Tuesday Afternoon, November 11, 2014

Thin Film
Room: 305 - Session TF+AS+EM-TuA

Thin Film: Growth and Characterization II

Moderator: Mark Davidson, University of Florida

2:20pm **TF+AS+EM-TuA1 A Statistical Optimization of Perpendicular Anisotropy and Damping for Ta-Inserted Double CoFeB/MgO Interface MTJ's**, *S. Gupta*, ***Samuel Schwarm***, *B. Clark*, University of Alabama

A statistical Design of Experiments was conducted on double-interface Ta-inserted CoFeB-MgO magnetic tunnel junctions (MTJ's). These MTJ's were deposited using a Shamrock planetary sputtering system. The thicknesses of the inserted Ta and the CoFeB electrodes were varied using Response Surface Methodology. The responses measured using magnetometry and ferromagnetic resonance were a) effective magnetization, b) damping constant and c) perpendicular anisotropy. The effect of annealing on the perpendicular anisotropy was also observed for these devices. As the Ta thickness is increased for fixed CoFeB thickness, the M-H loops indicate that the anisotropy is becoming perpendicular. After annealing, both magnetometry and FMR results show that the MTJ's indicate full perpendicular anisotropy. Interfacial perpendicular anisotropy, which can be extracted from the FMR measurements, scales with the inserted Ta thickness for both as-deposited and annealed samples.

2:40pm **TF+AS+EM-TuA2 1D Matlab Modeling of the Reaction-Diffusion System during the Selenization Process in the Two-Step CIGS Solar Cells Production Process**, ***Jurjen Emmelkamp***, *A. Mannheim*, TNO Technical Sciences, Netherlands

Introduction

In the two-stage fabrication process of CIGS thin-film solar cells first copper, indium and gallium precursor layers are deposited, followed by the selenization process where selenium vapor is provided at high temperature to form CIGS. Despite of the literature, many stages of the reaction-diffusion process are still a mystery. Several experimental techniques exist to analyze the selenization process, however, most of them are only useful to analyze the post-selenization product. In-situ XRD can be used to analyze the crystal structure during the selenization process, but the information is limited because depth profiles and amorphous intermediates are not measured. Modeling of the reaction-diffusion system during the selenization process can result in deeper understanding of the process and in a predictive model for the optimal process conditions that can lead to cheaper and more efficient CIGS solar cells.

The m odel

A relative simple 1D mathematical Matlab model is developed. Since many intermediate products and the CIGS end-product are crystals, and thus 3D systems, an 1D approach is very simplified. Intensive evaluation with experimental in-situ XRD and cross section EDX, as well as literature values, are used to tune the model specific parameters. Main parameters include diffusion and reaction constants of the different elements and binaries/ternaries, as well as the sticking factor at the surface for the uptake of selenium from the vapor phase. Using these parameters the (intermediate) reactions can be derived and fitted to the data from experiments and literature studies.

First the process temperature profile is calculated as function of time, followed by the calculating the uptake of selenium from the vapor phase. Additionally, the diffusion and reactions are modeled, using Fick's second law, error functions and multiple reflections at the solid interfaces. Based on phase diagrams the reaction kinetics of the most important reaction products are derived and are included into the model.

For reasons of memory limitations, the time and spatial mesh need to be relative coarse. For the spatial mesh this requires adaptive meshing, in order to adapt to small spatial variations and to mimic the overall and the specific layer growth well at small time changes.

Conclusions

The development of the model is still in progress, but the first results show good approximation of the selenium uptake and the formation of the first binaries and ternaries, such as $Cu_{11}In_9$, $Cu_{2-x}Se$, In_4Se_3 and InSe. This can be expanded easily to other intermediates, CIS, CGS and CIGS. However, further parameter fitting is required to mimic the experimental data better.

3:00pm **TF+AS+EM-TuA3 TiSiO Thin Films Deposited by Plasma Enhanced Chemical Vapor Deposition for Optical and Electrical Applications**, ***Antoine Goullet***, *S. Elisabeth, D. Li, M. Carette, A. Granier*, IMN, France **INVITED**

TiO_2 thin films are good candidates for the development of passive optical or electrical integrated devices. They exhibit high optical refractive index ($1.8<n<2.7$ at 633 nm) in combination with high transparency in the visible range and high dielectric constant ($50<k<100$). They are compatible with semiconductor technologies and can be synthesized at low temperature by plasma processes such as plasma enhanced chemical vapor deposition (PECVD). This technique is very attractive to tune film composition and properties such as film refractive index. PECVD is also known for its ability to prepare good quality amorphous or partially crystalline films at low temperature.

Titanium-silicon mixed oxide (TiSiO) materials can overcome some of the limitations given by TiO_2 material, e.g. columnar morphology and relatively low band gap energy.

In this study, TiSiO thin films are prepared without any intentional heating in low pressure inductively coupled discharges from titanium tetraisopropoxide (TTIP- $Ti(OC_3H_7)_4$) and hexamethyldisiloxane (HMDSO - $SiO_2(CH_3)_6$) precursors mixed with oxygen.

