such thin films can be determined on monitor wafers using XRR. µ-spot XRF can be used to control the layers thickness and chemical composition on patterned wafers. The main trend for advanced Cu interconnects is to reduce the thickness for barrier and liner layers. Due to its high sensitivity XRR is perfectly suited to control the Atomic Layer Deposition (ALD) of Ta, TaN and W ultra-thin films as well as the more conventional PVD TiN/Ti films stack. As the heavy constitutive elements of such films also exhibit a high XRF efficiency, XRF metrology also allows the reliable film thickness monitoring. XRF was also used to control the Cu deposition and CMP processes on 300mm wafers. Cu dishing and erosion were characterized using XRF with a measurement precision, which strongly depends on the pattern design.

P-I.05 10:20

A SIMPLE SOLUTION TO SYSTEMATIC ERRORS IN DENSITY DETERMINATION BY X-RAY REFLECTIVITY: THE XRR-DENSITY EVALUATION (XRR-DE) METHOD

P. Bergese, E. Bontempi and L.E. Depero, INSTM and Chemistry for Technology Laboratory, Università di Brescia, 25123 Brescia, Italy

X-ray reflectivity (XRR) is a non-destructive, accurate and fast technique for determining the density. Sample-goniometer alignment is a critical experimental factor and the overriding error source in XRR density determination. With commercial single-wavelength X-ray reflectometers alignment is difficult to control and strongly depends on the operator.

In the present work the contribution of misalignment on the error of the density evaluation is discussed, and a novel procedure (named XRR-Density Evaluation method) to minimize the problem will be presented. The method allows to overcome the alignment step through the extrapolation of the correct density value from appropriate non-specular XRR data sets. This procedure is operator-independent and suitable for commercial single-wavelength X-ray reflectometers. To test the XRR-DE method single crystals of the TiO_2 and $SrTiO_3$ were used and in both cases the densities values differed from the nominal ones less than 5.5%. Thus, the XRR-DE method can be applied to evaluate the density values of thin films, for which only the optical reflectivity is today used. The advantage is that this method can be considered thickness independent.

10:40 **BREAK**

Session II : Current trends in optical spectroscopies
Session chair : M. Modreanu, M. Losurdo,

P-II.01 11:00 -Invited-

THE ULTIMATE IN REAL TIME ELLIPSOMETRY: MULTICHANNEL MUELLER MATRIX SPECTROSCOPY

R.W. Collins, Chi Chen, Ilsin An* and N.J. Podraza, Dept. Physics & Astronomy, University of Toledo, Toledo OH 43606, USA; *Permanent address: Dept. Physics, Hanyang University, Ansan, Korea

Spectroscopic ellipsometers with multichannel detection systems have been developed and applied extensively over the last 15 years for in situ and real time analysis of multilayered film structures during their fabrication and processing. Real time measurement techniques are desired in research due to their ability to separate surface, interface, and bulk characteristics of the films that make up a multilayer. Inevitably, however, one sacrifices precision and accuracy for high-speed real-time operation, and the goal of recent instrumentation development is to minimize this sacrifice. The first multichannel ellipsometers employed a rotating polarizer configuration, and these exhibited several disadvantages stemming from their inability to measure the fourth component of the 4x1 Stokes vector of the light beam reflected from the sample. A series of advances over the years has led to the dual rotating-compensator multichannel ellipsometer with the ability to extract the full 4x4 Mueller matrix of the sample in a single optical cycle of the two synchronized compensators. Application of multichannel Mueller matrix spectroscopy include: (i) simultaneous measurement of spectra in the bulk isotropic and surface-induced anisotropic dielectric functions of cubic crystals, (ii) measurement of the optical properties, structure, and local orientation of sculptured thin films, and (iii) measurement of surface roughness thickness on three different in-plane scales during the processing of thin films.

P-II.02 11:40 -Invited-

LIGHT AND MATTER: ADVANCED POLARIZATION SPECTROSCOPY IN FUNCTIONAL MATERIALS PHYSICS

M. Schubert[1], T. Hofmann[1], G. Leibiger[1], K. Streubel[2], A. Jaeger[2], A. Kasic[3], E. Schubert[4], B. Rauschenbach[4], M. Sousa[5] and J.-P. Locquet[5], [1]Universität Leipzig, Germany, 2OSRAM Opto Semiconductors Regensburg, Germany, [3]Linköpings universitet, Sweden, [4]Institut für Oberflächenmodifizierung Leipzig e.V., Germany, [5]IBM Research GmbH, Rüschlikon, Switzerland

The investigation of the bound and unbound charge excitation spectrum is of basic interest for understanding fundamental physical properties of materials. Represented by the complex response functions, and observed by ellipsometry, bound and unbound charge excitations within complex nano-scale architecture systems reveal structural, vibrational, electronic, and free-charge-carrier properties. The use of ellipsometry at the forefront of nanotechnology and solid state physics research will be addressed in this review. Contemporary tools permit feasible measurements from the terahertz region into the deep ultra violet. In particular, the concept of generalized ellipsometry is portrayed, which is capable to characterize materials and nanostructures of reduced symmetry. Unprecedented, ellipsometry at far infrared wavelengths and external magnetic fields is capable of "weighing" the inertial effective electron mass in semiconductor layer structures as well as in correlated electron systems, and permit, for example, nondestructive analysis of free-charge-carrier properties in complex optoelectronic device structures. Results on materials with novel electronic properties will be presented. Special emphasize will be given to birefringence in three-dimensional subwavelength silicon nano-architectures, conduction band anti-crossing in boron diluted semiconductors, charge condensation phenomena in III-V quantum confinement structures, charge and polarization-coupling in high-k metal-oxide thin films, and spectroscopic observation of Landau level splitting in charge correlated systems.

P-II.03 12:00

GENERALIZED ELLIPSOMETRY IN UNUSUAL GEOMETRIES

G.E. Jellison, Jr., J.D. Hunn, D.E. Holcomb and C.M. Rouleau, Oak Ridge National Laboratory, Oak Ridge TN 37831-6030, USA

Most ellipsometry experiments are performed by impinging polarized light onto a sample at a large angle of incidence, and the results are usually interpreted in terms of thin film thicknesses and isotropic optical functions of the film or substrate. Here, however, we describe briefly generalized ellipsometry experiments performed using the two-modulator generalized ellipsometer (2-MGE) in either the transmission or normal-incidence configuration. In both cases, microscope optics and serial measurements can be used to create an image of the sample comprised of diattenuation, retardation, direction of the fast axis, circular diattenuation, and polarization factor. Three examples will be presented. First, transmission mode measurements are used to determine the birefringence of z-cut crystals by tilting the sample slightly off normal incidence. Second, In transmission, the 2-MGE can also be used to measure birefringence introduced by the application of an external voltage; we will focus on semi-insulating GaAs. Finally, normal incidence 2-MGE measurements can be used to characterize optical cross-polarization generated from anisotropic samples; we will show examples from highly oriented pyrolytic graphite (HOPG) and cross sections of nuclear fuel particles.

P-II.04 12:20

INVESTIGATION OF THE OPTICAL ANISOTROPY OF PET AND PEN FILMS BY VIS-FUV TO IR SPECTROSCOPIC ELLIPSOMETRY

A. Laskarakis, S. Logothetidis, Aristotle University of Thessaloniki, Department of Physics, 54124 Thessaloniki, Greece

In the last years, a significant amount of research is being performed in the field of polymer research for novel applications, such as flexible electronic devices, photovoltaic cells, high performance optics, data storage, etc. Toward this direction, in this work, the optical anisotropy of biaxially stretched Poly(Ethylene Terephthalate) (PET) and Poly(Ethylene Naphthalate) (PEN) films has been extensively investigated. The optical properties of the films have been studied in terms of their optical, electronic and vibrational response, by Fourier Transform IR Spectroscopic Ellipsometry (FTIRSE) (900-3500 cm-1) and Vis-fUV Variable Angle SE (1.5-6.5 eV) techniques. The films optical anisotropy is the result of the stretching procedure during their fabrication, which results to the structural rearrangement of the macromolecular chains parallel to the stretching direction and to a higher structural symmetry. During the SE spectra analysis, the films have been approximated as uniaxial materials with their optic axis parallel to the sample/ambient interface leading to the accurate determination of the principal components ε|| and ε┴ of the dielectric function ε(ω). The detailed study of the electronic transitions has been performed in the Vis-fUV region, where the characteristic features corresponding to the n->π* electronic transitions of the carbonyl -C=O group and the 1Ag->1Bu transition due to the π->π* excitation of the π-electron structures have been identified and analysed. Furthermore, the FTIRSE spectra allowed the accurate identification and assignment of the characteristic features of ε(ω) to the vibrational modes of the various bonding structures consisting the PET and PEN macromolecular chains.

12:40 **LUNCH**

Tuesday, May 31, 2005 — Afternoon
Mardi 31 mai 2005 — Après-midi

Session III : Methodological advances in X-ray
Session chairs: L. Kirste, : V. Holy

P-III.01 14:00 -Invited-

ANOMALOUS X-RAY SCATTERING FROM SELF-ASSEMBLED SEMICONDUCTOR NANOSTRUCTURES

Vaclav Holy, Department of Electronic Structures, Charles University Prague, Czech Republic, Julian Stangl, Guenther Bauer, Institute of Semiconductor Physics, Kepler University Linz, Austria, Tobias Schuelli, ESRF Grenoble, France

X-ray scattering is frequently used for structure investigations of self-organized semiconductor quantum dots and wires. The method studies shapes and local chemical composition of both free-standing and buried nanostructures. Usual x-ray scattering methods reached their limits due to very small volumes of scattering objects and consequently very low intensities. The sensitivity of the scattering method can be further improved using anomalous scattering with energy close to an absorption edge of constituting atoms. In the talk, the principle of anomalous scattering will be discussed. The applicability of the method will be demonstrated on several experimental examples (Ge quantum dots on Si, PbSe quantum dots in PbSe/PbEuTe superlattices, InAs quantum dots on GaAs). Further development of anomalous scattering will be discussed including x-ray diffraction spectroscopy EDAFS on semiconductor nanostructures.

P-III.02 14:40

1500 K IN-SITU RECIPROCAL SPACE MAPPING ON A LABORATORY X-RAY DIFFRACTOMETER

R. Guinebretière, A. Boulle, R. Bachelet, O. Masson, P. Thomas, SPCTS CNRS UMR 6638, ENSCI, 47 Av. A. Thomas, 87065 Limoges Cedex, France

One of the challenges in the coming years in the microelectronic field is the introduction of oxide compound thin films as functional materials into new devices. Oxide materials often require high processing temperature that profoundly affect their microstructure. The knowledge of their behaviour as a function of temperature is therefore of primary importance. X-ray diffraction (XRD) reciprocal space mapping (RSM) is a non destructive characterization technique allowing the analysis of the microstructure of epitaxial thin films on a quantitative level.

P-III.03 15:00

TOWARDS ULTRA FAST HIGH RESOLUTION X-RAY DIFFRACTION ON PSEUDOMORPHICALLY GROWN EPITAXIAL LAYER STRUCTURES

A. Kharchenko(a), J.F. Woitok(a), P.F. Fewster(b), V. Kogan(a), (a)PANalytical Application Development Centre, Almelo, The Netherlands, (b)PANalytical Research Centre, Sussex, Brighton, U.K.

A new experimental set-up has been realized on a commercially available diffractometer that enables the measurement of a complete high resolution X-ray diffraction pattern on epitaxial layer structures within seconds. The proposed set-up consists of a newly designed X-ray mirror and a solid-state multistrip detector. By means of a specific diffraction geometry the diffraction pattern from pseudomorphically grown epitaxial layer structures can be rapidly and easily obtained without movement of the sample or the detector. Due to the unique properties of the detector a high gain in data collection time is accomplished. Measurements performed on different AlGaAs and SiGe based structures confirmed the high data quality of the diffraction data with respect to resolution and large dynamic range. Individual layer properties were extracted by full pattern simulations based on the dynamical theory of X-ray diffraction.

P-III.04 15:20

NOVEL METHODS AND UNIVERSAL SOFTWARE FOR HRXRD, XRR AND GISAXS DATA INTERPRETATION

A. Ulyanenkov, Bruker AXS, Östliche Rheinbrückenstr. 49, 76187 Karlsruhe, Germany

A large diversity of modern nanomaterials demands reliable techniques for sample characterization. High-resolution x-ray diffraction (HRXRD), x-ray reflectometry (XRR) and grazing-incidence small-angle scattering (GISAXS) are well-established and non-distructive methods for determining of thickness, crystallinity, composition, porosity and interface roughness of thin films and multilayers. Whereas the hardware component of x-ray apparatus provides the data acquisition, the software part is necessary for reliable data interpretation. Therefore, modern x-ray measurement techniques require a flexible and universal physical theories and numerical tools for data evaluation.

P-III.05 15:40

STRUCTURAL CHARACTERISATION OF SB-BASED HETEROSTRUCTURES BY BOTH X-RAY REFLECTOMETRY AND X-RAY DIFFRACTOMETRY

C. Renard(a), O. Durand(a), X. Marcadet(a), J. Massies(b), O. Parillaud(a), (a)TRT, THALES 91404 Orsay Cedex, France, (b)CRHEA ,CNRS, Valbonne, France

The application of band-gap engineering concepts to the combination of arsenide and antimonide materials makes it possible to obtain unique properties particularly well suited for mid IR quantum cascade laser (QCL) applications. Two arsenide/antimonide mixed systems are very attractive : InAs/AlSb which can be epitaxially grown on GaSb or InAs substrates and InGaAs/AlAsSb which for specific alloy compositions is lattice matched to InP. Both are very promising systems to fabricate QCLs operating at room-temperature in the l ~ 3-5 µm atmospheric window region. We present here an overview of a wide range of techniques based on X-ray reflectometry (XRR) and X-ray diffractometry (XRD), applied on both (InAs/AlSb)N and (InGaAs/AlAsSb)N superlattices. We show that a Fourier transform analysis allows an accurate and fast determination of the individual layer thicknesses. Using a simulation software with the results from a Fourier analysis as a starting point for the fitting procedure, the r.m.s. roughnesses values at the interfaces has been determined, in two similar (InAs/AlSb)N superlattices but with different InAs/AlSb interface roughness values. In addition, we show that lateral correlation properties of interfaces profiles, giving the in-plane morphological roughness, can be extracted from small-angle incoherent-scattering-signal experiments. Then, a study on a InGaAs-cap layer /(InGaAs/AlAsSb)N superlattice grown on a InGaAs/InP buffer layer illustrates the complementary between XRR and XRD for the determination of both top-layer and deep-layer thicknesses, by means of Fourier transform analysis

16:00 **BREAK**

Session IV : Applications : Optical spectroscopies
Session chairs : G.E. Jellison, R.W. Collins

P-IV.01 16:20 -Invited-

OPTICAL IN-SITU SPECTROSCOPY DURING EPITAXIAL GROWTH PROCESSES

T. Zettler, E. Steimetz, K. Haberland and S. Uredat, LayTec GmbH, Helmholtzstr. 13-14, 10587 Berlin, Germany

In the last decade optical in-situ sensors for real-time monitoring and real-time control of epitaxial thin-film growth processes (metal-organic vapor phase epitaxy, molecular beam epitaxy) evolved into a key technology for compound semiconductors. Methods like optical reflectance, reflectance-anisotropy, emissivity corrected pyrometry and substrate curvature sensing are now applied routinely in multiple-wavelength or spectroscopic sensors. This development has been driven by the increasing complexity of epitaxial thin-film processes for electronic and opto-electronic devices and by the need for control of extremely thin layers in these structures (often only a few atomic monolayers thick). In addition, the industry's demands for shorter process development times, reduced system down-times and higher yields motivated sensor developments enabling real-time access to key growth parameters by direct optical sensing of the growing layers. To illustrate this, examples will be given on monitoring of layer thickness, layer composition, lateral growth uniformity, interface properties, surface roughness, substrate temperature and strain-induced substrate bending.

Finally, we will also discuss the current status of optical sensor integration into thin-film growth systems, including remote monitoring by real-time LAN based optical sensors and active feed-back control of growth parameters.

P-IV.02 17:00

ELLIPSOMETRIC CHARACTERIZATION OF NANOCRYSTALS IN POROUS SILICON

P. Petrik, M. Fried, É. Vázsonyi, T. Lohner, O. Polgár, I. Bársony, J. Gyulai, Research Institute for Technical Physics and Materials Science, P.O. Box 49, 1525 Budapest, Hungary

Porous silicon layers (PSLs) were prepared by electrochemical etching of p-type single-crystallin silicon (c-Si) wafers having different dopant concentrations to obtain systematically changing sizes of nanocrystals (walls). The microstructure of the porous material was characterized using spectroscopic ellipsometry with multi-layer effective medium approximation (EMA) models. The dielectric function of PSL is conventionally calculated using EMA mixtures of c-Si and voids. The porousity of PSL is expressed by the concentration of voids. Some PSLs could be described only by adding fine-grained polycrystalline silicon reference material to the EMA model (Bársony et al., Mat. Res. Soc. Symp. Proc. 342 (1994) 91; Fried et al., Thin Solid Films 276 (1996) 223). Modified model dielectric functions (MDF) of c-Si have been shown to fit composite materials containing nanocrystalline regions, either by fitting only the broadening parameter (Tsunoda et al., J. Appl. Phys. 91 (2002) 2936) or also other parameters of the parametric oscillator in MDF (Kurihara et al., J. Appl. Phys. 96 (2004) 3247). The broadening parameter correlates with the long-range order in the crystalline material, i.e. with the size of nanocrystals. Recently, we have demonstrated the usability of the MDF model for PSLs by using EMA with dielectric function data based on the MDF model calculated with different broadening parameters, in spite of using pc-Si in the EMA. In this work we fit the broadening and/or gap-energy parameters of MDF to investigate the correlation with wall size of PSL measured by complementary techniques. The longer term goal of this work is to provide a method for the quantitative characterization of nanocrystal size using quick, sensitive, and non-destructive optical techniques.

P-IV.03 17:20

RAMAN AND INTERFEROMETRY BASED STRESS METROLOGY FOR CHARACTERIZATION OF SI/SIGE, SOI AND OTHER NOVEL SEMICONDUCTOR STRUCTURES

Wojciech J. Walecki, Talal Azfar, Kevin Lai, Manuel Santos II, and Ann Koo, Frontier Semiconductor, 1631 North 1st Street, San Jose CA 95112, USA

Innovative materials have emerged as an alternative to simple scaling for achieving improved device performance [1]. Engineered substrates such as Si/SiGe structures and silicon on insulator (SOI) are the most promising solution for increasing mobility [1].

Raman spectroscopy has been recognized as one of the most versatile non contact tools for characterization of stress in SOI and Si/Ge structures as well as composition variation within volume of the substrate wafer [1,2]. In our paper we report recent progress in commercial high resolution (0.6 cm-1 and below) dual wavelength Raman scatterometry for strained Si/SiGe and SOI applications. We report measurements at two different excitation wavelengths (325 nm, and 532 nm) at which the impingent radiation is absorbed at two different depths allows accurately map stress and alloy composition within the wafer. We present estimates for trade-off between throughput and accuracy of the stress and composition measurement. We also compare results of stress measurement on Si wafers obtained using Raman spectroscopy with results obtained using coherence optical interferometry [3]. We discuss benefits of the combined Raman interfermetric tool for characterization of multi-layered stressed structures. 1. C. Mazure, I. Cayrefourcq, G. Celler, M. Kennard, A. Tiberj, Solid State Tech., "Engineered substrates require strain metrology", 111, November, 2004 2. J.C. Tsang, P.M. Mooney, F. Dacol, J.O Chu, J. Appl. Phys. 75, p. 8098, 1994. 3. W. Walecki, F. Wei, P. Van, K. Lai, T. Lee, SH Lau, and A. Koo Koo, "Interferometric Metrology for Thin and Ultra-Thin Compound Semiconductor Structures Mounted on Insulating Carriers", CS Mantech Conference, May 3-6, 2004, Miami Beach, Florida

P-IV.04 17:40

EFFECTS OF UV - PHOTON IRRADIATION ON SiOx (0<x<2) STRUCTURAL PROPERTIES

Nicolae Tomozeiu, R&D Oce Technologies B.V., Postbus 101, 5900 MA Venlo, The Netherlands

Thin films of a-SiOx (0<x<2) were prepared by reactive r.f. magnetron sputtering from a polycrystalline-silicon target in an Ar/O2 gas mixture. The oxygen partial pressure in the deposition chamber was varied so as to obtain films with different values of x. The plasma was monitored, during depositions, by Optical Emission Spectroscopy (OES) system. Energy Dispersive X-Ray (EDX) measurements and Infra-red (IR) spectroscopy were used to study the compositional and structural properties of the deposited layers.

