	Experiment title:	Experiment number:
	Refle-XAFS study of ultra-thin Y_2O_3 oxides and Y_2O_3/Si interface	SI 836
Beamline: BM 08	**Date of experiment**: from: 23/11/02 to: 29/11/02	**Date of report**: 26/2/08 (updated)
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Report:

The scaling down of the gate dielectric thickness is the most difficult issue in the development of next generation ultra-large scale integrated (ULSI) devices. Gate dielectric with equivalent oxide thickness (EOT) less than 1-1.5 nm will soon be required for sub-0.1 μm devices. The scaling down of SiO_2 thickness is limited by exponential leakage current increase or dielectric breakdown. To reduce leakage current while maintaining the same gate capacitance, a thicker film with a higher dielectric constant (*high-k*) is required. Several oxides, such as Ta_2O_5, TiO_2, ZrO_2, HfO_2, Y_2O_3, $SrTiO_3$, as well as silicates, such as $ZrSi_xO_y$, are currently considered. Although research and development worldwide has focused mostly on amorphous oxides, a suitable candidate has not been identified yet. On the other hand, epitaxial crystalline oxides on silicon could offer advantages such as higher dielectric constant and better control of interfaces with respect to other growth techniques. Several requirements related to electrical and structural properties, interface engineering and thermal stability must be fulfilled. To address these issues the use of complementary characterization techniques is mandatory and in particular surface sensitive techniques are requested to investigate the composition and the micro-structure of ultra thin (< 10 nm) films on silicon.

In this experiment we have used X-ray absorption in the reflection mode (Refle-XAFS) on the GILDA beamline in order to probe the local structure of Y_2O_3 epilayers, in a thickness range 2-20 nm, grown on Si(100) by electron beam evaporation; information on the oxide – silicon interface was also sought and obtained. Y_2O_3 grows hetero-epitaxially on Si(001) and it is a good candidate for SiO_2 replacement due to its predicted thermodynamic stability in contact with silicon and its relatively high k (14-18).

X-Ray absorption spectroscopy (XAS) measurements at the Y K-edge were performed to study the interface atomic environment and the evolution of the epilayer structure with thickness and *in-situ* post deposition annealing. Complementary information on the epitaxial quality, the film thickness and the roughness of the surface and of the interface were obtained by reflection high energy electron diffraction (RHEED), high resolution x-ray diffraction (HRXRD) and x-ray reflectivity (XRR).

Y_2O_3 layers were grown on 2” p-type Si(001) wafers in a MBE system by the group of A. Dimoulas at the Institute of Material Science, National Center for Scientific Research, Demokritos, Athens, Greece. Y_2O_3 was evaporated by means of an e-gun from a sintered ceramic target. The oxide growth rate was ~ 0.4 Å/s for all films. Some samples were subsequently *in-situ* annealed for 30 min at 500 °C.

In Fig. 1 we report the Magnitude of the Fourier Transform (FT) of data obtained on the samples as a function of thickness and treatment (“ann” indicates annealed samples). The data for the 20 nm thick film is virtually identical to that obtained on a polycrystalline Y_2O_3 powder (not shown). The first peak (1.5 – 1.7 Å) is related to Y – O atomic correlations (first shell) while the peaks in the 2 – 4 Å range are related to Y – Y correlations (“second” shell); this signal is typical of the bixbyite structure. It is clear from the figure that with decreasing thickness the signal from coordination shells higher than the first decreases – indicating a higher degree of structural disorder; moreover the first peak shifts to lower energies.

The origin of the changes in the first peak position has been clearly identified. For all samples except the 2nm as deposited one the first peak can be fitted with Y – O atomic correlations; for the 2 nm as-deposited sample we have been able to reproduce the signal with Y – Si atomic correlations. This is shown in Fig. 2, in which we report in k-space the filtered contribution from the first shell and its fit. The bottom curves are for the as-deposited sample (Y-Si correlations) while the top curves are for the annealed sample, in which Y-Si correlations are not present.

In-house XRR data on the same samples indicate the presence of a 1 – 2 nm interface layer in the 2 nm as-deposited samples.

These results indicate that in as-deposited samples an interface layer in which Y is directly bonded to Si is present; with annealing these atomic correlations disappear. We conclude that interface bonds are formed directly between Y and Si (and not via oxygen), possibly forming a disordered silicide phase which is unstable under annealing.

These results have been presented as an oral contribution at the European Materials Research Society Spring Meeting in June 2003 and have been published in Phys. Rev. B [2].

[1] S. Spiga, C. Wiemer, G. Tallarida, M. Fanciulli, M. Malvestuto, F. Boscherini, F. D’Acapito, A. Dimoulas, G. Vellianitis, and G. Mavrou “Structural characterization of epitaxial Y_2O_3 on Si (001) and of the Y_2O_3/Si interface”, Materials Science and Engineering B **109**, 47 (2004).

[2] M. Malvestuto, R. Carboni, and F. Boscherini F. D’Acapito S. Spiga, M. Fanciulli, A. Dimoulas, G. Vellianitis, and G. Mavrou, Phys. Rev. B **71**, 075318 (2005).

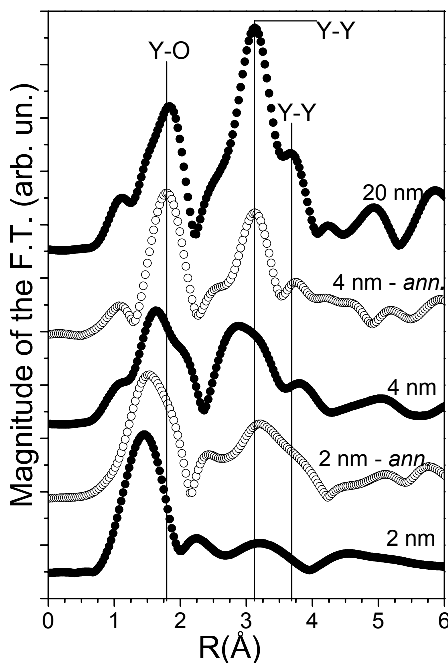

Fig. 1

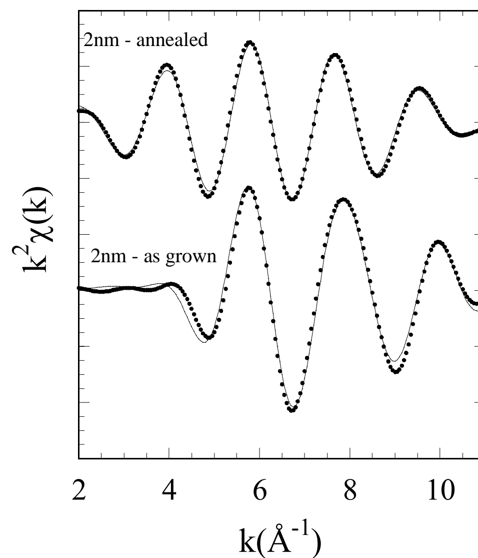

Fig. 2