Dear M. Stellmach,

Please find on page two the camera ready abstract. I cordially request an oral presentation.

My address etc. follow:

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Sincerely,

Erik Svedberg

Asymmetric Interface Broadening in Epitaxial Mo/W (001) Superlattices grown by Reactive Magnetron Sputtering on MgO (001) Substrates

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Asymmetric interfacial broadening in sputtered epitaxial Mo/W superlattices (SL) using both Ar and Kr discharges is reported. The different atomic masses of Mo and W, implies that the conditions during sputtering of W on Mo can be expected to be different than the conditions prevalent during sputtering of Mo on W. Possible effects on the sputtering process should also be different in Ar and Kr discharges, since the fluxes and energies of the backscattered neutrals strongly depend on the gas-to-target mass ratio. Special interest is taken in the effect of the interfaces due to their importance in phenomena such as giant magneto resistance.

100 periods composed of alternating 44 Å Mo and 54 Å W layers were deposited at ~700°C in a dual magnetron HV sputtering system, first in Ar and then in Kr. MgO (001) substrates were cleaned and annealed prior to these depositions.

Conventional θ-2θ x-ray diffraction (XRD) was carried out in the low angle region (1-10° 2θ) and high angle region around the Mo/W 002 Bragg reflection (50-66° 2θ). Single crystal Mo and W SL were observed with more than 10 superlattice peaks indicating that the SL had well defined and ordered layers.

In order to deduce the interface broadening and possible asymmetries in the broadening of W on Mo compared to Mo on W, either XRD or high resolution electron microscopy can be used. However, both techniques demand extensive simulations with several fitting parameters and the latter also requires tedious sample preparation. With XRD it is difficult to achieve a unique fit unless the films have a very high crystalline quality allowing high resolution rocking curves or reciprocal space maps to be recorded to provide additional information. Consequently in metallic SL, the fitting procedure of low-angle diffractograms does not lead to an unambiguous determination of the interfacial structure. An alternative approach to deduce interface broadening during sputter deposition is to simulate the growth process and use the simulated compositional profiles as input parameters for the x-ray simulations.

To simulate the growth process, the TRIM90 code was initially used to calculate the number of Ar and Kr atoms reflected from the targets. The results from these calculations were then used to determine the average energy of these particles impinging at the substrates, taking into account that the atoms have to cross the sputtering gas to reach the sample surface. At the substrate, the TRIDYN code was then employed to dynamically calculate the intermixing effects occurring during growth. The bombardment of the growing W on Mo interface by energetic argon species reflected from the W target caused significant elemental intermixing with a typical width of ~1.2 nm. For comparison, the Mo on W interface width is only 0.5 nm. Finally, simulations of the low-angle diffractograms were made with the Philips GIXA software in order to validate the interfacial mixing from the XRD data. The compositional profiles used for the asymmetric interfaces were taken directly from the TRIDYN calculated profiles. The low angle x-ray diffractograms from SL with asymmetrically broadened interfaces were compared with the measured x-ray diffractograms. The good overall fit of the simulations to the measured diffractograms is a indicator that the interface broadening is indeed asymmetric.