Structural modifications of SiOx thin films have been induced by UV photons' bombardment (wavelength of 248nm) using a pulsed laser. IR spectroscopy and x-ray photoemission spectroscopy (XPS) were used to investigate the structural changes as a function of x value and incident energy. SiOx phase separation by spinodal decomposition was revealed. The IR peak position shifted towards high wavenumber values when the laser energy is increased. Values corresponding to the SiO2 material (only Si4+) have been found for laser irradiated samples, independently on the original x value. The phase separation process has a threshold energy that is in agreement with theoretical values calculated for the dissociation energy of the investigated material. For high values of the laser energy, crystalline silicon embedded in oxygen rich silicon oxide was revealed by Raman spectroscopy.

P-IV.05 18:00

ABSORBANCE SPECTRA OF POLYCRYSTALLINE AND MULTI-LAYERED OLIGOTHIOPHENES CRYSTALS

L. Raimondo, M. Campione, M. Laicini, M. Moret, A. Sassella, S. Tavazzi, INFM and Dipartimento di Scienza dei Materiali, Università di Milano Bicocca, Via Cozzi 53, 20125 Milano, Italy, P. Spearman, School of Chemical and Pharmaceutical Sciences, Kingston University, Kingston upon Thames KT1 2EE, U.K.

In recent years an increasing attention has been devoted to the research on organic semiconductor materials both in single crystal and thin film form for their potential in device applications. For example, oligothiophenes are often considered as representative of a wide class of materials based on conjugated molecules. Recent studies have been focused on the investigation of the peculiarities of crystal optics and light propagation in these highly anisotropic materials, which present strong optical transitions of Frenkel origin. Interesting features have also been predicted for layer-by-layer organic heterostructures and for organic nanoaggregates embedded in matrices of different species. In this respect, the non-destructive nature of optical techniques allows to investigate the molecular packing, the growth mode, the macroscopic order, and the quality of the samples. In this context, we focus our attention on quaterthiophene crystals whose dielectric tensor has been recently calculated on the basis of the known crystallographic data and taking into consideration Frenkel exciton states. Using a 4 x 4 matrix method, it is possible to simulate the optical spectra of different types of samples, either polycrystalline or multi-layered. Since the spectral features are strongly affected by the orientation of either the crystalline domains or the different layers, the comparison between the measured and simulated absorbance spectra taken in different experimental configurations allows deducing the sample macroscopic structural features, as reported here for the case of quaterthiophene samples. We discuss that these materials can demonstrate interesting negative refraction properties and furthermore the twin structures may be important producing non reflective interfaces.

Session V : Advanced material characterization : high-k metal oxides
Session chairs : G.E. Jellison, M.F. Gartner

P-V.01 14:00 -Invited-

BAND EDGE ELECTRONIC STRUCTURE OF TRANSITION METAL/RARE EARTH OXIDE DIELECTRICS: THEORY AND EXPERIMENT

G. Lucovsky, Dept. of Physics, NC State Univ., Box 8202, Raleigh NC 27695-8202, USA

This paper addresses band edge electronic structure of transition metal/rare earth (TM/RE) non-crystalline and nano-crystalline elemental/complex high-k oxide dielectrics. Experimental approaches include X-ray absorption spectroscopy from TM, RE and oxygen core states, photoconductivity, and visible/vacuum ultra-violet spectroscopic ellipsomentry, as well as ab initio theory applied to small clusters. High-k conduction band edge states are distinguished from SiO_2, Si oxynitrides, and Al_2O_3 by being comprised of localized TM/RE d-states, rather than delocalized/free-electron like s-states. Two factors contributing to additional differences are local/crystal field effects that split these d-states into doubly and triply degenerate groups, and Jahn-Teller (J-T) term-splittings that remove these degeneracies reducing band gaps and band offset energies. The average d-state energies track with systematic trends in TM/RE atomic d-state energies, and significantly limit high-k options to Zr, Hf, Y, La, and trivalent RE oxides. Deposited dielectric films are typically nano-crystalline, and this results in intrinsic band edge defects from J-T splittings of TM/RE d-states at grain boundaries. These localized defects contribute to trap-assisted tunneling, trapping and Frenkel-Poole transport, degrading device performance and reliability. Approaches for optimization of dielectric films are addressed, including limits imposed on the continued and ultimate scaling of the equivalent oxide thickness (EOT).

P-V.02 14:40 -Invited-

VACUUM ULTRAVIOLET SPECTROSCOPIC ELLIPSOMETRY AND NANOSCALE DEVICE APPLICATIONS: AN INDUSTRIAL PRIMER

N.V. Edwards, Freescale Semiconductor, Inc. and SEMATECH, Austin, Texas

The recent commercialization of Vacuum Ultraviolet spectroscopic llipsometry (VUV SE) instruments means that it is now possible to routinely erform SE measurements at wavelengths below 190 nm, considerably extending the vailable spectral range for in-house industrial analytical characterization. his ability to obtain optical constants over a spectral range that spans ultiple inspection wavelengths and lithographic technology nodes has meant that the instrument has played an often critical role in lithographic design nd strategy. An overview of lithographic design and metrology challenges for ext generation lithography will be presented; however, it should be noted that he new industrial VUV capability has implications for the characterization of other materials of importance to the Si industry beyond the obvious applications for lithographic work. These are materials that are nominally transparent at long wavelengths but that possess unique absorption signatures in the VUV, such as newly emerging high-k gate materials (e.g. Al_2O_3, HfO_2, ZrO_2, Y_2O_3) as well as more familiar dielectrics (e.g. SiO_xN_y, organo-silicate glasses, Si_3N_4, SiOF, and TEOS). We review recent progress concerning materials characterization for advanced technology nodes with VUV SE, citing diverse examples from semiconductor processing to demonstrate the capabilities of the instrument. These capabilities include increased access to unique VUV spectral features as a means of tuning process parameters and increased ability to determine the thickness of thin films grown on Si. We also address the initial challenges that had to be overcome in order to develop optical constants at short wavelengths and to enable this sort of materials characterization.

P-V.03 15:20

STRUCTURAL-OPTICAL STUDY OF HIGH-DIELECTRIC-CONSTANT OXIDE FILMS COMBINING 0.75-6.5 EV ELLIPSOMETRY AND XRD

Maria Losurdo, Maria M. Giangregorio, Pio Capezzuto, Giovanni Bruno, Institute of Inorganic Methodologies and of Plasmas, IMIP-CNR and INSTM UdR Bari, Bari, Italy, Roberta G. Toro, Graziella Malandrino, Ignazio L. Fragalà, Dipartimento di Scienze Chimiche, Università di Catania, and INSTM, UdR Catania, Catania, Italy, Raffaella Lo Nigro, IMM, sezione di Catania, CNR, Catania, Italy

The scaling down in microelectronics technology requires new high-k dielectrics to replace the traditional SiO_2 gate insulator in CMOS devices and ferroelectric materials in capacitive elements.

Here, we evaluate a group of high-k oxides. Among the rare-earth oxides, praseodymium oxide Pr_2O_3, has a high-k of 26-30, thus it can be an appropriate candidate for the replacement of SiO_2 gate insulator. On the other hand, recently, much attention is being paid to an unusual cubic perovskite material $CaCu_3Ti_4O_{12}$ (CCTO), which have a very high-k of the order of 104 almost constant in the temperature range 100K-600K thus showing improved physical properties with respect to the currently used ferroelectric materials. Therein, we investigate the microstructure and its correlation with optical properties in the 0.75 - 6.5 eV photon energy range of Pr_2O_3 and CCTO films grown by metalorganic chemical vapour deposition (MOCVD) on a variety of substrates including Si(100), $LaAlO_3$ (100)and $Pt/TiO_2/SiO_2/Si(100)$ crossing spectroscopic ellipsometric measurements and X-ray diffraction. We focus on the following aspects: - The interrelation between the optical properties and different structural aspects (crystallinity, grain orientation, size,..) caused by processing conditions; - Interface formation depending on substrate lattice parameters and deposition conditions since control of the substrate/oxide interface is crucial for applications; - Optical parameterization of the Pr_2O_3 and CCTO thin films depending on the microstructure. In particular, parameterization (Drude+Lorentzian oscillators) of optical properties and their variation upon annealing conditions, which may cause change in the electrical as well as optical behaviour of films, is discussed.

P-V.04 15:00

INVESTIGATION OF THERMAL ANNEALING EFFECT ON MICROSTRUCTURAL AND OPTICAL PROPERTIES OF HfO_2 THIN FILMS

M. Modreanu, J. Sancho-Parramon, Tyndall National Institute, Cork, Ireland, O. Durand, B. Servet, Thales R&T, Orsay, France, M. Stchakovsky, C. Eypert, Horiba Jobin-Yvon, Thin Film Division, Chilly-Mazarin, France, C. Naudin, HORIBA Jobin-Yvon Raman Division Villeneuve d'Ascq, France, A. Knowles, HORIBA Jobin-Yvon Ltd Raman Division , Middlesex , U.K., F. Bridou, M-F. Ravet, Laboratoire Charles Fabry de l'Institut d'Optique, CNRS, Unité mixte de Recherche 85801, Bat 503, Centre Scientifique d'Orsay, 91403 Orsay Cedex, France.

During the recent years, there has been a growing interest in the study of the physical properties of hafnium dioxide (HfO2) for its use as a possible high-k material to replace SiO2 as the gate dielectric of future MOSFETs and for its application to optical coatings technology as a high-refractive index material. In the present paper we focus on the study of the impact of the different post-deposition thermal treatments on optical and microstructural properties of thin (30 to 150 nm) films of HfO2 obtained by Plasma Ion Assisted Deposition (PIAD). After deposition, the HfO2 films were annealed in N2 ambient for three hours at 300, 350, 450, 500 and 750oC. Several characterisation techniques including High-Resolution TEM (HRTEM), X-ray Reflectometry (XRR), X-ray Diffraction (XRD), Spectroscopic Ellipsometry (SE), UV Raman and FTIR were used for the physical characterisation of the as-deposited and annealed HfO2. The results indicate that the HfO2 films are amorphous in as-deposited state and a transition to crystalline phase occurs for temperature greater than 500oC. HRTEM, SE, XRR and FTIR results show that an increase in the interfacial layer was observed only for high temperature annealing. The amorophous HfO2 samples exhibit band tails which are attributed to the presence of the defects within the HfO2 films. Following the transition to a crystalline phase the absorption edge is shifted to higher energy and the band tails associated with the defects are not observed

16:00 **BREAK**

Session VI : Advanced material characterization : oxides
Session chairs : O. Durand, M. Modreanu

P-VI.01 16:20 -Invited-

RECENT ADVANCES IN HIGH-RESOLUTION X-RAY DIFFRACTOMETRY APPLIED TO NANOSTRUCTURED OXIDE THIN LAYERS

A. Boulle, R. Guinebretière, A. Dauger, Science des Procédés Céramiques et de Traitements de Surface CNRS UMR 6638, ENSCI, 47-73 avenue Albert Thomas 87065 Limoges Cedex, France

Nanostructured oxide thin layers are the subject of intense research in the field of micro- and nanoelectronics as well as in optoelectronics and photonics. However, in contrast with metallic or semiconductor layers, oxide layers are much more difficult to grow with a high crystalline quality level which results in very broad and complicated reciprocal space features. Therefore it is often extremely challenging to obtain reliable information concerning the nanostructure of oxide layers using X-ray diffraction.

In this communication we will adress some important issues that can be encountered in the study of nanostructured oxide layers and explain how these affect the diffracted intensity distribution: - roughness and thickness fluctuations combined or not with lattice spacing fluctuations, - highly localized strain fields associated with planar defects, - strain gradients and strain fields associated with misfit dislocations, - cationic interdiffusion at the interface. Recent X-ray diffraction reciprocal space mapping experiments performed on epitaxial SrBi2Nb2O9 and Zr(Y)O2 deposited on various oxide substrates (SrTiO3, Al2O3, MgO...) will be used as representative examples

P-VI.02 17:00

EVIDENCE FOR BA DIFFUSION IN ULTRA THIN $SRTIO_3$/BASRO/SI FILMS MEASURED BY XRD AND GIXD

M. Sousa(a), C. Marchiori(a), A. Guiller(a), M. Seo(b), J. Fompeyrine(a), H. Siegwart(a), D. Caimi(a), C. Rossel(a), R. Germann(a), J.P. Locquet(a), (a)IBM Research GmbH, Sauemerstrasse 4, 8803 Rueschlikon, Switzerland, (b)Institute of Physics of Complex Matter, EPFL Ecublens, 1015 Lausanne, Switzerland

For the semiconductor industry, it is very crucial to find a substitute to the SiO2 as gate oxide in order to keep improving device performance by scaling. Among the different candidates, the perovskite SrTiO3 is of interest because of its high permittivity κ and because it can be grown epitaxially on Si (001). While depositing this material, the formation of a thin interfacial SiO2, which will affect the equivalent oxide thickness (EOT) dramatically, is likely. In order to overcome this issue, a BaSrO intermediate layer is grown prior to the SrTiO3, and allows us to obtain a thin crystalline template at low temperature and low oxygen pressure. The aim of this work was to characterize by X-ray Diffractometry (XRD) and Grazing Incidence X-ray Diffractometry (GIXD) the interfacial reaction between BaSrO and SrTiO3. Ultra-thin samples with a stack of 1 unit cell (UC) BaSrO and 10 UC SrTiO3 have then been grown by molecular beam epitaxy with different thermal budget for the crystallization step on Si (001). The analysis shows that the crystallization time and temperature have an influence on the SrTiO3 lattice parameter, in plane and out of plane, which can be correlated with a diffusion of Ba in the film.

P-VI.03 17:20

DENSITY, THICKNESS AND COMPOSITION MEASUREMENTS OF TiO_2-SiO_2 THIN FILMS BY COUPLING X-RAY REFLECTOMETRY, ELLIPSOMETRY AND ELECTRON PROBE MICROANALYSIS

A. Hodroj, H. Roussel, A. Crisci*, F. Robaut*, Ulrich Gottlieb, J.-L. Deschanvres, Laboratoire des Matériaux et du Génie Physique CNRS, Ecole Nationale Supérieure de Physique de Grenoble, BP 46 38402 St Martin d'Hères France *Consortium des Moyens Technologiques Communs Institut National Polytechnique de Grenoble BP 75 38402 St Martin d'Hères France

Mixed TiO_2-SiO_2 thin films were deposited by aerosol atmospheric CVD method by using di-acetoxi di-butoxi silane (DADBS) and Ti tetra-butoxide as precursors. By varying the deposition temperatures between 470°C and 600°C and the ratios between the Si and Ti precursors (Si/Ti) from 2 up to 16, films with different composition and thickness were deposited. The coupled analysis of the results of different characterisation methods was used in order to determine the variation of the composition, the thickness and the density of the films. First EPMA measurements were performed at different acceleration voltages with a Cameca SX50 system. By analysing with specific software the evolution of the intensity ratio Ix/I_{std} versus the voltage, the composition and the mass thickness (product of density by the thickness) were determined. In order to measure independently the density, x-ray reflectometry experiments were performed. By analysing the value of the critical angle and the Kiessig fringes, the density and the thickness of the layers were determined. The refractive index and the thickness of the films were also measured by ellipsometry. By assuming a linear interpolation between the index value of the pure SiO_2 and TiO_2 films, the film composition was deduced from the refractive index value. XPS measurements were also performed in order to obtained an independent value of the composition. The coherence of the results is analysed and discussed.

P-VI.04 17:40

DEVELOPMENT OF A NEW COUPLED GXRR WITH VUV-SE WITH NEW MODELLING FOR High-k GATE OXIDES

Jean-Louis Stehlé(a), Patrick Evrard(a), Christophe Defranoux(a), Alice Elbaz(b), Enrico Bellandi(b), (a)SOPRA, 26 rue Pierre Joigneaux, 92270 Bois-Colombes, France, (b)ST Microelectronics, Central R&D, via Olivetti 2, 20041 Agrate Brianza, Italy

The 45 nm technology node of the ITRS roadmap may require to replace the nitrided gate oxides by new high-? materials such as Hafnium oxides and aluminates (HfxAlyOz). This materials are usually deposited by ALD (atomic layer deposition). Their overall Equivalent Oxide Thickness (EOT), including the interfacial oxide layer, is required to be 1 nm, according to the 2003 ITRS.

In this paper we will present the results obtained by a combination of GXRR and VUV-SE. The same sample position is analyzed with two optical non destructive techniques, the GXRR which works at a wavelength of 1.54Å (hard X-Rays) where all materials are transparent and the refractive index is close to 1. Therefore this technique does not require to know the refractive index in order to determine the layer thickness. The UV extended spectroscopic ellipsometer (VUV-SE) has a spectral range from 1.9 to 9eV. The measurement goniometer is enclosed in an N2 purged chamber. Such UV extension allows to study the band gap energy of most high-?dielectrics. SE beam diameter is about 6 x 10 mm6mm. The sample holder is mounted on a Rho-Theta mapping chuck. The system is automated with robot handling and pre-alignment option. Samples of 300 mm can be measured. The two techniques can be used sequentially and the average measurement time for a sample using both GXRR and VUV-SE on 5 measurement sites is less than 2 hours. In our approach, we first analysed the X-Ray measurement for obtaining the layer thickness, regardless of its refractive index. The ellipsometric spectra was then analysed, tanking care of the bottom interface layer in order to calculate the refractive index, keeping the thickness obtained from the first technique.,The results of the measurements will be presented and the improvements given by the new regression analysis will be given. he combination of the two non destructive techniques, GXRR and VUV-SE, allows to collect complementary information about high-??gate dielectrics. The GXRR is very accurate for roughness, thickness and the top-layer density. VUV SE using the thickness data obtained by the X-Ray measurement, allows determining the refractive index, and the interface oxide layer thickness.

P-VI.05 18:00

YTTRIUM OXIDE, Y2O3, X-RAY INVESTIGATION OF THIN FILMS: INTERNAL STRESS AND MICROSTRUCTURE

F. Paumier, R.J. Gaboriaud, F.P. Pailloux, Laboratoire de Métallurgie Physique, Université de Poitiers, CNRS, SP2MI, BP 30179, 86962 Chasseneuil-Futroscope cedex, France

Y2O3 has attracted much attention because of several physical properties (high k value (10-18), wide band gap (5.5 eV), a high thermal stability up to 2300°C) particularly relevant for MOS structure. Y2O3 thin films are deposited by ion beam sputtering on Si, MgO and SrTiO3. This deposition technique promotes a very particular structure in the thin films whatever the substrate. Y2O3 layers are studied by means of X ray diffraction and HRTEM. It has been shown that two cubic crystallographic phases coexisted (fm3m and cubic C). This work pays a particular attention to the microstructure of the fm3m cubic phase which is due to a strong disorder of the oxygen network induced by argon bombardment during the growth (penning effect). This disordered phase plays an important role on the residual stress (sinus square psi method) presents in the thin films. After annealing under air or vacuum only the cubic C structure is observed. The order-disorder transition is studied in situ by quantitative X ray diffraction versus the temperature (KJMA's theory) and the oxygen energy diffusion is determined.