Structure and chemical composition of the films are investigated by X-ray diffraction (XRD) and X-ray photoelectron spectroscopy (XPS). Information about film chemical bonds is also obtained from Fourier transform infrared spectroscopy (FTIR). Film morphology is characterized by scanning electron microscopy (SEM) and atomic force microscopy (AFM). Optical properties are mainly investigated by spectroscopic UV-Visible ellipsometry.

Capacitance-voltage (*C-V*) and current-voltage (*I-V*) measurements are performed by using MIS capacitors for evaluation of the mixed oxide film electrical performances.

TiO_2 thin films characteristics are investigated as a function of the plasma ion energy in the 25 – 175 eV range. Increasing the ion energy leads to more homogeneous and organized films with the transformation from anatase to rutile. To account for the columnar morphology of TiO_2 films, a gradient optical layer model was developed. The thin layer dispersion functions were described satisfactorily with the Tauc-Lorentz dispersion law.

TiSiO have been deposited by varying the HMDSO flow rate in the plasma operated in continuous or pulsed mode.

The thin films can be described as a mixture of silicon and titanium oxide at the atomic scale rather than two separate SiO_2 and TiO_2 phases. These mixed oxide layers are basically amorphous and exhibit good morphological properties provided the titanium content is lower than the silicon one.

On the whole these TiSiO layers offer a good compromise in terms of morphological, optical and electrical properties.

4:20pm **TF+AS+EM-TuA7 Kinetically-Limited Lattice Relaxation in Linearly- and Non-Linearly- Compositionally-Graded InxGa1-xAs/GaAs (001) Metamorphic Heterostructures**, ***Tedi Kujofsa***, *J.E. Ayers*, University of Connecticut

Metamorphic buffer layers allow tremendous flexibility to design novel InGaAs/GaAs semiconductor heterostructures for application in various microelectronic and optical devices. However, device fabrication, reliability and performance are limited by dislocation defects associated with the growth of highly mismatched systems such as InGaAs on GaAs substrate. Thus, understanding kinetically-limited lattice relaxation and development of a plastic flow model applicable to multilayered and compositionally graded heterostructure is desirable to provide guidance in designing InGaAs/GaAs devices. Previously, we reported a plastic flow model for ZnS_ySe_{1-y}/GaAs (001) heterostructures which predicts the non-equilibrium strain relaxation as well as misfit dislocation and threading dislocation densities. Here, we have extended our model to $In_xGa_{1-x}As$/GaAs (001) metamorphic buffer layers with arbitrary compositional grading profile. In addition, we have investigated the evolution of the kinetically limited in-plane strain of $In_xGa_{1-x}As$/GaAs (001) heterostructures with an emphasis on grading schemes employing a step, linear-, S- and power-law- lattice mismatch compositional profile. For each structure, we have studied the thickness and grading coefficient dependence on the average and surface kinetically-limited in-plane strain. In addition, we show that the use of compositionally graded buffer layers enables the design of $In_xGa_{1-x}As$/GaAs (001) heterostructures with high surface strain values which enhance the

sweeping of threading defects and therefore yielding device structures with minimal defect.

5:00pm **TF+AS+EM-TuA9 Superconducting Properties of NbN and NbTiN Thin Films**, ***Matthew Burton***, *M.R. Beebe, R.A. Lukaszew, D. Beringer*, College of William and Mary

Thin films of NbN and NbTiN are promising materials currently researched for improvements in superconducting radio frequency (SRF) technology and applications. At present, bulk niobium SRF accelerating cavities suffer from a fundamental upper limit in maximally sustained accelerating gradients; however, a scheme involving multi-layered superstructures consisting of superconducting-insulating-superconducting (SIS) layers has been proposed to overcome this fundamental material limit of 50 MV/m [1]. The SIS multi-layer paradigm is reliant upon implementing a thin shielding material with a suitably high Hc1 which may prevent early field penetration in a bulk material layer and consequently delay the high field breakdown. It has been predicted that for thin superconducting films — thickness less than the London penetration depth (~200 nm in the case of NbN) — the lower critical field Hc1 will be enhanced with decreasing thickness. Thus, NbN thin films with a high Hc1 value are possible candidates for such SIS structures. We note though that since the intrinsic resistivity of NbN is rather large, efforts are also devoted to NbTiN which has similar superconducting properties but much lower intrinsic resistivity which is preferable for this application. Here we present our study on the structure and superconducting properties of a series of NbN and NbTIN thin films and correlate the effects of film microstructure and surface morphology on relevant superconducting properties such as the critical temperature, Tc, the lower critical field, Hc1, and the residual resistance ratio.

[1] A. Gurevich, Appl. Phys. Lett., 88, 012511 (2006).

