Electronic Materials and Processing
Room: 9 - Session EM+MI-ThA

Semiconductor Heterostructures II + Heusler Alloys
Moderator: J.E. Ayers, University of Connecticut, B.D. Schultz, University of California, Santa Barbara

2:00pm **EM+MI-ThA1 Dislocation Compensation in Ungraded ZnS_ySe_{1-y}/GaAs (001) Heterostructures**, ***T.M. Kujofsa***, *J.E. Ayers*, University of Connecticut

Control of strain and dislocation dynamics are important in determining the performance and reliability of semiconductor devices such as light-emitting diodes and photo-detectors. Experimental studies of ZnS_ySe_{1-y} /GaAs (001) heterostructures show that a dislocation compensation mechanism is active in structures involving abrupt interfaces. This mechanism involves the bending over of threading dislocations associated with misfit segments of one sense by misfit dislocations having the opposite sense, and it allows removal of threading dislocations from device structures.

Semiconductor device structures may be designed to take advantage of the dislocation compensation with the aid of a dislocation dynamics model accounting for misfit-threading interactions. To develop such a model we studied strain relaxation in ZnSe/GaAs (001) and ZnS_ySe_{1-y} /GaAs (001) heterostructures to determine the kinetic material parameters associated with dislocation glide and multiplication. Based on these results and by including misfit-threading interactions we developed a dislocation dynamics model which predicts dislocation compensation in arbitrary ZnS_ySe_{1-y}/GaAs (001) heterostructures.

Whereas our previous experimental work involved graded structures, this work focuses on the study of theoretical heterostructures comprising a device layer (DL) of ZnS_ySe_{1-y} on a ungraded buffer layer (BL) of ZnS_ySe_{1-y} deposited on a GaAs (001) substrate. We show that for a given device layer thickness and compositional change at the buffer-device layer interface there exists an optimum thickness of the ungraded buffer layer where the mobile threading dislocation density can be removed entirely. The optimum buffer layer thickness decreases monotonically with the compositional difference between buffer and device layer.

2:20pm **EM+MI-ThA2 Dynamical X-ray Diffraction from Semiconductor Heterostructures with Asymmetrical Dislocation Densities**, ***P.B. Rago***, *J.E. Ayers*, University of Connecticut

We extend the dynamical theory of Bragg x-ray diffraction to include asymmetrical dislocation densities on the two types of active slip systems in zinc blende semiconductor heterostructures with (001) orientation. In such structures the dislocations exist in eight active slip systems of two basic types distinguished by the orientation of their misfit segments, which are oriented along either the [1-10] or [110] direction. Variation of the incident x-ray beam azimuth results in a change in the shape of the diffraction profile if the two types of slip systems exhibit an asymmetry in dislocation densities. Our work allows simulation of the x-ray diffraction profile of an arbitrary zinc blende semiconductor heterostructure, and through comparison to experimentally measured data, the two dislocation densities of an experimentally measured sample can be extracted. In this work we have demonstrated use of the model by applying it to the ZnSe/GaAs (001) and HgCdTe/CdTe (001) material systems.

3:40pm **EM+MI-ThA6 Epitaxial Growth and Electronic Bandstructure of the Semiconducting Half Heusler Compound CoTiSb**, ***J. Kawasaki***, University of California Santa Barbara, *L. Johansson, M. Hjort, R. Timm*, Lund University, Sweden, *B. Shojaei*, University of California Santa Barbara, *A. Mikkelsen*, Lund University, Sweden, *B.D. Schultz, C. Palmstrom*, University of California Santa Barbara **INVITED**