P-VI.06 18:20

NANOSTRUCTURE CHARACTERIZATION OF HIGH K MATERIALS BY SPECTROSCOPIC ELLIPSOMETRY

L. Pereira, H. Aguas, E. Fortunato, R. Martins, Departamento de Ciência dos Materiais, Faculdade de Ciências e Tecnologia, Universidade Nova de Lisboa and CEMOP, Campus da Caparica, 2829-516 Caparica, Portugal

In this paper we present a complete study of the optical properties of high k materials such as tantalum oxide and titanium oxide determined by spectroscopic ellipsometry, where a Tauc Lorentz dispersion model based in two or one oscillator was used. The samples were deposited at room temperature by radio frequency magnetron sputtering and then annealed at temperatures ranging from 100 to 500ºC. The use of two Tauc Lorentz oscillators allowed a better fitting of the titanium oxide films, suggesting that they are nanocrystalline, even when deposited at room temperature.
Concerning the tantalum oxide films two different behaviours where observed related to the film's structure. For films annealed at temperatures above 400 ºC, the model proposed fits quite well the experimental data, suggesting a transition from amorphous to nanocrystalline, as it was also confirmed by XRD data. On the other hand, for tantalum oxide samples annealed at lower temperatures a simple Tauc Lorentz dispersion model fits quite well the experimental data, as it is normal obtained in amorphous films. These results demonstrate that spectroscopic ellipsometry is an effective technique to characterize high k dielectrics, supplying important information concerning not only the optical parameters of the materials but also on films compactness, nanostructure and density.

19:00

AWARD CEREMONY

The symposium organizers and the candidates to the graduate student award are requested to attend.

CONFERENCE RECEPTION

Thursday, June 2, 2005 — Morning
Jeudi 2 juin 2005 — Matin

Session VII : Optical metrology : materials and devices (I)
Session chairs : M. Modreanu, B. Servet

P-VII.01 9:00 -Invited-

MODULATED REFLECTANCE AND REFLECTANCE CHARACTERISATION OF OPTOELECTRONIC DEVICE STRUCTURES

T.J.C. Hosea, Advanced Technology Institute, University of Surrey, Guildford, Surrey GU2 7XH, U.K.

It is of vital importance to semiconductor device manufacturers to be able to characterise wafers by a non-destructive methods. Ideally these should be applicable in air, at room temperature, and without the need for special mounting, so that full-sized pre-fabrication wafers can be assessed. Modulated reflectance (MR) spectroscopy is a well-known suitable optical technique. Here, the reflectivity R of a semiconductor is periodically perturbed externally, yielding spectra with detailed derivative-like features arising from ground-state, and other possible higher-energy optical transitions, from which can be extracted many material parameters crucial to efficient device operation. The talk will discuss applications of MR to assessing structures such as quantum dot lasers and Raman amplifiers, and for the extraction of built-in electric fields. The MR technique often entails the simultaneous measurement of the ordinary R spectrum, for the purposes of normalisation. Though perhaps the simplest optical technique, reflectivity is not used extensively to characterise semiconductor wafers quantitatively, due to the rather broad and featureless spectra which commonly result. However, the R spectra of modern multi-layer structures such as resonant-cavity LEDs, show much more detail. The talk will discuss how such R spectra may also be exploited to extract layer thicknesses and compositions, and even information about the active quantum-well layer absorption spectrum.

P-VII.02 9:40 -Invited-

PHOTOREFLECTANCE STUDY AT THE MICROMETER SCALE

C. Bru-Chevallier, H. Chouaib, A. Bakouboula, T. Benyattou, Laboratoire de Physique de la Matière, INSA de Lyon, Bâtiment Blaise Pascal, 7 avenue Jean Capelle, 69621 Villeurbanne Cedex, France

Photoreflectance (PR) spectroscopy has proven to be a very efficient non-destructive tool to get information on various semi conducting epitaxial structures. Indeed, due to its derivative nature, modulation spectroscopy is very sensitive to every direct optical transitions in semiconducting quantum structures. It also allows to optically measure internal electric fields in space charge layers, through Franz Keldysh oscillation analysis. Up to now, most of the PR studies have been reported using large spot size.

Owing to the very important potentialities expected from the direct optical characterization at the device scale, it is very challenging to try to push PR technique to the micrometer spatial scale. We have developed an experimental set-up which allows to get µPR spectra on epitaxial structures on a 5µm wide spot. Due to a very low signal intensity, experimental conditions have to be very carefully controlled : the signal/noise ratio strongly depends on the pump-probe power ratio. We will give experimental results recorded on antimonide based Heterojunction Bipolar Transistors, which give the local electric field at the junction, eventually under operation. A second part of the paper will be devoted to µPR analysis performed on tuneable VCSELs with InP/air Bragg mirrors. In such VCSELs, both the cavity Fabry Perot peak and the active region quantum well ground state are giving transitions in the µPR spectrum. This is very valuable in the case of a tuneable structure.

P-VII.03 10:20

PHOTOREFLECTANCE SPECTROSCOPY CHARACTERISATION OF STRAINED SILICON EPIWAFERS

P.V. Kelly, M.E. Murtagh, V. Guénebaut and S. Ward, Optical Metrology Innovations Ltd. (OMI), 2200 Cork Airport Business Park, Cork Airport, Co. Cork, Ireland

Engineered epitaxial wafer substrates, traditionally found in the compound semiconductor industry, are now emerging into the wider silicon industry with the requirement for strained silicon substrates. This technological development requires similar advances in characterisation tools for engineered strained silicon substrates. A key requirement is for a diagnostic tool with ultra thin film sensitivity capable of measuring the strain in layers as thin as 10 nm of silicon. This paper presents the state-of-the-art in the application of photoreflectance (PR) spectroscopy to the characterisation of engineered epitaxial wafer substrates. PR is an electro-absorptive modulation reflectance spectroscopy technique capable of measuring the E_1 direct interband transition energy, and critically, its splitting and energy shifting under strain. PR has a fundamental advantage of sensitivity to ultrathin silicon, because the E_1 transition energy, in the ultraviolet, lies at the onset of strong optical absorption in the silicon, and the signal is dominated by the contribution from the top 10-20 nm of the silicon. The underlying physics and example results are presented in this paper, along with a description of the photoreflectance method as applied to silicon. The photoreflectance behaviour of silicon-germanium alloys is also discussed.

10:40 **BREAK**

Session VIII : Optical metrology : materials
Session chairs : T.J.C. Hosea, C. Bru-Chevallier

P-VIII.01 11:00 -Invited-

ADVANCES IN MODULATION SPECTROSCOPY: STATE-OF-ART PHOTO-REFLECTANCE METROLOGY

M.E. Murtagh, P.V. Kelly, V. Guénebaut and S. Ward, Optical Metrology Innovations Ltd. (OMI), 2200 Cork Airport Business Park, Cork Airport, Co. Cork, Ireland

Engineered compound semiconductor epitaxial wafer substrates are the basis for most r.f. electronics and photonics devices. The emergence of GaN technologies paralleling existing GaAs technologies has expanded the scope of the compound semiconductor industry, most notably in the area of blue emitter devices. These advances in technologies require similar advances in both characterisation and statistical-process-control (SPC) metrologies. In particular is the requirement for diagnostic tools to have sufficient sensitivity and accuracy to semiconductor material and device parameters. Advances in the application of photoreflectance (PR) spectroscopy to the characterisation of engineered compound semiconductor epitaxial wafer substrates are presented in this paper. Probing the electric field modulated density-of-states, PR is an electro-absorptive modulation reflectance spectroscopy technique which yields important band structural information such as transition (interband) energy levels, critical point type and resonance, mole fraction, lattice strain and significantly, interfacial (surface) electric field levels. Novel methods are presented for the first time which overcome background (laser-induced) luminescence effects using an asynchronous switching modulation device. Novel optical designs can achieve micron scale spatial resolution. Dramatic reductions in signal acquisition time over previous PR spectrometers is demonstrated. The importance of dedicated operational algorithms or macro PR operation is emphasised. Results will be demonstrated for both III-V and III-nitride structures, confirming the importance and role PR will play as a successful commercial metrology tool for both existing state-of-art and next generation semiconductor characterisation/SPC equipment.

P-VIII.02 11:40

MODULATION SPECTROSCOPY OF Ga(In)NAs/GaAs QUANTUM WELL STRUCTURES CONTAINING Sb ATOMS

R. Kudrawiec, J. Misiewicz, Institute of Physics, Wroclaw University of Technology, Poland; H.B. Yuen, S.R. Bank, M.A. Wistey, H.P. Bae, James S. Harris Jr, Solid State and Photonics Laboratory, Department of Electrical Engineering, Stanford University, USA

Recently, the III-V-N compound systems with a small content of nitrogen (N<5%) have attracted great attention due to both their unusual fundamental properties and potential for long wavelength optoelectronic devices applications on GaAs substrates. Modulation spectroscopy, i.e. photoreflectance (PR) and contactless electroreflectance (CER), is a powerful tool to investigate optical properties of semiconductor systems. In this paper these techniques have been applied to determine the number of confined states and their energies for GaNAsSb/GaAs single quantum wells (SQWs), GaInNAsSb/GaAs SQWs as well as step-like GaInAsSb/GaNAs/GaAs QW structures tailored at 1.3 mm and 1.5 mm. The experimental data have been compared with the calculations in the envelope function formalism taking account the effect of strain. For GaNAsSb/GaAs SQWs excellent agreement between experimental data and calculation results have been found for band structure type-I with the conduction band offset ratio of 50 %. In the case of GaInNAsSb/GaAs SQWs four confined states for both electrons and heavy holes have been found for the calculations with the conduction band offset ratio of ~85%. Transitions related to the four confined states have been confirmed in PR spectra. In the case of the step-like GaInNAsSb/GaNAs/GaAs QW structures, besides the optical transitions in the GaInNAsSb/GaNAs QW, PR (CER) signal related to transitions between quantum states confined above the step-like GaNAs barriers has been observed. The role of Sb atoms in these structures will be discussed in this paper.

P-VIII.03 12:00

SIMULTANEOUS OPTICAL MEASUREMENT OF Ge CONTENT AND CARBON DOPING IN STRAINED EPITAXIAL SiGe FILMS

S.J. Morris and D. Le Cunff, Therma-Wave Inc., 1250 Reliance Way, Fremont CA94539, USA, D. Ristoiu, V. Vachellerie, F. Deleglise and D. Dutartre, ST Microelectronics, 850 rue Jean Monnet, 38926 Crolles Cedex, France

= Using a proprietary technique which has previously been shown able to decouple the effects of Ge and Boron on the optical properties of a B-doped SiGe film, we now apply the technique to decouple the effects of Ge and C and so perform simultaneous optical measurement of thickness, Ge-content and C-content for a set of Carbon-doped epitaxial SiGe films.

A set of Carbon-doped epitaxial SiGe layers were grown, each with the same nominal Ge-content but with the Carbon levels varying from zero to ~0.4%. The effect of the Carbon upon the optical properties of the SiGe was modelled as a "perturbation function" upon the ε2(E) optical function, and a mathematical formula was developed which could predict the whole form of this perturbation function for a given Carbon content. By combining the perturbational approach to the C-content with a conventional Alloy model for the Ge-content, the two material fractions could be measured independently using data from a standard production metrology tool (the Opti-Probe(r)). This was verified using XRD and SIMS as comparison techniques.

12:20 **LUNCH**

Session IX : Spatially resolved techniques-study of small objects
Session chairs : A. Gibaud, P. Mikulik

P-IX.01 14:00 -Invited-

SPATIAL MICROMETER-RESOLVED STRUCTURE QUALITY CONTROL OF SEMICONDUCTOR WAFERS AND LATERAL OVERGROWTH STRUCTURES BY SYNCHROTRON RADIATION ROCKING CURVE IMAGING

P. Mikulík, Institute of Condensed Matter Physics, Masaryk University, Kotlárská 2, 61137 Brno, Czech Republic, D. Lübbert, P. Pernot and L. Helfen, ISS and ANKA, Forschungszentrum Karlsruhe, Germany, D. Korytár, Institute of Electrical Engineering SAS, Vrbovská cesta 110, 92101 Pieštany, Slovakia, S. Keller, University of California at Santa Barbara, CA, USA, and T. Baumbach, ISS and ANKA, Forschungszentrum Karlsruhe, Germany

We present a review and recent advances on local lattice and structure quality control of semiconductor wafers and overgrown structures with spatial resolution downto one micrometer over an extended sample area. We employ synchrotron radiation diffraction rocking curve imaging (RCI) technique, which combines digital X-ray topography and conventional Bragg-diffraction rocking curve recording. Application of this method has been pushed from qualitative wafer structure characterization towards quantitative mapping of local crystalline misorientations and dislocation density and towards one-micrometer spatial resolution to study crystalline morphology of overgrown patterned structures.

Growth of compound materials in ingots, like SiC, GaAs, GaN, InP, leads to inherited imperfections. Regions of specific misoriented macrodefects and dislocation regions in ingots can be qualitatively mapped by RCI. Epitaxial lateral overgrowth (ELO) is an innovative crystal growth technique expected to achieve a better crystal quality. The overgrown layer shows significantly lower density of threading dislocations than in the wetting layer. With micrometer-resolved 2D detector, the RCI allows to monitor the lattice quality and lattice tilts in individual periods of the structure. Significant information can be obtained from individual sample areas as small as 2 micrometers in all three spatial dimensions, and to correct the findings of double-crystal diffraction rocking curve measurements.

P-IX.02 14:40 -Invited-

X-RAY SCATTERING: A POWERFUL PROBE OF LATTICE STRAIN IN MATERIALS WITH SMALL DIMENSIONS

Olivier Thomas, TECSEN UMR CNRS 6122, Université Paul Cézanne, Marseille, France

X-ray diffraction was recognized from the early days as very sensitive to atomic displacements. Indeed structural crystallography has been very successful in locating with great precision the position of atoms within an individual unit cell. In disordered systems it is the average structure and fluctuations about it that may be determined. In the field of mechanics diffraction may thus be used to evaluate elastic displacement fields. I will give examples from recent work where x-ray diffraction has been used to investigate average strains in lines, films or multilayers. In small objects the proximity of surfaces or interfaces may create very inhomogeneous displacement fields. X-ray scattering is again one of the best methods to determine such distributions. The need to characterize displacement fields in nanostructures together with the advent of third generation synchrotron radiation sources has generated new and powerful methods (anomalous diffraction, coherent diffraction, micro-diffraction, …). I will review some of the recent and promising results in the field of strain measurements in small dimensions via X-ray diffraction.

P-IX.03 15:20

PHOTOREFLECTANCE SPECTROSCOPY OF SELF-ORGANIZED InAs/InP (001) QUANTUM STICKS EMITTING AT 1.55µm

H. Chouaib, N. Chauvin and C. Bru-Chevallier, Laboratoire de Physique de la Matière, INSA de Lyon (UMR-CNRS 5511), Bâtiment Blaise Pascal, 7 Avenue J. Capelle, 69621 Villeurbanne, France, C. Monat, P. Regreny and M. Gendry, Laboratoire d'Electronique, Optoélectronique et Microsystèmes, (UMR CNRS 5512), Ecole Centrale de Lyon, 36 Avenue Guy de Collongue, 69134 Ecully, France

Photoreflectance (PR) spectroscopy is a sensitive optical powerful and a direct method for investigation of various semiconducting heterostructures. In the case of quantum dots, experimental conditions have to be very accurately controlled : because of the high photoluminescence (PL) background due to the laser pump, the signal-to-noise ratio of PR intensity strongly depends on the pump-probe power ratio.

In this work, we present PR measurements as a function of temperature performed on self-organized InAs/InP (001) quantum sticks (QSs) grown by solid source molecular beam epitaxy [1]. With a very weak excitation power, we observe three PR transition energies associated to the ground state and two excited states, respectively, in good agreement with both PL and PL excitation measurements, and with theoretical results previously developed for these InAs QSs using a simplified k.p model [2]. Moreover, the temperature dependence of the PR transition energies is also in good agreement with the Bose-Einstein behavior. In such a InAs/InP QS system, it has been previously assumed that the ground state is partially filled because of the non-intentional n doping of the InP layers [3]. The PR spectra analysis allows to further confirm this assumption, considering mainly the relative PR intensity of the different transitions. [1] M. Gendry et al., J. Appl. Phys., 95, 2004, 4761 [2] P. Miska et al., J. Appl. Phys., 95, 2004, 1074 [3] B. Salem et al., Phys. Rev. B 66, 2002, 193305

P-IX.04 15:40

NANOPHOTONICS AND NANOMETROLOGY WITH PLANAR X-RAY WAVEGUIDE-RESONATOR

V.K. Egorov, E.V. Egorov IMT RAS, Chernogolovka, Moscow District, 142432 Russia

Synchrotron systems and polycapillar optics can form X-ray beams for microsize photonic technology and metrology. X-ray beams of a nanosize range are possibly produced by the diffraction optics [1]. But in the last time, the alternative X-ray optics been suitable for nanodimention technology and metrology appears. This optics based on the total external X-ray reflection phenomenon forms superfine thread beams by capture the radiation into the planar narrow extended slit created by two dielectric reflectors and it's transportation by the flux superstream or waveguide-resonance manner [2]. Such device is called the planar X-ray waveguide-resonator (PXWR). Work contains experimental data described it's specific properties. Unique characteristics of PXWR allow to use this device for nanodiffractometry, reflectometry, small angle scattering, X-ray characteristical spectrometry of nanovolumes and TXRF. Moreover, PXWR can be served as the base element for operation on X-ray flux parameters. Experimental data described PXWR application for diffractometry and TXRF spectrometry are discussed, in details. Some attention is devoted to the model development of the superstream X-ray flux propagation through a planar narrow extended slit.

[1] H. Takano, Y. Suzuki, A. Takeuchi. Sub-100 nm hard X-ray microbeam generation with Freshnel zone plate optics // Japan J. Appl. Phys. 2003. v42. P. L132-L134. [2] V.K. Egorov, E.V. Egorov. The experimental background and the model description for the waveguide-resonance propagation of X-ray radiation through a planar narrow extended slit (Review) // Spectrochimica Acta. 2004. v59B. P. 1049-1069.

P-IX.05 16:00

GaN ON NANOPATTERNED GaN/Si(111) TEMPLATES: OPTICAL AND STRUCTURAL CHARACTERIZATION

L.S. Wang, B.Z. Wang, S. Tripathy and S.J Chua, Institute of Materials Research & Engineering, 3 Research Link, 117602 Singapore

The heteroepitaxial growth of GaN on silicon has attracted much interest for their use in light emitters in optoelectronic integrated circuits. In this study, we have used template based nanoscale epitaxy to realize high-quality GaN on Si(111) substrates. We have employed polystyrene-based nanosphere lithography to form the nano-hole array patterns on GaN/Si (111) template and then performed subsequent regrowth of GaN by metalorganic chemical vapor deposition. During the initial growth stage of GaN on such nano-patterned substrates, we have observed formation of nanoislands with hexagonal pyramid shape due to selective area nanoscale epitaxy. Such nanostructures are revealed single crystalline hexagonal phase GaN oriented along (0001) direction as characterized by x-ray diffraction (XRD) and high-spatial resolution optical spectroscopic methods, With further epitaxial regrowth, these nanoislands coalesce and form continuous GaN film. XRD, micro-photoluminescence (PL), scanning electron microscopy (SEM), transmission electron microscopy (TEM) and micro-Raman scattering have been used to assess the optical and microstructural properties. Micro-PL measurements show that the band-edge luminescence intensity from such GaN layers is significantly enhanced compared with GaN films simultaneously grown on Si(111). Combined PL and Raman data analyses show a reduction of biaxial stress. In addition, such epitaxial growth also leads to a reduction of defect density as revealed by TEM. Such GaN templates would be useful to realize III-Nitride based opto- and electronic devices integrated on Si substrates.