5:40pm **TF+AS+EM-TuA11 High-Throughput Assessment of the Composition Dependence of Initial Passivating-Al_2O_3-Scale Establishment in $Al_xFe_yNi_{1-x-y}$ Alloy Thin Films**, ***Matthew Payne***, *J. Miller, A.J. Gellman*, Carnegie Mellon University, DOE - National Energy Technology Laboratory

AlFeNi-containing alloys capable of forming passivating Al_2O_3 scales are designed for high-temperature structural applications requiring robust oxidation resistance. Mechanical considerations typically dictate that Al content be minimized, but a critical concentration, N_{Al}*, is minimally required to promote the initial establishment of a continuous Al_2O_3 layer. Current understanding of how N_{Al}* evolves across multi-component composition spaces is limited, being based largely on experiments that are constrained by the need for meticulous preparation and characterization of large numbers of single-composition samples. The study of properties across alloy composition space can be greatly accelerated using composition spread alloy films (CSAFs), materials libraries comprised of continuous lateral composition gradients. Properly designed CSAFs can contain every possible composition of a ternary alloy. In this work, ~120 nm-thick $Al_xFe_yNi_{1-x-y}$ CSAFs spanning the entire ternary range ($x = 0 \rightarrow 1$, $y = 0 \rightarrow [1-x]$) over an area of ~1 cm^2 were prepared. A variety of spatially resolved techniques were developed for effective, high-throughput characterization of early oxidation behaviors in the CSAFs. Energy-dispersive X-ray spectroscopy was used to measure changes in CSAF oxygen content as a function of both alloy composition and oxidation time. Raman spectroscopy allowed specific oxide phases formed in different regions of the composition space to be identified. X-ray photoemission depth profiling was performed at select locations of interest to determine composition and chemical state in CSAF cross-sections. These methods were used to study oxidation across $Al_xFe_yNi_{1-x-y}$ composition space in both dry and moist air at 700 K, and have enabled the identification of continuous boundaries separating regions of phenomenologically unique oxidation behaviors, including the N_{Al}*(x,y) boundary for each environment. The results enhance fundamental understanding of early-stage $Al_xFe_yNi_{1-x-y}$ oxidation and can contribute to the accelerated design of next-generation alloys.

6:00pm **TF+AS+EM-TuA12 Structural, Electrical, and Optical Characterization of Impurity-Dependent, Ultra-Low-Dislocation-Density Ge Epitaxially Grown on Si and Characterization of MOSFETs Fabricated on Ge-on-Si**, ***Swapnadip Ghosh***, *S.M. Han*, University of New Mexico

Building on a simple two-step MBE growth technique, we have investigated possible dislocation locking mechanisms by dopant impurities, coupled with artificially introduced oxygen (O). In the case of n-type Ge grown on Si, our materials characterization indicates that the dislocation density (DD) can reach the ~10^5 cm^{-2} level, compared to p-type and undoped Ge on Si (GoS). We note that our Ge film covers the entire underlying Si substrate at the wafer scale without mesas or limited-area growth. In this presentation, we will focus on the use of n-type impurity (phosphorus) diffusion from the Si substrate and the introduction of O at the Ge-Si interface. The O is introduced by growing a thin chemical SiO_2 layer on top of the Si substrate before Ge epitaxy begins. Z-contrast cross-sectional TEM images suggest the presence of O precipitates in n-type Ge, whereas these precipitates appear absent in p-type Ge. These O precipitates are known to lock the dislocations. Supporting the argument of precipitate formation, the TEM shows Moiré fringes due to various phase boundaries that exist at the precipitate/Ge-crystal interface. We speculate that the formation of phosphorus (P) segregation resulting from slow diffusion of P through precipitates at the precipitate/Ge-crystal interface facilitates dislocation locking. Impurity segregation in turn suppress O concentration in n-type Ge leading to the reduced DD that appears on the top surface of n-Ge compared to p-Ge film. The O concentrations (10^{17} to 10^{18} cm^{-3}) in the n- and p-type GoS films are measured using secondary ionization mass spectroscopy. We have then compared the structural and electrical characteristics of n-type Ge films with its p-type counterparts. In n-type Ge, the DD decreases from ~10^9 cm^{-2} near the Ge-Si interface to ~10^5 cm^{-2} at the film surface. In contrast, we observe 5×10^7 cm^{-2} DD at the film surface in p-type Ge. The full width at half-maximum for our n-type Ge(004) XRD peak is 100 arcsec, compared to 230 arcsec of p-type Ge. As a stringent test of the dislocation reduction, we have also fabricated and characterized high-carrier-mobility MOSFETs on GoS substrates.We also report p- and n-MOSFETs with μ_{eff} of 401 and 940 cm^2/V-s and a subthreshold slope of 100 and 200 mV/decade, respectively.These effective mobilitiesshow an exceptional 82 and 30% improvement over that of conventional Si channel MOSFETs. We also investigate the optical quality of ultra-low DD GoS film by measuring photoluminescence (PL). Then-type Ge PL main peak shows pronounced tensile-strain (×0.8%) than that of p-type, which is an indicator of direct bandgap shrinking at the Γ band-edge.

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