The Heusler compounds are an exciting class of intermetallics due to their ability to adopt a wide range of tuneable electrical and magnetic properties. These properties include ferromagnetism, paramagnetism, half-metallic ferromagnetism, large thermoelectric figures of merit, and both semiconducting and metallic behaviour. Additionally, some of the semiconducting Half Heuslers have been theoretically proposed be topological insulators, making the Heusler compounds a promising system for multifunctional heterostructure devices. However, due to challenges in controlling defects and stoichiometry, little is known about the experimental band structure of the semiconducting Half Heuslers. We demonstrate the epitaxial growth of the Half Heusler compound CoTiSb by molecular beam epitaxy. Samples consist of an InP (001) substrate, lattice matched $In_xAl_{1-x}As$ buffer layer, and CoTiSb layer. The films are single crystalline and of high structural quality, as measured *in situ* by reflection high energy electron diffraction (RHEED) and scanning tunnelling microscopy (STM) and *ex situ* by X-ray diffraction (XRD), with an out of plane lattice mismatch of less than 0.5%. For growth temperatures of less than 400°C the films grow in a layer-by-layer mode as demonstrated by RHEED intensity oscillations. Under stoichiometric growth conditions the films have a (2x1) surface reconstruction and for Sb-rich conditions the films have a (1x1) reconstruction. Electrical transport measurements show the resistivity of the films decreases as a function of temperature down to 10K, consistent with semiconducting behaviour, and using tunnelling differential conductance spectroscopy (dI/dV) we measure a band gap on the order of 160 meV. However, this band gap is much smaller than the value of 1.0 eV predicted by density functional theory. Angle resolved photoemission spectroscopy (ARPES) measurements were also performed at the MAX-Lab synchrotron facility in Lund, Sweden. A protective Sb capping and decapping scheme was developed to maintain the surface quality of the films as the samples are transported to the characterization facility and exposed to air. The structural, chemical, and electrical properties of the single crystal CoTiSb films will be presented to provide insights into the band structure of the semiconducting Half Heuslers. This work was supported in part by the Office of Naval Research and the National Science Foundation.

4:20pm **EM+MI-ThA8 Application of Magnetic Heusler Alloys to All-Metal Sensors for Ultrahigh-Density Magnetic Recording**, ***J.R. Childress***, HGST San Jose Research Center **INVITED**

Magnetic Heusler alloys are attractive materials for a number of applications in spintronics due to their potential high spin-polarization at the Fermi level, advantageous for spin-injection experiments and magnetoresistive devices. In the magnetic recording heads used in today's hard-disk drives (HDD's), the magnetoresistive thin-film sensors are multilayer spin-valves which operate in the current-perpendicular-to-film-plane (CPP) geometry, and rely on the spin-filtering properties of ultrathin MgO tunnel barriers (junction resistance < 1 Ohm-micron^2) to achieve large tunnel-magnetoresistance (TMR) values using standard CoFe and CoFeB magnetic alloys as electrodes. Sensors with lower resistance (and thus lower-noise) are continuously required as sensor dimensions are reduced to keep up with the increased areal density of recorded data (approaching 1 Tb/in^2). Intrinsically, an all-metal sensor can operate similarly to TMR sensors and will be able to achieve much lower resistances (~ 0.05 Ohm-micron^2) and lower noise, but also requires a relatively large giant magnetoresistance (GMR) ratio to achieve sufficiently large signal to noise ratios (SNR). A number of Co-based full-Heusler alloys have the required magnetization, high T_{Curie} and a predicted half-metallic behavior at low temperatures, and are therefore of interest for this application. But while the high spin-polarization in these Heusler alloys can significantly increase the GMR signal, integrating these materials in recording head sensors is a challenge due to their complex crystalline structure which typically requires high-temperature processing, and strong sensitivity to compositional disorder. In addition, the high polarization and low magnetic damping observed in these materials results in a high sensitivity to spin-torque excitations which limits the maximum allowable bias voltage, and is also a source of noise which limits the signal to noise (SNR) ratio. The geometrical, thermal, and magnetic constraints which influence the integration of Heusler alloys in magnetic recording head sensors will be presented, along with some examples of materials characterization and multilayer stack optimization required to improve the properties and robustness of the devices. It is found that practical spin-valves with Heusler alloy-based magnetic layers can be fabricated with CPP-GMR ratios which can be increased to >10%, more than 2x larger than for conventional ferromagnetic alloys. The outlook for applicability of such sensors to magnetic recording at high densities > 1 Tb/in^2 will be discussed.