16:20 **BREAK**

16:40-19:00 **POSTER SESSION**

POSTER SESSION

Thursday, June 2, 2005

16:40 – 19:00

P/P.01 OPTICAL MODELS FOR THE ELLIPSOMETRIC CHARACTERIZATION OF CARBON NITRIDE LAYERS PREPARED BY PULSED LASER DEPOSITION

P. Petrik, T. Lohner, Research Institute for Technical Physics and Materials Science, P.O. Box 49, H-1525 Budapest, Hungary L. Égerházi and Zs. Geretovszky, Department of Optics and Quantum Electronics, University of Szeged, P.O. Box. 406., H-6701 Szeged, Hungary

Amorphous carbon nitride (CNx) films were prepared by KrF excimer laser ablation of a graphite target in nitrogen atmosphere in inverse-PLD geometry. From the ellipsometric point of view, the challenging properties of these films were their exponential thickness distribution, accompanied by laterally varying chemical composition and structure. Optical models were developed to accurately describe the changes of film properties depending on distance from the ablation source, layer thickness, and nitrogen pressure. Multi-layer models were used to determine the surface roughness as well as the lateral and vertical inhomogeneities. Multiple angles of incidence and multiple wavelengths were applied in ranges of 66-75° and 400-1000 nm, respectively. The microspot capability (spot size of about 100 micron) of the spectroscopic ellipsometer used was exploited to decrease the error caused by the lateral inhomogeneity within the measurement spot. Material properties were derived using empirical dispersion models (Cauchy) as well as parametric dielectric function and oscillator models (Tauc-Lorentz, Forouhi-Bloomer). Further to layer thicknesses and dielectric functions, these models allowed the quantitative determination of the band gap as well as the oscillator parameters

P/P.02 SIMULATION OF X-RAY DIFFRACTION PROFILES IN MULTILAYERS BY DIRECT WAVE SUMMATION

S. Zamir, Department of Electrical Engineering, Technion-Israel Institute of Technology, Haifa 32000, Israel, and E. Lakin, E. Zolotoyabko, Department of Materials Engineering, Technion-Israel Institute of Technology, Haifa 32000, Israel

During last ten years there is an intensive development in the fields of quaternary III-V semiconductor alloys (e.g. InGaAsP/InP), crystalline/amorphous stack layers (e.g. Si-on-insulator (SOI)), layers and substrates of non-cubic symmetry (e.g. tetragonal BaTiO3, rhombohedral LiNbO3 and Al2O3, hexagonal GaN and AlN) directed to the design and fabrication of novel microelectronic and optoelectronic devices. An increasing complexity and diversity of material systems require further progress in characterization techniques. In order to meet these challenges we developed novel X-ray diffraction simulation routine based on the direct wave summation method. It permits introducing local variations of important parameters, such as defect-induced fluctuations of d-spacings and interface roughness, in order to describe partial or complete smearing of interference features in measured profiles. The simulations also take proper account for amorphous layers via their effect on phases of coherently scattered waves. Besides that, there is an option to perform coherent or incoherent summation of the contributions from individual layers that is essential in non-perfect multilayers. The developed routine can be used to simulate diffraction profiles taken with symmetric and asymmetric reflections for any multilayer structure with no limitations. Working examples for important material systems mentioned above are given

P/P.03 OPTICAL EMISSION SPECTROSCOPY DURING FABRICATION OF INDIUM-TIN-OXYNITRIDE FILMS BY RF-SPUTTERING

M. Koufaki, M. Sifakis, Physics Department, University of Crete, PO Box 2208, 71003 Heraklion, Crete, Greece, E. Iliopoulos, M. Androulidaki, E. Aperathitis, MRG, IESL, FORTH-HELLAS, PO Box 1527, 71110 Heraklion, Crete, Greece, M. Modreanu, Photonics Group, Tyndall National Institute, Lee Mattings, Prospect Row, Cork, Ireland.

Optical emission spectroscopy (OES) has been used as in situ diagnostic technique for identifying species in plasma during fabrication of indium-tin-oxynitride (ITON) thin films by rf-sputtering. The ITON films were fabricated in rf plasma containing a mixture of Ar-N2 gases and under different rf powers. The ITON films were characterized by employing different optical characterization techniques, like XRD, FTIR, AES and Reflectance- Transmittance in the whole DUV-IR spectrum range. The properties of ITON films were compared with those of Indium-Tin-Oxide (ITO) films fabricated in pure Ar plasma under the same sputtering conditions. A uniform distribution of nitrogen was found throughout the structure of the ITON films. The absorption edge of the ITON films deposited at 300-400W exhibited the strongest shift to shorter wavelengths and showed reduced infrared reflectance. Identification of species in the plasma during deposition of the ITON films under these conditions revealed that there was a correlation between plasma quality and the optical properties of the films. The potentialities of indium-tin-oxynitride film for use as a new transparent optical material for opto-electronic devices will be addressed

P/P.04 PHOTOREFLECTANCE SPECTROSCOPY OF SEMICONDUCTOR STRUCTURES UNDER HYDROSTATIC PRESSURE

R. Kudrawiec and J. Misiewicz, Institute of Physics, Wroclaw University of Technology, Wybrzeze Wyspianskiego 27, 50-370 Wroclaw, Poland

= Photoreflectance (PR) spectroscopy is very powerful tool to investigate optical properties of semiconductor systems. The derivative nature of this experimental method enables observation of a large number of sharp spectral features including those related to excited state transitions in low-dimensional structures, in contrast to common emission-type experiments such as photoluminescence (PL), which usually probes only the ground state. In addition, this techniques can probe different parts of semiconductor structures, i.e. quantum wells, barriers, step-like barriers, quantum dots as well as wetting layers in quantum dot structures. Very often PR spectra are very complicated due to an interference of PR signals related to different optical transitions associated with different parts of the investigated semiconductor structure. In order to identify and/or to separate them PR usually measurements at various temperatures or different modulation wavelengths are preformed. The other possibility to identify the optical transitions is the application of hydrostatic pressure. In this paper optical properties of semiconductor structures under hydrostatic pressure are investigated in PR spectroscopy. For the hydrostatic pressure experiments, the samples were mounted in a Be:Cu liquid-filled clamp-pressure cell with a sapphire window for optical access and with a maximum working pressure of 11 kbar. In this paper we focus on measurement aspects as well as optical properties of selected III-V semiconductor structures under hydrostatic pressure. For example it will be shown that a segregation of atoms in GaInNAs/GaAs quantum wells could be detected by the measurements of PR spectra at various hydrostatic pressure.

P/P.05 PHOTOREFLECTANCE AND CONTACTLESS ELECTROREFLECTANCE SPECTROSCOPY OF GAAS-BASED STRUCTURES: SIMILARITIES AND DIFFERENCES

R. Kudrawiec, M. Motyka, P. Sitarek, and J. Misiewicz, Institute of Physics, Wroclaw University of Technology, Wybrzeze Wyspianskiego 27, 50-370 Wroclaw, Poland

Photoreflectance (PR) and contactless electroreflectance (CER) spectroscopies are particularly useful because they are performed in contactless mode that is nondestructive for samples. In addition, these technique are very sensitive at room temperature that it is very important aspect of material characterization since devices normally operate around room temperature. The parameter which is modulated in the sample during PR and CER measurements is the same, i.e. it is the built-in electric field. However, the mechanism of the modulation of built-in electric fields is not equivalent for the two techniques. Hence some difference in PR and CER spectra could appear. In this paper these differences as well as similarities will be discussed. For example we show that the low energy oscillations (LEOs) often observed in PR spectra could be eliminated completely by applying the CER instead of PR. This finding confirms that the origin of LEOs is the modulation of the refractive index in the sample due to the generation of additional carriers by modulated pump beam. In the case of CER spectroscopy, any additional carriers are not generated during the modulation hence CER spectra are free of LEOs. This advantage of CER spectroscopy is very important in investigations of all semiconductor structures for which LEOs are present in PR spectra. Besides this mentioned difference between PR and CER other aspects associated with the difference in the mechanism of band bending modulation will be analyzed. We will consider the determination of the built-in electric field from the period of Franz-Keldysh oscillations observed in PR and CER as well as the detection of the sign of band bending by measuring CER.

P/P.06 CHARACTERIZATION OF GaN EPITAXIAL FILMS GROWN ON SILICON-ON-INSULATOR SUBSTRATES

S. Tripathy, L.S. Wang, and S.J. Chua Institute of Materials Research and Engineering, 3 Research Link, Singapore 117602

We report growth and characterization of GaN on (100) and (111) oriented silicon-on-insulator (SOI) substrates by metalorganic chemical vapor deposition (MOCVD). Prior to MOCVD growth, the Si(100) overlayers of the SIMOX SOI substrates were treated by KOH solution, which led to textured silicon microstructures. Growth of GaN on such surface leads to c-axis orientated textured GaN. This is evident from high-resolution x-ray diffraction (HR-XRD) studies. In addition, no crystallite cracking is observed in the GaN samples grown on KOH treated silicon surface. Significantly enhanced photoluminescence (PL) intensity and stress relaxation is observed from micro-PL and HR-XRD measurements. Furthermore, GaN grown on (111) oriented bonded SOI wafers shows good surface morphology and improved optical quality. Improved PL properties are also clearly observed from the GaN films grown by these methods, where the band-edge PL peak shows a blue shift when compared to the GaN epilayer simultaneously grown on bulk Si(111) substrate. HR-XRD measurements on GaN grown on bonded SOI (111) substrates reveal single crystalline hexagonal GaN oriented along (0001) direction. Micro-Raman measurements clearly show the hexagonal lattice structure with tensile stress relaxation. Such approach to realize GaN epitaxial layers is suitable for the integration of GaN-based optoelectronic structures on SOI based microelectronics.

P/P.07 DEFECT STRUCTURE OF In(GaAl)As/InP LAYERS SUBJECTED TO HIGH PRESSURE TREATMENT

J. Bak-Misiuk, A. Shalimov, Institute of Physics, PAS, Al. Lotnikow 32/46, 02-668 Warsaw, Poland, A. Misiuk, J. Kaniewski, J. Muszalski IET, Al.Lotnikow 32/46, 02-668 Warsaw, Poland, W. Wierzchowski IEMT, Wolczynska 133, 01-919 Warsaw, Poland, K. Wieteska IAE, 05-400 Swierk-Otwock, Poland, and W. Graeff DESY HASYLAB, Notkestrasse 85, D-22603 Hamburg , Germany

Strain state of In(GaAl)As/InP structures subjected to annealing under high hydrostatic pressure was investigated by X-ray diffraction methods. Due to differences in lattice parameters of the compounds it was possible to induce tensile as well as compressive strain in In(GaAl)As/InP layers by composition changes. The strain of the layer was calculated from the lattice parameter values determined from high resolution diffraction studies. Their defect structure was characterised by X-ray synchrotron topography. Fully strained, partially strained and fully relaxed layers were studied. The high temperature-high pressure (HT-HP) treatment was performed for 1 hour at 670 K under 1.2 GPa argon hydrostatic pressure. The HT-HP treatment results in defect and strain changes of thin layer structures. Type and density of dislocations present in In(GaAl)As layers before and after high temperature annealing were calculated assuming Kaganer's model. After the HP-HT treatment contribution of 60° and 90° misfit dislocations to defect stucture of the layers was modified.

P/P.08 CALCULATED STRUCTURAL, ELECTRONIC AND OPTICAL PROPERTIES OF SNO_2

B. Amrani[1,2], I. Chiboub[1], M. Tahiri[1], S. Hiadsi[1] 1 Laboratoire Traitement de Surface et Structure des Matériaux 2 Laboratoire de Physique Quantique et de Modélisation Mathématique, Département de Physique, Université de Mascara

In this paper we report a theoretical study of the structural, electronic and optical properties of SnO2. The study is focused on the first-principles all electron full-potential linearized augmented plane wave calculations within the density-functional theory. The results of bulk properties, including lattice constants, bulk modulus and derivatives and band structures are obtained and compared using both the local density approximation (LDA) and the generalized gradient approximation (GGA) for the exchange-correlation functional. We find that the GGA does not give a significant improvement over LDA.

P/P.09 LASER REFLECTOMETRY IN SITU MONITORING OF InGaAs GROWN BY AP-MOVPE

M. M. Habchi, A. Rebey, A. Fouzri, B. El Jani, Unité de Recherche sur les Hétéro-Epitaxies et Applications, Faculté des sciences, 5000 Monastir, Tunisia

In this study, InGaAs layers on GaAs (001) substrates were successfully grown by atmospheric-pressure metalorganic vapour phase epitaxy(AP-MOVPE). Growth temperature (Tg) as growth parameter, was varied from 420°C to 680°C to obtain films with different indium composition (xIn). Furthermore, high resolution X-ray diffraction (HRXRD) measurements were used to determinate xIn. The changes of xIn and crystal quality have been studied as a function of growth conditions. On the other hand, laser reflectometry (LR) at 632.8 nm wavelength, was employed to in situ monitor epitaxy. Reflectivity-time signal was enabled to evaluate structural and optical properties of samples. We have fit experimental data to determinate the variation of optical constants and growth rate of InGaAs at 632.8 nm versus xIn. In addition, the fitting provided InGaAs thickness as a function of growth time. Finally, scanning electronic microscopy (SEM) was used to study surface morphology and determinate alloy thickness. The results reveal good agreement between LR and SEM.

P/P.10 APPLICATION OF SPECTROSCOPIC ELLIPSOMETRY TO THE INVESTIGATION OF THE OPTICAL PROPERTIES OF COBALT NANOCRYSTALS EMBEDDED INTO SILICA LAYERS.

M. Gilliot (1), A. En Naciri (1), L. Johann (1), C. d'Orleans (2), D. Muller (2), J.P. Stoquert (2), J.J. Grob (2).
(1) Laboratoire de Physique des Milieux Denses, 1Bd Arago, 57078 Metz Cedex 3, France (2) Laboratoire PHASE 23 rue du Loess BP 20 CR F-67037 Strasbourg Cedex 2, France

Spectroscopic ellipsometry is used to investigate optical properties of cobalt- implanted silica thin films. The films under investigation are 250 nm thick thermal SiO_2 layers on Si substrates implanted with Co^+ ions at energy of 160 keV and at fluences of 10^17 ions/cm² for different temperatures of substrate during implantation (77K, 295K and 873 K).
Changes due to Co^+ implantation are clearly observed in the optical response of the films. Optical behaviours are furthermore different for the three implantation temperatures. To understand the optical responses of these layers, the ellipsometric experimental data are compared to different models including interference effects and metal inclusions effects into the dielectric layer. The simulated ellipsometric data are obtained by calculating the interferences of an inhomogeneous layer on a Si substrate. The material within this layer is considered as an effective medium which dielectric function is calculated using the Maxwell-Garnett effective medium approximation. We show that although the structures of these layers are very complicated because of ion-induced damage during implantation, such quite simple models can provide relatively good agreement. The possibilities of ellipsometry for the study of the optical properties of such clusters-embedded films are discussed. We especially provide the evidence that ellipsometry can give interesting information about the optical properties of nanostructured layers. This is of special interest in the field of nanocrystals optical studies on a non-transparent substrate where ellipsometry appears to be a suitable characterization technique.

P/P.11 ULTRATHIN InAs AND MODULATED InGaAs LAYERS IN GaAs GROWN BY MOVPE STUDIED BY PHOTOMODULATED REFLECTANCE SPECTROSCOPY

P. Hazdra, J. Voves, Department of Microelectronics, Czech Technical University in Prague, Technická 2, CZ-16627, Prague 6, Czech Republic and E. Hulicius, J. Pangrác and Z. Šourek, Institute of Physics, Academy of Sciences, Cukrovarnická 10, 162 53 Prague, Czech Republic

Photomodulated reflectance (PR) spectroscopy in combination with photoluminescence and photocurrent measurement was used for the characterisation of highly strained submonolayer and supermonolayer multiple InAs quantum wells (MQW) and modulated InGaAs layers on GaAs grown by metal-organic vapour phase epitaxy. Structures were grown in AIXTRON 200 reactor at 500°C on (100) oriented GaAs substrates by periodic interruption of the InAs and GaAs growth. The layers were analysed by X-ray diffraction and scanning tunnelling microscopy. The origin of various PR spectral features was proposed using simulation of electronic states in these structures with a theoretical model accounting for influence of stress and quantum states coupling. Optical transitions between ground and excited states identified on a series of structures with different modulations/thicknesses were used for interpretation of resulting electronic band structure of MQWs. Optimised modulated InGaAs layers were embedded into the AlGaAs/GaAs waveguides and used as active regions of highly efficient (~35%) near infrared (1.1μm) lasers.

P/P.12 IN SITU ELLIPSOMETRY OF SURFACE LAYER OF NONMETALLIC TRANSPARENT MATERIALS DURING ITS FINISH PROCESSING

L.V. Poperenko, A.Y. Filatov, Physics Department, T. Shevchenko National Kyiv University, 6 Acad. Glushkov Ave., 03022 Kyiv, Ukraine

For modern technology applications it is important to develop non-contact methods of control of the modification of dielectric materials surface layer. The aim of the work is to determine the level of roughness changes in the surface layer of nonmetallic material, optical glass BK-7, and to control it by in situ ellipsometry. The probing light spot was formed at a second (lower) reflective surface of the plate being studied during its mechanical processing at direct observation of these changes. The fine mechanical polishing was carried out for 2 hours by using the grinding-polishing machine installed directly on the sample table of ellipsometer LEF-3M. The angle of light incidence was close to 70 deg. The ellipsometric parameters, Delta and Psi, were determined within the mechanically processed area. For this purpose, the probing light beam passed two times through the sample and then returned to the initial (air) medium, where its polarization state was studied. The polarized beam falls on lower plate surface polished by conventional technology using grinding-polishing CeO_2-based instrument "Aquapol"(grain size 1 micron). The time dependences of the ellipsometric parameters during the surface layer treatment were studied. In these dependences the tendency of changes of ellipsometric parameters (Delta - from 165 to 134 deg , Psi - from 24 to 36 deg) indicates the surface roughness enhancement.

P/P.13 EVALUATION STRATEGIES FOR MULTILAYER, MULTIMATERIAL ELLIPSOMETRIC MEASUREMENTS

O. Polgár, P. Petrik, T. Lohner, M. Fried Research Institute for Technical Physics and Material Sciences, H-1525 Budapest, POB 49, Hungary

In order to extract the physical properties from an ellipsometric measurement an optical model of the sample has to be assumed first, because the theory of ellipsometry consists on one-directional computation only (there is no reverse function). Then the ellipsometric evaluation is an iterative optimising procedure with high time consumption feature and the reliability depends strongly on the a-priori information. The faster the computers are today, the more exactly the physical properties of either the sample or the process can be evaluated. However the increasing number of the parameters and so the dimensions of the search space leads to a combinatorial explosion. In order to avoid that, and to fulfil in parallel the ever-increasing demand of gaining more reliable data, complex optical models with embedded physical functions, which describe the physical properties with less parameter, can be useful. In the case of larger search space is needed (either less a-priori information is available or more parameters are used) the error surface of the parameter space can be quite "hilly" and may contain even numerous local minima. In the lack of precise a-priori information the Levenberg-Marquardt gradient search is generally started out of the decreasing area of the global minimum and therefore it's inappropriate to find the solution. Therefore there is a hard need of more complex evaluating strategies, which combines the algorithms to make the evaluation more reliable. Different point selection strategies, an extended criteria function and combined algorithms [O. Polgár et al. Thin Solid Films 455-456C (2004) 95-100.] were applied on porous silicon multilayer and polycrystalline measurements to demonstrate a higher convergence speed (effectiveness) and more reliability.

P/P.14 HIGH RESOLUTION X-RAY DIFFRACTION OF GAN GROWN ON SI(111) BY MOVPE

N. Chaaben, T. Boufaden, A. Fouzri, and B. El Jani. Unité de Recherche sur les Hétéro-Epitaxies et Applications, Facultés des Sciences, 5019 Monastir, Tunisia.

High temperature (1080°C) GaN layers have been grown on Si (111) substrate by Metalorganic Vapor Phase Epitaxy (MOVPE). AlN buffer layer was used with various thickness and growth temperature. Single crystal GaN layers have been obtained on buffer layer with growth temperature of 1080 °C and thickness of 40 nm.

High resolution X-ray diffraction (HRXRD) was used for crystalline characterization. Symmetric and asymmetric GaN reflections were combined for tilt and stress measurements. Curvature radiuses of substrates were also measured. Complementary studies by scanning electron microscopy (SEM) were performed to evaluate respectively the morphological and optical qualities of GaN.

P/P.15 TRANSFORMATION OF HYDROGEN SILSESQUIOXANE PROPERTIES WITH RIE PLASMA TREATMENT FOR ADVANCED MULTIPLE-GATE MOSFETs.

J. Penaud, F. Fruleux, E. Dubois, I.E.M.N, Microélectronique Silicium, Avenue Poincaré, B.P.69, 59652, Villeneuve d'Ascq, France

Keeping in line with Moore's law requires increasing efforts in the development of alternative electronic devices. Multiple-gate transistors are very promising in order to suppress short channel effects and to increase the current drive. Nevertheless, the realization of such devices represents a strong challenge for silicon process technology. We propose an original and easy process to fabricate a triple gate MOSFET with sidewall extending into the buried oxide (Pi gate). One of the key steps is to use the fluable oxide Hydrogen Silsesquioxane (HSQ) as an isolated matrix for the thin silicium fins. Our aim is to engineer the properties of the HSQ in term of planarity and etching selectivity. SEM characterisation has shown that HSQ exhibits excellent planarization and gapfill capability, while AFM analyses, on 100 nm HSQ thickness films deposited by spin on, has measured an RMS roughness as lower as 3 nm. Different oxygen plasma treatments were applied to densify the HSQ films. FTIR Spectroscopy has shown very interesting qualitative and quantitative informations: chemical and physical transformations from a Si-O-Si cage-like structure to a Si-O-Si network one have been observed. It is shown that exposure to oxygen plasma at high power (290 W) for a long time (20 min) improves the resistance to 1% hydrofluoric acid. This densification technic holds the remarkable property to transform HSQ to a SiO2-like structure.

P/P.16 STABILIZATION OF THE ANATASE PHASE IN TIO2 (Fe^{3+})NANOSTRUCTURED COATINGS

C. Trapalis[1], M. Gartner[2], G. Kordas[1], M.Anastasescu[2], M. Zaharescu[2] M. Modreanu3, [1]Institute of Materials Science, National Center for Scientific Research "Demokritos", 153 10, Athens, Greece; [2]Institute of Physical Chemistry, Spl. Independentei 202, Bucharest 77208, Romania; [3]Tyndall National Institute, Lee Maltings, Prospect Row, Cork, Ireland

TiO2 has been shown to be an excellent photocatalyst for the degradation of several environmental contaminants. The photocatalytic activity of TiO2 is influenced by the crystal structure (anatase, rutile), dopants, surface area, size distribution and porosity, as well as by the surface hydroxyl group density. Multilayered TiO2(Fe3+, PEG) films were deposited on SiO2/glass substrate by sol-gel method The influence of Fe3+ and PEG concentrations, the number of coatings and calcinations time and temperature on the optical and microstructural properties of the TiO2 film were studied.

As-deposited TiO2(Fe3+,PEG) films were very porous, but after the thermal treatment at 500C, the PEG decomposed and burned out leading to the film densification. Homogeneous nanostructured films (as SEM image have shown) resulted, where the amorphous and the anatase phases coexist. XRD analysis showed that no rutile phase is observed in the films deposited on SiO2/glass as compared to those deposited directly on glass and that the presence of the anatase phase in the films without PEG is more evident in 3 layers film. The intensity of the main peak of anatase from 25 grade decreases with the increase of PEG concentration. The optical gap of the TiO2 (Fe3+, PEG) films is in the range of 3.03-3.05 eV and does not depend essentially on the PEG content.

P/P.17 Cu NANOPARTICLES FORMATION IN Cu:SiO_2 SOL-GEL THIN COATINGS

C.C. Trapalis[1] , G. Kordas[1], M.F. Gartner[2], P. Osiceanu[2], M. Anastasescu[2], M. Zaharescu[2] ;[1]Institute of Materials Science, National Center for Scientific Research Demokritos, 153 10, Athens, Greece; [2]Institute of Physical Chemistry I.G.Murgulescu,Romanian Academy, 202 Splaiul Independentei, 77208, Bucharest, Romania

Metal nanoparticles formation in dielectrics is a perspective direction of solid-state chemistry and more than that glass-metal nanocomposites are the subject of an ongoing investigation for applications including nonlinear optical properties, photonic devices, ceramic antibacterial coatings, medical tools and appliances. Such glasses and thin coatings can be prepared via the sol-gel route.

In the present work, the metal nanoparticles formation and the optical properties of nanostructured Cu:SiO2 sol-gel thin coatings were studied. It is proved that the Cu:SiO2 coatings prepared by sol-gel route show high absorption at 571 nm due to metal nanoparticles formation after thermal treatment at reductive atmosphere. Spectroellipsometric results pointed out the transformation of CuO from as prepared samples in Cu2O in samples heated in oxidative condition and in metallic Cu in samples heated in reductive conditions. This observation is supported by SEM and XPS analysis. The differences in the optical properties were attributed to differences in the distribution of copper in the coating, to the formation of copper nanoparticles, as well as to the diffusion of the metal in the glass substrate during the high temperature thermal treatment.

P/P.18 PHOTOLUMINESCENCE STUDY IN COMPOSITIONALLY STEP GRADED InxAl1-xAs/GaAs

N. Yahyaoui, S. Aloulou and M. Oueslati, Unité des nanomatériaux, Département de Physique, Faculté des Sciences de Tunis Compus Universitaire, le Belvédaire, Tunis 1060, Tunisie

Doped InxAl1-xAs/GaAs heterostructure lattice mismatched to GaAs are important for device applications including heterojonction bipolar transistors and modulation doped field-effect transistors. However such applications are limited in composition and thickness due to strain relaxation and the formation of lattice defects induced by the lattice mismatch between interfaces. In general the approach to growing highly lattice-mismatched epilayers is to interpose a buffer layer between the substrate and the active layers. The ideal buffer layer must be fully relaxed prevent dislocations from propagating into active layers. For this purpose, linearly graded buffer layers have been used for the lattice-mismatched systems.
The samples used in this study G30 and G40 are InxAl1-xAs epilayers grown on semi-insulating GaAs (001) substrate by Molecular Beam Epitaxy (MBE). Compositionally step graded, x@0.15/step buffer layers were used to relax the mismatch strain between these heterostructures and their substrates. The G30 and G40 active layer compositions are respectively x=0.46 and x=0.41 where the DX centers are resonant. These samples show intense PL spectra at T=300K with a main broad band at energies 1.58eV and 1.70eV corresponding to the direct band gaps in G30 and G40 respectively. In this paper we present a detailed study of the evolution of G30 and G40 PL spectra versus power excitation, temperature and excitation energy.

P/P.19 BAND STRUCTURE INVESTIGATIONS OF GaN FILMS USING MODULATION SPECTROSCOPY

V.P. Makhniy, M.M. Slyotov, V.V. Gorley, P.P. Horley, Yuri Fed'kovych, Chernivtsi National University, 2 Kotsyubynsky Str., 58102, Chernivtsi, Ukraine, and Yu.V. Vorobiev, J. Gonzalez-Hernandez, CINVESTAV Unidad Queretaro, Libramiento Norponiente 2000, Fracc. Real de Juriquilla, 76230 Queretaro, QRO, Mexico

Despite of numerous applications of gallium nitride in optoelectronics, some important physical parameters of this material are still not thoroughly investigated. First of all it is true for quantitative values characterizing band structure of the material, as well as position of impurity and defect levels. In this paper we discuss the spectra of main optical characteristics (transmission, reflection and luminescence) measured in lambda-modulation mode for epitaxy-grown GaN films. From the analysis of experimental data obtained, we determined the magnitude of valence band splitting caused by spin-orbital interaction (47 meV) and crystalline field (10 meV). Analyzing dependence of band structure on excitation level and the temperature, recombination centers were identified and mechanisms of irradiative transitions were determined. It was shown that the formation of impurity bands in the spectrum is connected with LO-phonons with the energies, correlating well with another published data.

P/P.20 OPTICAL AND X-RAY CHARACTERIZATION OF PROPOLIS

S.I. Drapak(a), A.P. Bakhtinov(a), S.V. Gavrylyuk(a), I.T. Drapak(b) Z.D. Kovalyuk(a) (a) Frantsevich Institute of Materials Science Problems, the National Academy of Sciences of Ukraine, Chernivtsi Department, 5 Iryna Vilde Str., Chernivtsi, 58001, Ukraine. (b) Chernivtsi Yuriy Fedkovich National University, Optoelectronic Department, 2 Kotsyubynskii Str., Chernivtsi, 58012, Ukraine.

Propolis, a honey bee glue, is widely used in medicine and fragrance-cosmetic industry. Recently [1, 2] it was established the possibility of the formation of photosensitive hybrid organic-inorganic (InSe, Si) heterojunctions on the base of this substance. In this communication we present the results of optical and X-ray studies of both initial composition of propolis films and thin films obtained from alcohol solution. It is established from researches of optical absorption spectra α(hν) at Т = 300 К that particularities of vibration spectra (wavelength range of 2.8-3.9 μm) and optical absorption, whish corresponds to π-π^* electron transitions in energy range of 3.1-3.25 eV at α(hν) > 10^(-3) cm^(-1), do not depend from the way of obtaining of amorphous films. The optical band gap of the substance (both initial composition of propolis and thin films obtained from alcohol solution) hν = 3.0-3.1 eV, whish was calculated by extraploting the straight line portions of the (αhn)^2 to α=0, is in good agreement with energetic position of photoluminescence maximums. Difference of absorption spectra at α < 10^(-3) cm^(-1) is determined by structure of amorphous films, definite from X-ray investigations

P/P.21 STRUCTURAL AND OPTICAL PROPERTIES OF DOPED TIN DIOXIDE THIN FILMS DEPOSITED BY CVD ON DIFFERENTS SUBSTRATES.

R. Outemzabet(a,b), N. Gabouze(b), H. Cheraga(b) and N. Kesri(a). (a) U.S.T.H.B. Faculté de physique, Laboratoire de semiconducteurs B.P. 32 El-Alia Bab-Ezzouar, Alger, Algérie. (b) U.D.T.S. 2, Bd Frantz Fanon, B.P. 399 Alger-Gare, Alger, Algérie.

Antimony doped tin dioxide SnO2-Sb thin films have been fabricated by atmospheric pressure chemical vapor deposition (CVD) at temperature varying between 350°C and 420°C in a horizontal reactor, from a mixture of hydrated SnCl2, SbCl3 and O2 gas. The SnO2-Sb films were grown on glass substrates and onto polished and porous n-type silicon. SnO2-Sb films fabricated for different dopant concentration (Sb/Sn varying from 4% to 0.66%) were characterised employing different optical characterisation techniques, like XRD, transmittance and reflectance in the wavelength range of 300 to 2500 nm and ellipsometry. X-ray diffraction measurements showed that as-prepared films are polycrystalline with 200 as preferred orientation. The microstructure of SnO2-Sb films depend strongly on deposition conditions and doping concentration. Examination of the surface by scanning electron microscope (SEM) showed that SnO2 and SnO2-Sb thin films are textured made up of many pyramidal grains with average grain size of 200 nm. The surface morphology was found to be independent on the kind of the substrate. The optical results provide information on film thickness, variation of transmittance and optical parameters upon antimony dopant concentration. The influence of the doping on the photoresponse of Sb-SnO2/porous Si/C-Si device is discussed.

P/P.22 OPTICAL AND X-RAY CHARACTERIZATION OF FERROELECTRIC STRONTIUM-BISMUTH-TANTALATE (SBT) THIN FILMS

M. Fried1, P. Petrik1, Zs. E. Horváth1, T. Lohner1, C. Schmidt2, C. Schneider2, H. Ryssel2,3 1 Research Institute for Technical Physics and Materials Science (MFA), Konkoly Thege Miklós ut 29-33, H-1121 Budapest, Hungary, 2 Fraunhofer Institute of Integrated Systems and Device Technology (IISB), Schottkystrasse 10, 91058 Erlangen, Germany, 3 Chair of Electron Devices (LEB), University of Erlangen-Nuremberg, Cauerstrasse 6, 91058 Erlangen, Germany

Strontium-Bismuth-Tantalate (SBT) is a new kind of dielectric layer material for use in semiconductor devices. The MOCVD made layers of SBT were characterized by Spectroscopic Ellipsometry (SE) using the Adachi model [S. Adachi, Phys. Rev. B 35 (1987) 7454-7463]. The evaluated optical parameters were correlated with the physical and chemical behavior examined by X-ray diffraction (XRD) and Rutherford backscattering (RBS).
As a result, it was possible to fit the measured spectra with the Adachi model in a wide range covering the region of the band gap. The Adachi model provides electronic layer-parameters like the transition energy E0 and broadening Gamma. Our investigations established a correlation between XRD-determined average grain-size and the electronic layer-parameters.

P/P.23 AN OPTICAL STUDY OF THE CORRELATION BETWEEN GROWTH KINETICS AND MICROSTRUCTURE OF MICROCRYSTALLINE Si GROWN BY SiH4-H2-He PECVD

M.M. Giangregorio1, M. Losurdo1, A. Sacchetti1, P. Capezzuto1, F. Giorgis2, G. Bruno1 1IMIP-CNR, via Orabona 4 - 70126 Bari, Italy 2 Physics Department, Polytechnic of Torino, Corso Duca degli Abruzzi 24, I-10129 Torino, Italy and Materials and Microsystems Laboratory (cLab), Lungo Piazza d'Armi 6, I-10034 Chivasso (Torino) Italy

The higher doping efficiency, enhanced carrier mobility and reduced optical absorption of hydrogenated microcrystalline silicon make mc-Si:H suitable for photovoltaics and electronics.
Therein, the effect of He dilution, deposition temperature (60-230°C), film thickness, substrate and of the in-situ substrate pre-treatments on the crystallite nucleation kinetics, growth/crystallization dynamics and on the mc-Si microstructure is discussed for mc-Si films deposited using SiH4-H2-He plasma enhanced chemical vapour deposition (PECVD). Non destructive optical probe also operating in real time including laser reflectance interferometry (LRI), spectroscopic ellipsometry (SE), and Raman spectroscopy are used for investigation of the correlation between the growth dynamics and film microstructure. From the diagnostic point of view, we focused on setting a structural model able to fit simultaneously LRI, SE and Raman data. From the process point of view, real time LRI highlighted the existence of a "crystallite induction time" that depends on the substrate pre-treatment and plasma phase. The "crystallite induction time" impacts on the film microstructure. Longer "crystallite induction time" results in a lower density of crystalline nuclei which grow laterally yielding to complete suppression of the amorphous incubation layer and to the growth of very dense, fully crystalline layers at a temperature as low as 120°C. The He dilution effect on the microstructure depends on deposition temperature. Amorphization of the network and its initiation by the presence of an extremely high void density in the incubation layer occur for He-diluted deposition at 230°C. In contrast, for T<160°C, He-dilution results in fully densed microcrystalline layers without incubation layer

P/P.24 OPTICAL CHARACTERISATION OF ROOM TEMPERATURE UV-BLUE EMMITING SiO_xN_y THIN FILMS

M. Modreanu, Tyndall National Institute, Lee Maltings, Prospect Row, Cork, Ireland, M. Gartner, Institute of Physical Chemistry, Spl. Independentei 202, Bucharest 77208, Romania; N. Tomozeiu, R&D Oce Technologies B.V. Postbus 101, 5900 MA, Venlo, The Netherlands

Silicon oxynitride (SiOxNy) thin films obtained by Low Pressure Chemical Vapour Deposition (LPCVD) are widely used in microelectronics and optoelectronics industry for passivating coatings and thin gate dielectrics.
In the last period, new applications in Micro-Opto-Electro-Mechanical-Systems as low stress membranes and optical wave-guides have been reported. Properties as: the ability to control its refractive index (of growing interest for integrated optoelectronic devices) by deposition parameters, the inertness and low mechanical stress recommend SiOxNy as a suitable material for such applications. The purpose of this paper is the investigation of the optical and microstructural properties of LPCVD SiOxNy thin films and the correlation of deposition parameters with material properties and its internal structure. Fourier Transform Infrared Spectroscopy, Variable Angle Spectroscopic Ellipsometry and Photoluminescence Spectroscopy were used to characterise the optical and microstructural properties of as-deposited and annealed SiOxNy films. SiOxNy thin films show a strong photoluminescence (PL) signal at room temperature (RT) in UV-blue spectral range. The PL peaks at 380nm and 425nm are resonantly excited with 280nm and 320nm light, indicating transition energies of 4.42eV and 3.26eV.

P/P.25 POLARIZED RAMAN SCATTERING OF WURTZITE GAN FILMS: THE DOUBLE MIXED NATURE OF THE 740 cm^{-1} BAND.

P.C. Ricci, A. Anedda, C.M. Carbonaro, R. Corpino, M. Marceddu, M. Salis, Dipartimento di Fisica, Università di Cagliari, and INFM, UdR Cagliari, sp n° 8, Km 0,700, I-09042 Monserrato (CA), Italy

Promising to a wide range of technology device manufacturers, gallium nitride exhibits: wide bandgap for optical and optoelectronic device in the visible and UV spectrum, high thermal conductivity, excellent thermal expansion and lattice match to GaN-based devices and good chemical stability. An exhaustive study of the polarized Raman scattering of wurtzite GaN films is presented, focusing on the nature of band at 740 cm-1 observed in the X(Z,Z)X configuration. The origin of this band has been assigned to the mixed contribution of the A1 and E1 longitudinal phonons coupled individually with the free carrier excitation. The spectral profile of the 740 cm-1 Raman band has been reconstructed through a linear combination of the A1-E1 longitudinal phonon plasmon coupled modes. The percentage of the mixed character has been calculated at 50 % and the phonon propagation direction has been estimated at 45° with respect to X axis of the crystal.

P/P.26 DONOR-ACCEPTOR PAIRS IN $AgGaS_2$

A. Anedda[1], C.M Carbonaro[1], R.Corpino[1], M. Marceddu[1], P.C. Ricci[1], I.M. Tiginyanu[2] and V.V. Ursaki[2]. 1) Dipartimento di Fisica, Università di Cagliari, Cittadella Universitaria SP Monserrato-Sestu Km 0,700, 09042 Monserrato (Ca), Italy and INFM, unità di Cagliari, 2) Laboratory of Low-Dimensional Semiconductor Structures, Technical University of Moldova, 2004 Chisinau, Moldova

AgGaS2 is a wide gap ternary semiconductor, which crystallizes in the chalcopyrite structure. Photoluminescence (PL) is characterized by a band peaked around 500 nm, related to donor-acceptor pairs recombination (DAP). However the exact nature of defects involved in DAP has not been clarified.

We performed PL measurement from 10K up to room temperature at different excitation powers. AgGaS2 excitation was provided by the 3rd harmonic (355 nm) of a Nd:YAG laser, with maximum power density on the samples of 150KW/cm2; excitation power has been varied over 5 orders of magnitude. We observed a band at 502.4 nm, with full width at half maximum of 36 nm, asymmetric in the low energy side. In the 10-293K range this band is interested by an enhancement of its half maximum width. Temperature dependence of intensity indicates an activated behavior, with activation energy of 55 meV. From the spectral distribution at the low energy side of the band, we estimated the energy of acceptor levels in 415 meV from valence band. These results are in good agreement with ionization energies of donors and acceptors, as theoretically determined. The efficiency of the recombination process exhibits a linear dependence from excitation power density. Above 150K an enhancement in the recombination efficiency has been observed. Such a results suggests that DAP emission could be inhibited by non-radiative processes, which become less efficient above 150K.