5:00pm **EM+MI-ThA10 Growth of Epitaxial Co_2MnSi/MgO/Co_2MnSi Magnetic Tunnel Junctions by Molecular Beam Epitaxy**, ***S. Patel***, *A. Kozhanov, B.D. Schultz, C. Palmstrøm*, University of California, Santa Barbara

Epitaxial magnetic tunnel junctions (MTJs) have the potential to be used as low-energy non-volatile random access memory. The use of half metallic ferromagnets as electrodes has drawn great interest due to the predicted 100% spin polarization at the Fermi level. Co2MnSi is predicted to be half-metallic[1], with a Curie temperature of 985K [2], and is a strong candidate for use in magnetic random access memory devices. These devices, however, are highly sensitive to interfacial and bulk disorder, which may result in the loss of a minority spin gap [3]. Therefore it is critical to understand the fundamental properties of the Heusler alloy films and correlate these properties with device performance. We have successfully grown highly-ordered, epitaxial Co2MnSi(001) films by molecular beam epitaxy (MBE) using a "seeded growth" technique to form a crystalline seed layer on various substrates, including MgO (001) and a Sc0.3Er0.7As lattice-matched diffusion barrier layer on GaAs (001). The lattice mismatch between GaAs and Co2MnSi is only -0.06% and x-ray diffraction of the MBE grown thin films show the two are nearly lattice matched. These films also have relatively smooth surfaces and coercivities down to 4 oersteds for stoichiometric films. Composition is also found to play a large role in the magnetic properties of the films. Off-stoichiometry films display lower saturation magnetization as well as higher coercivities. We have subsequently been able to grow epitaxial MTJ heterostructures of Co2MnSi/MgO/Co2MnSi with different switching fields for the top and bottom electrodes. We have characterized the structure of each layer and interfaces with reflection high-energy electron diffraction (RHEED), low-energy electron diffraction (LEED), scanning tunneling microscopy (STM) and cross-sectional transmission electron microscopy (XTEM) and the corresponding magnetic properties using vibrating sample magnetometry (VSM) and a superconducting quantum interference device (SQUID) to better understand the fundamental properties of these epitaxial heterostructures. This work was supported in part by the Semiconductor Research Corporation under award number 2011-IN-2153.

References

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[3] B. Hülsen, M. Scheffler, and P. Kratzer. Physical Review B 79 (9), 094407 (2000)

5:20pm **EM+MI-ThA11 Fabrication of Highly Ordered Co_2FeAl Thin Films by Reactive Ion Beam Deposition for Spintronic Devices**, ***Y.S. Cui***, University of Virginia, *S. Schäfer, T. Mewes*, University of Alabama, *M. Osofsky*, Naval Research Laboratory, *J.W. Lu, S.A. Wolf*, University of Virginia

Co_2FeAl (CFA) is a full Heusler alloy that has potentially very low damping parameter and high spin polarization, highly desired for spintronic devices such as magnetic tunnel junctions and spin valves. CFA with B2-type chemical ordering has shown an extremely low Gilbert damping parameter among the Heusler alloys, which facilitates spin dynamics such as spin current driven magnetization switching. A large tunnel magnetoresistance (TMR) has been reported in B2-CFA based magnetic tunnel junctions, which is ascribed to its intrinsic high spin polarization efficiency. The high spin polarization efficiency originates from the half-metal gap in some of its energy bands with certain symmetry. It was predicted by theory that both low damping parameter and high spin polarization can only be achieved with a high chemical ordering existing in the CFA crystal structure. We will present the synthesis of high quality CFA thin films, prepared by a novel deposition technology, Reactive Biased Target Ion Beam Deposition (RBTIBD). The surface roughness (RMS) was observed as low as 0.14 nm. It was determined that CFA thin films grew on MgO(001) epitaxially along both in-plane and out-of-plane directions with a B2-type chemical ordering, according to the results obtained in XRD and TEM. The chemical ordering can be significantly improved by properly choosing the post annealing parameters. The ferromagnetic resonance (FMR) measurements suggested an extremely small damping parameter (~0.002). The damping parameter was strongly correlated with the chemical ordering of B2 structure. In addition, the impact of chemical ordering on the spin polarization efficiency of CFA films based on PCAR measurements will be discussed.

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