P/P.27 X-RAY TRIPLE-AXIS DIFFRACTOMETRY INVESTIGATION OF SI/SIGE/SI ON SILICON-ON-INSULATOR SUBJECTED TO IN-SITU LOW-TEMPERATURE ANNEALING

T. D. Ma, H. L. Tu, National Engineering Research Center for Semiconductor Materials, General Research Institute for Nonferrous Metals, No. 2, Xinjiekouwai Street, 100088 Beijing, P. R. China, G. Y. Hu, B. L. Shao, A. S. Liu, National Center of Analysis and Testing for Nonferrous Metals and Electronic Materials, General Research Institute for Nonferrous Metals, No. 2, Xinjiekouwai Street, 100088 Beijing, P. R. China

X-ray triple-axis diffractometry (TAD) was used to characterize heterostructure Si/SiGe/Si on Silicon-on-insulator (SOI) subjected to in-situ low-temperature annealing. Crystallographic tilt, lattice constant and relaxation percentage were examined respectively. In particular there are two peaks appearing in the (004) reciprocal lattice mappings (RLMs) of the epitaxial Si layers. The (004) RLMs indicate that Si cladding is in tensile strain. Whereas the offset in (004) RLMs of the Si layers underneath SiGe layer could not be explained satisfactorily although the thermal remnant stress was taken into consideration. Two peaks with different k// and k┴ were also found in (113) asymmetrical RLMs of the epitaxial Si layers. It is deduced from comprehensive analyses on (004) and (113) RLMs that Ge diffusion leads to the offset in (004) RLMs of the Si layers underneath SiGe layer. And the average concentration of Ge determined by TAD is mole fraction 0.85% which is very difficult to be measured so accurately by other methods.

P/P.28 THE X-RAY DIFFRACTOMETRY MORPHOLOGY INVESTIGATION OF THICK POROUS SILICON LAYERS

Anastacya A. Migunova, Analitical Centre, Institute of Nuclear Physics, Almaty, Kazakhstan

The thick porous silicon layers (TPSL) are a perspective material for preparation photon crystals, gas sensors and microchannel plates.

Different TPSL kinds were formed by two ways with variation of 1)Si-wafers parameters: (100)n- and p-types, few resistivities; 2) anodizing conditions: an electrolyte composition, current density j and etching time. The different TPSL-morphotypes constitution was studied by cross-section and topographic SEM and energy-dispersive analysis, X-ray diffractometry with D8 ADVANCE (Bruker). (100)n-TPSL are an array of microcolumnar crystallites, p-material is it of microtubes. Them length is determined by etching time and can be realised on all substrate thickness. The crystallite diameter depends on j and electrolyte composition. TPSL can have thin top random nanocrystallites layer which is variable composition SiOx semiamorphous phase with the O amount to 45 at.% on a surface. For etching time more than 1 h this layer can approach 100 mkm thickness, and diffractograms change from mono- to polycrystalline kind. The X-ray diffractometry was realized in usual geometry, grazing beam configuration, rocking curves were also taken. The degree of the mismatch TPSL lattice parameters and microstrains/stress are evaluated. The alternating layers with different assigned porosity are obtained by periodic modulation of current density.

P/P.29 STUDIES OF COMPACTION AND DECOMPACTION OF SIO_2 LAYERS ON SILICON SUBSTRATES BY INTERFEROMETRY AND SPECTROSCOPIC ELLIPSOMETRY

W. Rzodkiewicz, A. Panas and H. M. Przewocki, Institute of Electron Technology, Al. Lotników 46, 02-668 Warsaw, Poland.

Thermal oxidation of silicon is a fundamental step in VLSI technology. In semiconductor devices, stresses and strains are known to affect process yield and microelectronic device reliability. Therefore, there is a need for better understanding of generation mechanisms of elastic and non-elastic strains (compaction and decompaction) in the Si-SiO2 system.

In this paper, the influence of the strain on the optical properties of Si-SiO2 system has been investigated by spectroscopic ellipsometry (SE), interferometry and weighing methods. Subtle changes of densification (compaction degree) in silicon dioxide layers on silicon substrates has been determined by weight technique (relying on measurements of the silicon dioxide layer mass and calculations of the volume). Whereas, elastic stresses in the oxide layers have been measured by Fizeau fringes image analysis method. A comparison is made between the density of the silicon dioxide (ρ) with the results of calculations made using ρ=f(n) relations (where n is the refractive index) given in the literature. Our results remain in agreement with the experimental results of Taniguchi.

P/P.30 STRUCTURE OF Pt-Fe/Fe MULTILAYERES INVESTIGATED BY XRD, SAXS, TEM AND COMPUTER SIMULATIONS

N. Zotov, J. Feydt, T. Walther and A. Ludwig, Caesar, Ludwig-Erhard-Allee 2, 53175 Bonn, Germany

Double-period [(Pt/Fe)m Fe]n multilayers were prepared using a combinatorial sputter deposition approach. Such multilayers are expected to be suitable candidates for the synthesis of exchange-spring magnets consisting of soft- and hard-magnetic phases by thermal annealing.

The structure of the as-deposited multilayers was studied by wide-angle (WAXS) and small-angle X-ray scattering (SAXS), transmission electron microscopy as well as simulations of the X-ray scattering intensities with a newly written program. Texture measurements show that the multilayers have narrow angular distribution along the growth direction. WAXS and SAXS simulations give superlattice periods of the first Pt/Fe multilayer of about 24-27 Å, non-cumulative modulation variations and indicate the presence of interdiffusion at the interfaces. The second modulation period (124-175 Å) is generally incommensurate to the first one and the two sub-lattices scatter incoherently due to the presence of rough discontinuous interfaces. The out-of-plane coherence lengths (150-250 Å) decrease while the strains increase with increasing thickness of the additional Fe layers. SAXS non-specular scans indicate that there is no vertical correlation between the interface roughnesses. The in-plane correlation lengths are 1500-2000 Å.

P/P.31 SPECTROELLIPSOMETRIC CHARACTERIZATION OF SPUTTERED AMORPHOUS SILICON GERMANIUM THIN FILMS

T. Lohner, M. Serényi, Z. Zolnai, P. Petrik, Á. Nemcsics, N. Q. Khánh, Research Institute for Technical Physics and Materials Science, 1121 Budapest, Konkoly Thege M. ut 29-33, Hungary

Hydrogenated amorphous silicon-germanium thin films were prepared using radio frequency sputtering on top of bare or oxidized single crystalline silicon. Sputtering was done with a mixture of high purity argon and hydrogen. The layers have been investigated by spectroscopic ellipsometry (SE). To determine the Ar and Ge content of the films, Rutherford backscattering (RBS) measurements were performed. Multilayer optical models were developed for interpretation of the SE spectra. Both effective medium approximation (EMA) and parametric semiconductor model were applied to determine the dielectric function of the amorphous SiGe layers. The optical model for the film deposited on silicon dioxide covered silicon consists of five phases: air, roughness layer, parametric semiconductor layer, silicon dioxide layer and single crystalline silicon substrate. The layer thickness values obtained by SE and RBS exhibit satisfactory agreement. It was observed that the precision concerning the determination of the thickness of the amorphous SiGe layer deposited on 1 micron thick silicon dioxide covered silicon was several times better than that one for SiGe layer deposited on bare silicon.

P/P.32 OPTICAL CHARACTERIZATION OF $In_XGa_{1-X}N$ ALLOYS EMBEDDED IN MULTILAYER STRUCTURES

M. Gartner[1], C. Kruse[2], M. Modreanu[3], D. Hommel[2], [1] Institute of Physical Chemistry "I.G.Murgulescu" of the Romanian Academy, 202 Splaiul Independentei, 060021, Bucharest, Romania [2] Institute of Solid State Physics, University of Bremen, Otto-Hahn-Allee NW 1, D-28359 Bremen, Germany [3] Tyndall National Institute, Lee Maltings, Prospect Row, Cork, Ireland

We combined the utilization of spectroscopic ellipsometry (SE), raman spectroscopy, photoluminescence (PL) and reflectance measurements to investigate the optical properties, the microstructure and the quality of the InGaN/GaN/sapphire layers. The multilayered structures were grown on (0001) sapphire substrate by molecular beam epitaxy (MBE) and metal-organic vapor-phase epitaxy (MOVPE). The stoichiometry of the layers grown by MBE was adjusted by monitoring the surface reconstruction using reflection of high-energy electron-diffraction (RHEED).

SE measurements of InXGa1-XN/GaN complex heterostructures were performed in situ and ex situ. The analysis of SE data was done using a parametric dielectric function model, established by the analysis of individual layers. A dielectric function database, optical band gap, the microstructure and the alloy composition of the layers were derived. The SE band gap data are compatible with the reflectance and PL data. It was found that the GaN band gap changes with temperature after a Bose-Einstein equation $E(T)=Eg-0.22865[1+2/(exp(700 /T)-1)]$. The variation of the InGaN band gap with In content (x) in the $0<x<0.15$ range evolves after the linear law $Eg=3.44-4.5x$ The purity and the stability of the GaN crystalline phase, as well as the stress of the samples were investigated by Raman Spectroscopy. For example, the point defects can induce supplementary stress in the sample, which can be detected in the Raman spectra due to a shift of the main E1(LO) band. The spectrum of a hexagonal GaN sample without defects is dominated by the E2(TO), located at 568.63 cm-1, while in the spectrum of a GaN sample with defects E2 is shifted at 576.62 cm-1.

P/P.33 OPTICAL CHARACTERISTICS AND MICROSTRUCTURE OF RF-SPUTTERED BARIUM TITANATE THIN FILMS

A. Ianculescu1, M. Gartner2, B. Despax3, V. Bley3, Th. Lebey3, R. Gavrila4 1 "Politehnica" University of Bucharest, Department of Oxide Materials Science and Engineering, 1 Gh. Polizu, 78216, Bucharest, ROMANIA 2 Institute of Physical Chemistry of the Romanian Academy, 202 Splaiul Independentei, 77208 Bucharest, ROMANIA 3 "Paul Sabatier" University, Department of Electrical Engineering, 118 Route de Narbonne, 31062 Toulouse, FRANCE 4 National Institute of Microtechnologie, 32B Erou Iancu Nicolae, 72225 Bucharest, ROMANIA

Crystalline BaTiO3 thin films were successfully deposited on platinum coated Ti/SiO2/Si substrate by RF magnetron sputtering. In order to investigate the optical properties and the microstructure of the annealed thin films, Spectroscopic Ellipsometry (SE), Atomic Force Microscopy (AFM) and High Resolution Electron Microscopy (HRTEM) were used. The dependence of the structural and microstructural properties (texture, degree of crystallinity), as well as of the optical characteristics on the deposition parameters was analysed. Samples with the same characteristics could be obtained by varying of different technological parameters of the deposition process. The films thickness increases with the decrease of both deposition pressure and distance between sample and discharge centre. The films annealed at 900°C, for 8 hours, exhibit a direct band gap energy ranged between 3.57 - 3.59 eV. The roughness values (10 - 20 nm) of the surface layer estimated from SE coupled with the Bruggeman Effective Medium Approximation (B-EMA) and from AFM measurements were in good agreement. Cross-section and surface SEM analyses were carried out in order to check the thickness values obtained by spectroellipsometry and to emphasize the growth mechanism, as well as to determine the average grain size of the films. The deposited films show densely packed, non-columnar structure and hexagon-like crystallite.

P/P.34 AN XPS STUDY ON ION BEAM INDUCED OXIDATION OF TITANIUM SILICIDE

P. Osiceanu, Institute of Physical Chemistry "I.G. Murgulescu", Spl. Indep. 202, Bucharest 77208, Romania

The 3d metal silicides layers are of great interest for VLSI techonology as interconnect material and gate electrodes. Titanium silicides films grown on Si(100) substrate were investigated by "in situ" XPS depth profiling after athermal ion beam induced oxidation. The composition and stoichiometry of these films were quantitatively determined as chemical state relative concentrations vs. sputter time.The initial sample TiSi2 has been athermal oxidized by O2+ ions at 12 keV energy and normal incidence and then sputter etched with Ar+ ions at 2.5 keV and normal incidence. Narrow energy windows have been placed on the main pfotoelectron lines of Ti(2p), Si(2s), O(1s) and N(1s). While the silicon is found to be almost full oxidized over a large range in the sampling material, the titanium oxidation states are mixed , the suboxides being imbeded into the "bulk""of the film. The presence of titanium in its suboxides forms spread over a wide sampling depth suggest its "catalytic - like" behavior in the silicon oxidation process. Some trace of titanium nitride is detected revealing the very high reactivity of titanium in titanium silicide even in its oxidized form.

P/P.35 CHARACTERIZATION OF Si NANOCRYSTALS INTO SiO_2 MATRIX

Gravalidis C., Logothetidis S., Hatziaras N., Laskarakis A., Fragkis N., Tsiaousis I., Department of Physics, Aristotle University of Thessaloniki, GR-54124, Thessaloniki, Greece

Silicon nanocrystals (nc-Si) have gained great interest due to their excellent optical and electronic properties and their applications in optoelectronics. The aim of this work is the explanation of growth mechanism of nc-Si into SiO2 matrix from SiO/SiO2 multilayers annealing, using x-rays and optical techniques. The multilayers were grown by e-beam evaporation in UHV conditions from SiO and SiO2 evaporation materials and annealed at high temperatures (500-1100 οC) in N2 atmosphere. X-Rays Diffraction, X-Rays Reflectivity and Transmission Electron Microscopy were used for the structural characterization and Spectroscopic Ellipsometry from IR to FUV for the study of optical and electronic properties. The ellipsometric results gave evidence of the formation of a SiO2 matrix after the annealing process. Additionally the X-Rays diffraction identified the formation of Si crystal phases, fact proved also from HREM. The origin of these nc-Si is enhanced from the XRR results, which gave correlations between the SiO and SiO2 layers thickness, proving the growth of SiO2 matrix, as was found from FTIRSE, with portions of nc-Si inside. Using the above results we describe the growth mechanism of nc-Si into SiO2 matrix under N2 atmosphere.

P/P.36 MODELLING OF LASER REFLECTANCE EVOLUTION DURING MOVPE GROWTH OF GaN ON 2D AND 3D NUCLEATION LAYER

H. Fitouri, Z. Benzarti, I. Halidou, T. Boufaden and B. El Jani Unité de Recherche sur les Hétéro-Epitaxies et Applications, Faculté des Sciences de Monastir, 5019 Monastir, Tunisie

The SiN treatment of the sapphire substrate for GaN growth induces a spectacular effect on the in situ reflectometry monitoring signal. Different growth modes are observed. The evolution of the reflectometry signal is simulated by the scattering theory approximation. The point by point analysis revealed that the roughness (rms) increases in the first region where the growth mode is dominated by the formation of isolated and three-dimensional hillocks. The rms attains a maximum value exceeding that authorized by the Rayleigh criterion. Another approach based on the effective medium approximation is used to simulate the entire reflectometry signal evolution. An effective refractive index and a growth rate profiles are determined. Obtained results agree the observations done by the in situ ellipsometry monitoring.

P/P.37 NEW CALIBRATION METHOD FOR A UV/VIS PHOTOTHERMAL DEFLECTION SPECTROSCOPY SET-UP

Jordi Sancho-Parramon, Josep Ferré-Borrull, Anna Krasilnikova* and Salvador Bosch Departament de Física Aplicada i Òptica, Universitat de Barcelona Diagonal 647, 08028 Barcelona, Spain * Optical Coatings Group, ENEA, Via Anguillarese 301, 00060 Roma, Italy

Photothermal deflection spectroscopy (PDS) is a useful technique for the determination of the optical absorption of low-absorbing materials. The technique is based on the heating of the sample under investigation by a normally incident beam of light, inducing a gradient of refractive index in the surrounding medium of the sample (mirage effect). This gradient is therefore related to the sample absorption and can be estimated by the deflection of a laser beam travelling parallel and close to the sample surface. In order to improve the sensitivity of the technique, the sample is immersed in a medium (generally, a liquid) with a high rate of variation of the refractive index with the temperature.

One of the main drawbacks of this technique is the need of a reference sample with very well known absorption, for the calibration of the setup. A typical approach for referencing consists in implementation of a highly absorbing sample with assumed absorption equal to 100% that leads to an unavoidable systematic error. We present a new method for referencing, based on the use of samples with various levels of absorption. The samples are single thin films of amorphous carbon deposited by r.f. sputtering under various conditions (deposition time, substrate, etc). The optical constants of the samples are accurately determined from spectrophotometric measurements that has enabled the computation of the corresponding optical absorption in the liquid used for amplification of the mirage effect. The calibration method is cross-checked by comparison of the measurements for the several reference samples and is finally applied to the study of the absorption of single dielectric thin films.

P/P.38 OPTICAL CHARACTERIZATION OF ns-SiN:H IN THE INFRARED BY SPECTROSCOPIC ELLIPSOMETRY

Jordi Sancho-Parramon, Salvador Bosch and Adolf Canillas Departament de Física Aplicada i Òptica, Universitat de Barcelona Diagonal 647, 08028 Barcelona, Spain

The optical properties of dielectric materials in the infrared spectral range are determined by the presence of vibrational absorption bands. Infrared spectroscopic ellipsometry (IRSE) has emerged as a powerful technique for the optical characterization of these materials. Typically, the IRSE measurements are fitted considering the contribution of an oscillator for each of the vibrational absorption bands. Thus, when several bands must be considered, a large number of parameters is required for the correct description of the data, increasing the difficulties on the numerical inversion of the data due to the multiplicity of solutions.

This work is focused on the accurate optical characterization of nanostructured amorphous silicon nitride (ns-SiN:H) by means of IRSE in the spectral range between 950 and 3500 cm-1. The samples investigated consist of single layers of ns-SiNH deposited on metallic substrates. The analysis of the measured data reveals the presence of a significant number of vibrational absorption bands. In order to fit the data, two different strategies are tested: i) fitting all the available experimental data optimising all the required parameters in a single step (the standard numerical approach), and ii) fitting the data in a progressive way, introducing at each step new absorption bands and thus extending the fitted spectral range. The first approach leads to solutions where some of the vibrational bands (those of lowest intensity) are ignored, while the second strategy is able to account for those bands, leading more meaningful results.

P/P.39 ENERGETICS AND PARAMETERS IN TGS FERROELECTRIC TRANSITION

C. Berbecaru, H.V. Alexandru, F. Stanculescu, A. Dutu, Faculty of Physics, University of Bucharest; V. Ciupina, "Ovidius" University of Constanta, Romania.

An extended Landau type-model for the second order phase transition was cheeked in pure and doped TGS crystals. Gibbs free energy in three-terms polynomial expansion was used. Temperature dependence of coefficients was calculated using experimental data on a large temperature interval. The second coefficient, is always dominant and sharply increases <5 oC near the transition point, when a DC bias field is considered. The third coefficient "naturally" increases near the Curie point, some constant values found in the literature, fit quite well our curves, but only in a few distinct points, 5-10 oC near the Curie Point. Gibbs free energy curves GE(P,T) versus polarization, show peculiar behavior depending on the external field, in the temperature range 3¸5 oC near the Curie point. The energy corresponding to the internal field Eint " PS /3eo, is higher or comparable to kBT, only at T £ Tc - 10 oC.
The equation of state E(P,T), which is supposed to represent the hysterezis loop P(E) gives the coercive field two order of magnitude higher than measured values. We conclude that the free energy of TGS is a non-analytical function. Some other models, taking into account short and long-range interaction, have to be considered (H.V.Alexandru, C.Berbecaru, Mater. Science in Semicond. Processing 5 (2003) 159-165).

P/P.40 OPTICAL PROBING OF THE WEAK DIELECTRIC TENSOR COMPONENT IN QUATERTHIOPHENE CRYSTALS

S. Tavazzi, A. Borghesi, M. Laicini, A. Papagni, L. Raimondo, S. Trabattoni INFM and Dipartimento di Scienza dei Materiali, Università di Milano Bicocca, Via Cozzi 53, I-20125 Milano, Italy P. Spearman School of Chemical and Pharmaceutical Sciences, Kingston University Kingston upon Thames, KT1 2EE, United Kingdom

Recently, molecular-based materials have been attracted a great interest due to their suitability in nanotechnology applications. A crucial point is to understand the intrinsic properties of these solids which are highly anisotropic and often possess strong optical transitions. This is the case of oligothiophenes that crystallize in the monoclinic system with two or four molecules per unit cell, so that the Frenkel-Davydov exciton model predicts a splitting of the molecular singlet states into multiplets of bands. In addition to these neutral Frenkel excitons (FE), there exist excited states of charge-transfer (CT) origin where the promoted electron is transferred to nearest neighboring molecular sites. CT states influence the creation of charge carriers and their study is fundamental for the comprehension of the optical and electrical properties. However, their absorption is usually masked by FE vibronic satellites and the intensity is in general weak. In this paper, we report polarized reflectance and absorbance spectra of quaterthiophene single crystals recorded at low temperature. For generic experimental configurations, a wave with mixed transverse and longitudinal character propagates. A strong directional dispersion in the optical spectra is observed and for some angles of incidence a stopping band is detected due to the real part of the dielectric function being negative. Exploiting experimental configurations at oblique incidence which do not excite the FE states (for wave vector propagating along the FE transition moment), it is also possible to detect evidence of CT bands, otherwise buried under the FE bands occurring in the same energy region.

P/P.41 BST SOLID SOLUTIONS, TEMPERATURE EVOLUTION OF THE FERROELECTRIC TRANSITIONS

H.V. Alexandru, C. Berbecaru, A. Dutu, Faculty of Physics, University of Bucharest; A. Ioachim, National Institute of Materials Physics, Bucharest-Magurele Romania

Solid solutions Ba1-xSrxTiO3 (BST) are of high technological importance, particularly in microwave domain. Barium titanate has "naturally" three transitions, between four stable ferroelectric phases: (1) cubic - (2) tetragonal - (3) rhombic - (4) rhomboedric. Jaffe [1] has given the dependence of the transition temperatures up to the Sr concentration of about 30 %. We have extrapolated these temperatures and we have found that some phases might disappear at higher Sr concentrations.
A family of solid solutions with x = 25, 50, 75, 90 % was prepared by standard solid-state reaction and sintered at 1260 oC [2]. The permitivities and the dielectric losses were measured (1 KHz), on a large temperature range (± 200 oC). The composition x = 25 % shows three peak values of permitivity as expected, while the composition x = 0.50 % only two peak values, corresponding to phase transitions cubic-tetragonal-rhomboedric, phase (3) being excluded. Compositions with x ³ 0.75 % Sr shows only one peak value corresponding to a genuine transition cubic-rhomboedric. The cubic transition to several lower phases shows almost a linear decrease of the Curie Point with the increase of Sr fraction. At x ³ 80 % Sr concentration, the Curie Point appears to fall more rapidly than linear. To our best knowledge, there is for the first time this effect is reported. Some other data will be reported in the lecture. References: [1] B.Jaffe et al, Piezoelectric Ceramics, Acad. Press 1971. [2] H.V.Alexandru, C.Berbecaru et al, Mater.Sci.Eng. B, in press

P/P.42 REDUCTION OF GAAS DRY ETCH DAMAGE BY A CL_2/Ar NEUTRAL BEAM ETCHING

Byoung-Jae Park, Do-Haing Lee, Dong Yul Lee*, Dong Woo Kim* and Geun-Young Yeom Department of Materials Science & Engineering, Sungkyunkwan University, Suwon, Korea * Samsung Electromechanics, Korea

Plasma etching is essential in the fabrication of compound semiconductor devices due to the requirements of anisotropic profiles and submicron features for optoelectonic integrated circuits, microwave devices, lasers, etc. In the application to these devices, dry etch damage is a potential concern because it may affect device performance through the enhanced non-radiative carrier recombination, degraded mobility, decreased carrier density, etc.
In this study, a Cl2-based directional radical (or neutral) beam was formed by the low angle reflection of the energetic directional Cl2-based reactive ions generated by a Cl2/Ar inductively coupled plasma (ICP) gun, and, using the directional radical beam, GaAs was etched and its etch characteristics such as etch rates and etch damage were investigated. As a comparison, GaAs was etched by a conventional Cl2 ICP in addition to the Cl2-based neutral beam. Both techniques showed anisotropic etch profiles even though the neutral beam etching showed a significantly lower etch rate than that by the ICP. When dry etch damage of the etched GaAs was investigated by using PL and PRS, no damage could be observed when the neutral beam etching was used while the ICP etched GaAs showed a significant damage. No damage by the energetic neutral beam etching appears to be related to the insignificant reaction of the neutrals with the electrically active surface states during the etching.

P/P.43 BAND GAP STRUCTURE PECULIARITIES OF GaAs MODIFIED TO PATTERNED As_2O_3 - GaAs MEDIA

T.Ya. Gorbach, L.A. Matveeva, P.S. Smertenko, V. Lashkarev Institute of Semiconductors Physics, National Academy of Sciences of Ukraine, 45 prospekt Nauki, 03028 Kyiv, Ukraine; and M. Kuzma, Institute of Physics, Rzeszów University, Rejtana 16a, 35-309 Rzeszów, Poland

To probe the band gap structure of patterned dendritic As2O3 - GaAs media, which was prepared by wet etching in HNO3 solution, the electroreflectance (ER) spectroscopy has been carried out in GaAs (or As2O3 - GaAs)- 0.1 N KCl system by classic modulation technique in the energy range from 1.1 to 3.5 eV in low field mode at 273 K. As diagnostic indicators, the energies of Eo (Ã8V - Ã6C transition) and E1 (L4,5 - L6 transition) at the critical points of Brilloun zone Ã and L, respectively, both energies of spin-orbit splitting Do, D1 and the phenomenological broadening parameters Ã 0, Ã1 were used. The ER spectra analysis has shown the existence of redshifts in E0, E0+Do, E1 and E1+D1 at the fundamental gap; changes in Ã0, Ã0+Do, Ã1, Ã1+D1, the multioscillatory structure presence and the spin-orbit signal distortion. Another important features of ER spectra were the additional peaks between E0, E0+Do at 1.65-1.75 eV and the additional transition at 1.1-1.3 eV and 2.0-2.6 eV. The magnitude of these features is a function both the oxide thickness and the thickness or degree of disorder and nonstoichiometry (Ga-vacancies, free As) at As2O3 - GaAs interface. Possibility that the observed peculiarity may be due to the interface nature and multiquantum wells formation is discussed.

P/P.44 IMPLANTATION DOSE OF Si^+ INTO SiO_2 EFFECTS ON THE ELLIPSOMETRIC PARAMETERS

M. Mansour(a), A. En Naciri(a), L. Johann(a), V. Dzhagan(b), M.Ya. Valakh(b), V.O. Yukhymchuk(b), (a)Laboratoire de Physique de la Matière Dense, 1Bd Arago, CP 87811, 57078 Metz Cedex 3, France, (b)Lashkaryov Institute of Semiconductor Physics, NAS of Ukraine, Prospekt Nauki 41, 03028 Kyiv, Ukraine

Nanocrystalline semiconductor based on silicon nanocrystal (nc-Si) has recently attracted much intention, because those systems show a highest potential application in a visible light emission device. The optical and electrical properties are investigated to understand the origin of the remarkable photoluminescence behaviour and the expansion of the gap energy in such layer.
Among the different method to characterize optical properties, ellipsometry is a very sensitive measurement technique that uses polarized light to characterize isotropic and anisotropic thin films. This technique is based on the measurement of the parameters y and D called ellipsometric angles. In this letter, we report the study of ellipsometric responses of nanocrystalline silicon implanted in a host matrix SiO2 on the Si substrate. The measurements are performed in air at room temperature of the sample with different doses of 4x1016 cm-2, 6x1016 cm-2 and 2x1017 cm-2. We observe that the ellipsometric parameters ψ and ∆ change with implantation doses, and hence the dielectric function of nc-Si. We found the correlation between the change of the implantation doses and ellipsometric responses. The real and the imaginary part of the dielectric function of nc-Si are determined for different doses using Tauc Lorentz dispersion combined with the Bruggeman effective medium approximation. It is demonstrated that spectroscopic ellipsometry is a useful technique to characterise the nanostructured material. The behaviour of the photoluminescence (PL) band maximum with a variation of the implantation dose is also discussed.

P/P.45 PYROELECTRIC COEFFICIENT MANIPULATION IN DOPED TGS CRYSTALS

H.V. Alexandru, C. Berbecaru, L. Ion, A. Dutu, F. Ion, University of Bucharest; L. Pintilie, National Institute of Materials Physics, Bucharest-Magurele, Romania; R.C. Radulescu, Galway-Mayo Institute of Technology, Dublin Road, Galway, Ireland

High quality L or D alanine doped TGS crystals were grown at 52 oC in paraelectric phase [1]. Smaller permitivity and lower dielectric losses (up to one order of magnitude), are typical for such doped crystals and higher figures of merit make these materials attractive for IR detection devices. Internal bias field of ~1 kV/cm, induced by L/D alanine dopant, stabilizes the polarization components P+ and P- in opposite directions, with peculiar dependence on the measuring AC electric field [2].
Pyroelectric coefficient measurements were performed at constant heating rate of the samples, using a computer controlled He cryostat and Keithley 6517 electrometer. The temperature dependence of P+ polarization, pined by L dopant (obtained by computer integration of the pyro coefficient), compare well with P+ component of the hysteresis loops, Sawyer-Tower measured and computer recorded in conjunction with Tektronics TDS 210 digital oscilloscope. Pyroelectric coefficient of the doped samples could be adjusted on specific temperature intervals and polarization also tailored with positive or negative values. The pyroelectric coefficient could be made almost constant on 25-40 oC intervals, for EDC " 0.8 Kv/cm. References: [1] C.Berbecaru et al, Mater.Sci.Eng.B -in press, [2] H.V.Alexandru et al, Sensors and Actuators A 113 (2004) 387-392

P/P.46 HIGH-K Mg-DOPED ZST FOR MICROWAVE APPLICATIONS

A. Ioachim, M.G. Banciu, M.I. Toacsen, L. Nedelcu, D. Ghetu, National Institute of Materials Physics, Bucharest-Magurele, H.V.Alexandru, C.Berbecaru, University of Bucharest, G. Stoica I.P.E.E. Curtea de Arges, Romania

High-k dielectric materials have a determinant influence on the electronic engineering and communications. Ceramic dielectrics offer cost-effective solutions for applications [1]. The (Zr0.8Sn0.2)TiO4 material (ZST), has been prepared by solid state reaction and characterized. The samples were sintered in the temperature range of 1260 ÷ 1320 0C for 2 hours. The effects of sintering parameters such as sintering temperature (Ts) and MgO addition (0.2wt%) on structural and dielectric properties were investigated. Mass density increases from 4.85 g/cm3 to 5.06 g/cm3 with the increase of sintering temperature. The effect of MgO addition is to lower the temperature in order to obtain well sintered samples with high mass density. The material exhibits a dielectric constant er ~ 36 and high values of the Q× f product greater than 45.000 at microwave frequencies.
The dielectric properties make the ZST material very attractive for microwave applications [2] such as filters, antennas, hybrid microwave integrated circuits, etc. [1] Y. Higuchi, H. Tamura, Journal of the European Ceramic Society, Vol. 23 (2003), pp. 2683 [2] A. Ioachim at al., Journal of Optoelectronics and Advanced Materials, Vol. 5, no. 5, (2003), pp. 1389

P/P.47 GIXR AND GISAXS STUDY OF SILICON OXINITRIDE FILMS

S. Bernstorff, Sincrotrone Trieste, SS 14, km 163.5, Basovizza (TS), Italy, P. Dubcek, B. Pivac, I. Kovacevic, R. Boskovic Institute, P.O. Box 180, Zagreb, Croatia, A. Sassella, A. Borghesi, Universita degli Studi di Milano-Bicocca, Milano, Italy

Thin films of silicon oxinitride have largely replaced pure silicon oxide films as gate and tunnel oxide films in modern technology due to superior properties in terms of the boron barrier, resistance to electrical stress and high dielectric strength. A single chamber system for PECVD vapor deposition was employed to deposit different films of SiOx:N,H with $0.85<x<1.91$. All films were previously characterized by RBS and FTIR to determine the soichiometry and the presence of various chemical bonds. We used grazing incidence x-ray reflectivity (GIXR) to determine the electron density profile across the depth, the roughness at the interfaces, and also to a certain extent the chemical composition by proper modeling of the structure of the film. We have shown the existence of a varation in the electron density profile which is a function of the stoichiometry of the film. Moreover, grazing incidence small-angle X-ray scattering (GISAXS) was used to study inhomogeneities (clustering) in the film as a function of the composition.

P/P.48 GRAZING INCIDENCE X-RAY REFLECIVITY STUDY OF HYDROGEN IMPLANTED SILICON

P. Dubcek, B. Pivac, Rudjer Boskovic Institute, POBox 180, 10000 Zagreb, Croatia, S. Bernstorff, Sincrotrone Trieste, SS 14km163,5, 34012 Basovizza(TS), Italy, F. Corni, R. Tonini, G. Ottaviani, Dipartimento di Fisica, Universita di Modena, Via Campi 213a, 41100 Modena, Italy

The Grazing Incidence X-ray Reflectivity (GIXR) technique was used to study monocrystalline silicon samples implanted with H2 ions at an energy of 32 keV and to the dose of 1E16 ions/cm2. All samples were subsequently isochronally annealed in vacuum at different temperatures in the range from 100 to 900 C. Although the hydrogen depth distribution was expected to be smooth initially, fringes in GIXR spectra were observed already in implanted but not annealed sample, revealing the presence of a well defined film like structure. Annealing enhances the film top to bottom interface correlation due to structural relaxation, resulting in presence of fringes in the larger angular range, already at low annealing temperatures. The thickness of the film decreases slowly up to 350 C where substantial changes in the roughness are observed, probably due to the onset of bubble formation, as observed by GISAXS in our previous study. Further annealing at higher temperatures restores the high correlation of the film interfaces, while the thickness decreases with the temperature more rapidly.

P/P.49 INFRARED SPECTROSCOPIC ELLIPSOMETER APPLICATION IN YIELD OPTIMISATION FOR IC MANUFACTURING

Jean-Louis Stehlé(a), Sophie Bourtault(a), Marc Bucchia(a), Christophe Defranoux(a), Cécile Guillotin (a), Dorian Zahorski(a), Laurens Kwakman(b), Chantal Trouillet(c), (a)SOPRA, 26 rue Pierre Joigneaux, 92270 Bois-Colombes, France, (b)PHILIPS Semiconductors, 850 rue Jean Monnet, 38920 Crolles, France, (c)STMicroelectronics, 850 rue Jean Monnet, 38920 Crolles, France

The complexity and costs of IC manufacturing requires tighter controls and more often on the products themselves. The accumulation of multilayers, particularly in ILD with double damascene, demands recurrent monitoring and the number of parameters per level is increased, particularly in case of ULK with etch stop, encapsulation and barrier layers. The Infra-Red Spectroscopic Ellipsometer (IRSE) measures in the mid Infra-red range from 1.7 to 17 µ where transparent regions and molecular bounds can be found. The sensitivity of this ellipsometer for thickness is better than 0.1 nm and the concentration of molecular bounds is given within 0.1%, particularly for SiN, SiH, CHx, O-Si-O and H-O which are very important for dielectric constant K. The electrical K value is also found at 30 THz and more representative of 30GHz clock than the DC and 1MHz CV probe. The barrier layer of TaN is measured in thickness and by using the Drude model as well as the sheet resistance. In conclusion, the IRSE300 with its box size of 100 x 250 µ can control the ILD multilayers in line, giving from one single measure thickness, composition and electrical information of multilayers together at 15 pattern wafers per hour for 5 points per wafer. Examples, results and modeling will be described.

P/P.50 CHARACTERIZATION OF COMPLEX MULTILAYERED MATERIALS BY BOTH FFT AND WAVELET TRANSFORM ANALYSIS ON X-RAY REFLECTOMETRY PROFILES. APPLICATION TO HETERO-STRUCTURES DEDICATED TO OPTOELECTRONIC DOMAIN

O. Durand, N. Morizet, Thales Research and Technology, Domaine de Corbeville, 91404 Orsay Cedex, France

For recent years, some innovative approaches are made on novel semi-conductor-based optical components, leading to more complexity and miniaturization. Realization of such devices needs the mastering of the material elaboration. Therefore, it is crucial to characterize precisely the stacking structure of these multilayered materials dedicated to optoelectronic applications, i.e. the layer thicknesses, the roughnesses, the superlattice periods, etc...

It is given here an approach of the structural analysis of thin-films materials by X-ray reflectometry with a scope centered on applications dedicated to real devices. Since the complexity of multilayered materials for optoelectronics is increasing dramatically, leading to complex X-ray reflectometry spectra, the extraction of information using simulation and fitting procedures is becoming very time-consuming, even hazardous. We propose methods based on the signal-treatment field, such as Fast Fourier Transform and wavelet transform, to extract the individual layer thicknesses from complex X-ray reflectivity profiles. Using the results from the signal-treatment tools, fitting procedures can then be used to assess the electronic density profile through the surface/interface roughness values.

P/P.51 SPECTROSCOPIC STUDY ON HIGH TC YBCO THIN FILMS OBTAINED BY PULSED LASER DEPOSITION

M. Branescu, National Institute for R&D of Material Physics, P.O. Box MG-7, Bucharest, Romania, P. Ionescu, "Horia Hulubei" National Institute for Physics and Nuclear Engineering, P.O. Box MG-6, Bucharest, Romania, A. Moldovan, National Institute for Lasers, Plasma and Radiations Physics, P.O. Box MG-36, Str. Atomistilor, Nr. 111, Bucharest, Romania

For small-scale applications of superconducting electronics, large area, multi-layer, epitaxially grown thin films with smooth surfaces and interfaces are required. Presently high temperature superconductor thin films for electronic applications are dominated by YBCO and related 123 materials. For these films, the microstructure is crucial to obtain high quality thin films with high reproducibility. Pulsed laser deposition (PLD) of the UV laser represents a particularly valuable tool, as the pulsed burst mode of operation revealed to provide particularly efficient energy transfer mechanisms of YBCO thin films. In this report we present the review of results obtained by authors from recent experiments which deals with the PLD and the post annealing processes of YBCO thin films that exhibit the TC around 90 K. Its have been epitaxially grown on LaALO3 substrates starting from sintered targets. Growth conditions were optimized to obtain epitaxial growth. We investigated the composition and the thickness of YBCO thin films using elastic recoil detection analysis (ERDA) and Rutherford Backscattering Spectroscopy (RBS). We used X-ray diffraction, optical Ellipsometric and Raman scattering spectroscopy to determine the superconducting phase, the mosaic spread, morphologic and micro-crystalline properties of these films. We have correlated the qualitative and quantitative information obtained by non-polarized Fourier Transform Raman spectra and polarized dispersive Raman spectra respectively, concerning the texture, thickness and oxygenation of YBCO thin films.

P/P.52 INTERFEROMETRIC EQUIPMENT FOR MORE PRECISE DETERMINATION OF ISOTROPIC AND ANISOTROPIC MATERIAL REFRACTIVE INDEXES

A.S. Andrushchak, B.V. Tybinka, M.V. Kaidan, Lviv Polytechnic National University, 5 Knyaza Romana Str., 79005 Lviv, Ukraine

The created automatic interferometric equipment allows measuring more accurately the refractive indexes for flat-parallel sample from any isotropic or anisotropic material. This is a non-destructive control express-method, after which the measuring sample can be used for future investigation.This equipment is based on our patent idea and consisted of: 1) the Michelson interferometer, 2) the rotation device and 3) optical registration system. The refractive indexes for investigated material are calculated on the basis of measured sample rotation angle and interferometric fringe shift using elaborated software. From theoretical calculation the precision of the refractive indexes determination is equal dn=4.4×10-6. Now from our previous test on created automatic equipment we have determined n=1.4594±0.0002 for fused-SiO2 and no=2.2845±0.0005 for LiNbO3 crystals. This computer-aided interferometric equipment has not analogues in the world practice. It can be used during scientific investigation and especially for non-destructive express-analysis of new and already existing anisotropic materials in industrial laboratories that guarantees more precise measurement of their refractive indexes and economy of valuable crystal raw materials.

P/P.53 QUANTITATIVE METHODS FOR NANOPOWDERS CHARACTERIZATION

T. Wejrzanowski(a), R. Pielaszek(b), J. Michalski(a), H. Matysiak(a), W. Wojkowski(b), K.J. Kurzydowski(a), (a) Warsaw University of Technology, Faculty of Materials Science and Engineering, Wooska 141, 02-507 Warsaw, Poland, (b)High Pressure Research Center of the Polish Academy of Science, Sokolowska 29, 01-142 Warsaw, Poland

The size, shape, and surface topology has a strong influence on powders properties, such as: mechanical, optical, catalytic, etc. In addition, when particles have a nanometer size the dispersion of these features are taking an important role.

There are a number of techniques, which could be used in order to characterize powders in terms of their particle size and shape. However, due to the scale of analysis, well beyond wavelength of visible light, most of them can not be applied for investigations of nanopowders. In this work the Transmission Electron Microscopy image analysis and X-ray methods are presented as a promising and complementary techniques. The examples of their applications for different kind of nanopowders are shown. The advantages and limitations of each method are described.

P/P.54 EVOLUTION OF NEAR BAND EDGE ABSORPTION OF SIO_X THIN FILMS UPON ANNEALING

I. Stenger, L. Siozade, B. Gallas, S. Fisson, G. Vuye, J. Rivory, Institut des Nano-Sciences de Paris, UMR CNRS 7588, Universités Paris 6 et Paris 7, 140 rue de Lourmel, 75015 Paris, France

Si nanocrystals (Si-nc) embedded in a SiO_2 matrix have been extensively studied because of their applications in Si-based optoelectronic devices. The near band gap absorption and the critical points positions have been measured previously by Spectroscopic Ellipsometry (SE) in the case of Si-nc in SiO_2. Indeed, this technique is very efficient to investigate the critical points for strong absorption values (extinction coefficient $k \geq 10^{-2}$). However, for low absorption values, in particular for materials diluted in a matrix in thin films, an additional technique is required.

SiO_x films ($1<x<2$), 0.2 – 0.5 µm thick, have been elaborated by electron-gun evaporation. A thermal annealing of these films induced a phase separation leading to the formation of Si nanocrystals embedded in a SiO_2 matrix. These films have been studied by SE and Photothermal Deflection Spectroscopy (PDS) measurements. The effective dielectric function of the thin films has been extracted from SE data in the 1.6 eV to 6.5 eV range. PDS measurements allowed us to reach lower absorption values in the spectral range from 0.62 eV to 3 eV. The influence of thermal annealing on the position of the Tauc band gap, and on the density of defects in the band gap will be studied. The influence of the initial composition, x, will be investigated as well.

P/P.55 OPTIMISATION GROWTH CONDITIONS OF BINARY COMPOUND In_2S_3 THIN FILMS DEPOSITED IN VACUUM BY THERMAL EVAPORATION TECHNIQUE

A. Timoumi, H. Bouzouita*, R.Brini, M. Kanzari and B. RezigLaboratoire de Photovoltaïques et Matériaux Semi-conducteurs (LPMS)Ecole Nationale des Ingénieurs de Tunis (E.N.I.T) BP 37 belvédère 1002 Tunis, Tunisie

$Cu(In,Ga)Se_2$-based solar cells that have been achieved record efficiency values in the thin-film photovoltaic technology contain a very thin interfacial CdS layer. However, there is a great interest in replacing CdS by a cadmium-free compound for environmental reasons and also in substitute the chemical bath deposition by a vacuum procedure, allowing a better match with the standard evaporation method used for the other steps of the device fabrication. Highly encouraging results have been reported for synthesis and deposited of In_2S_3 thin films by vacuum thermal evaporation technique (VTET). Experimental parameters have been adjusted in order to optimize the growth conditions, and to obtain a high band gap energy and low absorption material at low deposition temperature, as required for photovoltaic applications. Optimization of the deposition parameters has allowed us to achieve devices up to 18% efficient [1]. In order to improve our understanding of the influence of the deposition and annealed parameters on device performance we have investigated our indium sulfide material by X-ray analysis, EDAX, AFM, spectrophotometry and SEM. X-ray diffraction analysis confirmed the initial amorphous nature of deposited InS thin films and phase transition into crystalline In_2S_3 upon annealing at free air. The optical and structural properties of the films were studied as a function of the annealing temperature. Films show a good homogeneity and optical direct band gap energy about 2.2 eV. The structural modifications of the films are accompanied by changes in the other phases.

[1] N.Barreau, J.C.Bernède, H.ElMaliki, S.Marsillac, X.Castal, J.Pinel, Sol.Stat.Commun.122 (2002) 445.

Friday, June 3, 2005 — Morning
Vendredi 3 juin 2005 — Matin

Session X : Optical metrology : materials and devices (II)
Session chairs : M. Schubert, M. Modreanu

P-X.01 9:00 -Invited-

CHARACTERIZATION OF GRATINGS BY MUELLER POLARIMETRY IN CONICAL DIFFRACTION

Antonello De Martino, Tatiana Novikova, Sami BenHatit, Bernard Drévillon, Laboratoire de Physique des Interfaces et des Couches Minces, CNRS UMR7647, Ecole polytechnique, 91128 Palaiseau, France, Denis Cattelan, Département Couches Minces, Jobin Yvon, Groupe HORIBA, 5 av Arago, 91380 Chilly Mazarin, France

Optical techniques, such as spectroscopic ellipsometry (SE), coupled with suitable multiparameter fits, have been demonstrated to be useful tools for grating metrology. However, the results are heavily dependent on the chosen model, and the number of parameters which can be determined by such fits is limited by the set of measured data. Typically, SE is used to characterize 1D gratings in the usual planar diffraction geometry, with grating grooves perpendicular to the incidence plane : the grating Jones matrix is then diagonal, and it can be measured by any conventional ellipsometer. The resulting ellipsometric spectra, even though very sensitive to some grating features, are almost completely insensitive to others, such as groove asymmetry. More extensive sets of experimental data can be obtained if the grating is measured at different azimuthal angles, i.e. in conical diffraction geometries. As the grooves are no longer perpendicular to the incidence plane, the Jones matrix of the grating is no longer diagonal, and can be measured completely only by a generalized ellipsometer, or a Mueller polarimeter. We used this approach with photoresist gratings deposited on Si for nominal CDs down to 70 nm. The instrument was an original, homemade Mueller polarimeter based on ferroelectric liquid crystals, and operated in the visible. The measured spectra were fitted with a RCWA code suitable for conical diffraction, with rectangular and trapezoidal profiles. This approach proved to greatly reduce the parameter correlations observed with standard SE when groove asymmetry is included in the model, or for very small CDs.

P-X.02 9:40

LOW FREQUENCY RAMAN SCATTERING IN SOI : PROBING ELECTRON-PHONON INTERACTION AND CAVITY EFFECTS

F. Poinsotte, J. Groenen A. Zwick, V. Paillard, A. Mlayah, Laboratoire de physique des solides (LPST), Universite P. Sabatier, Toulouse, France and C.M. Sotomayor Torres, National Microelectronics Research Centre, Cork, Ireland and M. Prunnila, J. Ahopelto, VTT Centre for Microelectronics Espoo, Finland

We present an optical metrology method for layer-structured semiconductors devices, with typical thickness from a few to a few hundreds of nm, a range where acoustic phonons provide sensitive probing. It is based on low frequency Raman scattering and combines experiment and modelling.

Analysis of the photon-acoustic phonon-electron interactions allows to measure structural, optical and acoustic parameters. In addition to the characterization of thickness, composition and strain, the technique allows to directly probe the electron-phonon interaction, which limits to a great degree, charge carrier mobility. We show how acoustic and photo elastic cavities modify the electron-phonon interaction, by appropriate modelling of the inelastic light scattering process. Comparison between experiment and simulation is provided for silicon on insulator structures (SOI). In these structures which are of considerable interest to increase the operation speed of integrated circuits, the cavity effects are shown to be particularly important.

P-X.03 10:00

ANOMALOUS PSEUDODIELECTRIC FUNCTION OF GaN: EXPERIMENT, MODEL AND APPLICATION TO STUDY THE SURFACE PROPERTIES

S. Shokhovets(a), G. Gobsch(a), V. Lebedev(b), and O. Ambacher(b), Institute of Physics(a) and Center for Micro- and Nanotechnologies(b), Ilmenau Technical University, PF 100565, 98684 Ilmenau, Germany

Usually, a thin GaN/void (or oxide) surface layer (SL) on epitaxial GaN films is believed to account for values of the pseudodielectric function (PDF) measured by spectroscopic ellipsometry (SE) in the spectral region of 3.6-5.5 eV above the band gap. However, there is a wide spread of experimental data about an average trend which can be identified with a behaviour for growth under slightly N-rich conditions. In addition, sometimes (a) the void fraction significantly depends on the photon energy, (b) unphysically high or low void fractions are needed, (c) an “anomalous” PDF is found for which both the real and imaginary parts are higher than the values for an ideal abrupt ambient/GaN boundary that principally can not be modelled by a GaN/void SL. In the latter case a higher reflectance is often observed. We demonstrate that this “anomalous” behaviour is due to a thin SL with an absorptive component different from GaN both in magnitude and spectral dependence. The SL is likely formed during the cooling of samples after growth and subsequent exposure to air, with the deciding factors being growth and cooling conditions. Effects of thermal and wet chemical treatments studied by SE and reflectance, as well as application to characterise the surface properties will be presented.

P-X.04 10:20

CHARACTERIZATION OF OXIDE THIN FILMS USING OPTICAL TECHNIQUES

J.H. Hao, Department of Physics, The University of Hong Kong, Pokfulam Road, Hong Kong and Department of Optoelectronic Engineering, Huazhong University of Science and Technology, Wuhan 430074, P.R. China, J. Gao, Department of Physics, The University of Hong Kong, Pokfulam Road, Hong Kong

Thin films of oxide materials are playing a growing role as critical elements in optoelectronic devices and nanoscale devices. Many oxide materials are usually wide-band gap compounds. The interaction between light and electrons in semiconductors forms the basis for many interesting and practical effects, which are related to semiconductor composition, microstructure, energy band, carrier transport and others. In this work, we characterized WO3 and Ga2O3 materials by various optical probing techniques, like optical absorption, photo-Hall effect, and photoconductivity transients measurements. Analysis of the photo-Hall and photoconductivity data permits the determination of the contribution to the photoconductivity made by the carrier mobility and concentration. A theoretical model for dispersive carrier transport was proposed to explain the decay of the photoconductivity in oxide thin films. In addition, luminescent characterization was employed to study microstructures and energy band in oxide thin films. The broad emission from oxide host, consisting of several band peaks, was likely due to a recombination process. The dependence of the luminescent intensity on the annealing atmosphere and temperature was consistent a model that involved oxygen vacancies in the recombination. It is suggested that our optical characterization efforts have improved understanding of oxide thin films, and this should lead to the necessary advancements in a variety of devices.

10:40 **BREAK**

Session XI : Advanced material characterization : nitrides
Session chairs : O. Thomas, T. Baumbach

P-XI.01 11:00 -Invited-

X-RAY ANALYTICAL PROCESS MONITORING IN THE DEVELOPMENT OF GROUP-III-NITRIDE DEVICES

L. Kirste, S. Müller, R. Kiefer, R. Quay, K. Köhler, Fraunhofer-Institut für Angewandte Festkörperphysik (IAF), Tullastr. 72, 79108 Freiburg, Germany; N. Herres, Interstaatliche Hochschule für Technik Buchs NTB, 9471 Buchs (SG), Switzerland

Group-III-nitride layers are important materials for electronic and photonic applications. The physical properties of the epitaxial layers depend on structural features like phase purity, mosaicity, strains and chemical composition which can be analyzed by various X-ray diffraction techniques. After a brief overview on how X-ray diffraction techniques address problems common to III-V materials, we will concentrate on the following aspects:

- The influence of substrate defects on the properties of the group-III- nitride layers. The techniques applied are Lang X-ray topography and polarizing optical microscopy which are well suited to resolve dislocations, pipes, strains and polishing damages.

- The X-ray determination of the strain and composition of $Al_xGa_{1-x}N$ and $Ga_{1-x}In_xN$ layers. For these purposes we use a variant of the Bond technique which is based on an evaluation of the peak positions of the film alone without recurrence to substrate peaks. It is a safe and quick technique to accurately analyze even partially relaxed films

The evaluation of the layer´s defect structure from Reciprocal Space Maps (RSM) and Reciprocal Space Scans (RSS). Dislocations, stacking faults, and crystal size effects all tend to broaden X-ray peaks. Measurements of “rocking curves” are ineffective to single out the respective contributions. RSSs offer a quick and viable alternative to the rather time consuming RSMs.

P-XI.02 11:40

REAL TIME ELLIPSOMETRY FOR MONITORING PLASMA-ASSISTED EPITAXIAL GROWTH OF GaN

Giovanni Bruno, Maria M. Giangregorio, Pio Capezzuto, Maria Losurdo, Institute of Inorganic Methodologies and of Plasmas, IMIP-CNR and INSTM UdR Bari, via Orabona 4, 70126 Bari, Italy, April S. Brown, Tong-Ho Kim, Soojeong Choi, Dept of Electrical and Computer Engineering and Department of Physics, Duke University, 128 Hudson Hall, Durham NC, USA

III-nitrides have gained considerable interest because of their applications for optoelectronic devices covering the Vis-UV wavelengths. They are grown heteroepitaxially on substrates with lattice mismatch, requiring a multi-step approach including substrate pre-treatments, growth of buffer layers, nucleation and epitaxial growth. The quality of films depends on each of the above steps. Therefore, there is an increasing need for real time monitoring during growth for controlling process and material quality and for understanding the growth mechanism.

Herein we apply in situ real time spectroscopic ellipsometry for the investigation of the gas-surface interaction during both plasma-assisted-MOCVD (PA-MOCVD) and plasma assisted MBE. Specifically, we investigate the chemistry and kinetics of (i) the interaction of the SiC substrate with a remote hydrogen plasma for the in situ cleaning of SiC surface; (ii) the interaction of SiC with a remote nitrogen plasma that we use for pre-conditioning the SiC surface to the epitaxial growth; (iii)the early nucleation stage of GaN on SiC and (iv) the epigrowth dynamics. For the GaN growth by PA-MOCVD trimethylgallium (TMGa) and a N2 plasma are used as precursors, while for PA-MBE we use Ga and a N2 plasma. Kinetic ellipsometric data elucidate the impact of the surface temperature and of the H2 and N2 pretreatments on the SiC/GaN interface, on the GaN nucleation, i.e., GaN nuclei size and the nucleation mode (2D, 3D, hemispherical or columnar island nucleation), and growth, i.e., layer-by-layer or Stransky-Krastanov. Importantly, the comparison of PA-MOCVD and PA-MBE allows discerning processes governed by surface kinetics, which are independent of precursor and gas-phase reactions and, hence, can be optimized for both systems.

P-XI.03 12:00

STRUCTURAL CHARACTERISATION OF GAALN/GAN HEMT HETEROSTRUCTURES BY BOTH X-RAY REFLECTOMETRY AND X-RAY DIFFRACTOMETRY

N. Sarazin, O. Durand, M. Magis, M-A di Forte Poisson, J. Di Persio, Thales R&T, Domaine de Corbeville, 91404 Orsay Cedex, France

Wide Band Gap semiconductors, such as SiC and GaN, exhibit many attractive properties far beyond the capabilities of Si and GaAs :the unique combination of the wide band gap, the high breakdown field (over 2 MV/cm), the high saturation velocity and the ability to form high quality GaAlN/GaN heterostructures with good transport properties make them ideal candidates for high power, high frequency applications. GaAlN/GaN high electron mobility transistors (HEMTs) with very impressive power densities up to 30 W/mm at 4 GHz have been reported by Cree Research. In this paper, we report on a comparative study of the structural properties of GaAlN/GaN HEMT hétérostructures on sapphire using X-Ray reflectometry, High Resolution X-Ray diffraction and TEM. GaAlN/GaN HEMT heterostructures under study consisted of a 3µm insulating GaN buffer layer followed by 30nm undoped and Si doped GaAlN layer with Al content varying from 22% to 29% and finally a GaN cap layer (0nm and 5nm). First, a Fourier analysis on the X-ray reflectometry (XRR) profiles allows an accurate and fast determination of the top (GaN/GaAlN) bilayer thicknesses, in spite of a small electronic density contrast. Then, using a simulation software with the results of the Fourier analysis as a starting point for the fitting procedure, the electronic density profile has been determined, leading to the roughnesses at the interfaces and the surface. From a fit of the experimental X-Ray rocking curves, Al content of the high band gap layer have been extracted and the thicknesses of each layers, consistent with the results from XRR, were in addition confirmed at the atomic scale by TEM.

P-XI.04 12:20

STRUCTURAL AND OPTICAL CHARACTERIZATION OF GaN HETEROEPITAXIAL FILMS ON SiC SUBSTRATES

Mike Morse, Pae Wu, Soojeong Choi, Tong-Ho Kim, and April S. Brown, Dept of Electrical and Computer Engineering and Department of Physics, Duke University, 128 Hudson Hall, Durham NC, USA, Maria Losurdo and Giovanni Bruno, Institute of Inorganic Methodologies and of Plasmas, IMIP-CNR and INSTM UdR Bari, via Orabona 4, 70126 Bari, Italy

The microstructure of heteroepitaxial GaN is related to device performance.

Dislocations can significantly increase electron scattering and current leakage. Therefore, minimizing dislocation density is advantageous for device development and reliability. Therein, GaN samples were grown with and without AlN buffer layers on 4H and 6H-SiC substrates treated in different ways, i.e., with Ga flashing - 1/2 ML and 2ML Ga deposition and flash-off- to remove the SiC oxide and to establish the surface reconstruction and with and without nitridation. We exploit x-ray diffraction (XRD) and Williamson-Hall (WH) analysis for determining the microstructure, and therefore dislocation density, present in GaN films grown by molecular beam epitaxy (MBE) on 4H and 6H SiC substrates with differing surface treatments or buffers. X-ray rocking curves and w-2q scans for WH analysis were taken using a Philip's X'pert Pro MRD. The WH technique yields both edge and screw dislocation densities along with lateral coherence lengths. From the asymmetric rocking curve FWHM, we show the dependence of screw dislocation density on surface treatment and AlN buffer layers. These results indicate that modification of nucleation behavior mostly alters screw dislocation formation, but has little effect on edge dislocation density. The XRD studies and analysis are complemented with spectroscopic ellipsometry (SE) studies of the modifications of SiC surface using the various surface treatements and of the GaN nucleation on the various surfaces. The XRD and SE analysis of the amplitude and broadening of GaN exciton in the SE spectra shows the correlation between the microstructure and optical quality depending on SiC treatments and buffers.

12:40 **LUNCH**

Friday, June 3, 2005 — Afternoon

Vendredi 3 juin 2005 — Après-midi

14:00 **ROUND TABLE**

Advances in optical and X-ray metrology

Session chairs : O. Durand, G.E. Jellison