High Resolution X-ray Reflectometry: Theory, Practice, Accuracy and Precision

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High resolution X-ray reflectometry is widely used for the characterization of thin film systems that are of interest to the semiconductor industry. Critical parameters such as layer thickness, chemical composition, and interfacial roughness (both at the free surface and at the various buried interfaces in a multilayer structure) are typically obtained using X-ray reflectometry methods. Important semiconductor materials such as high-k dielectrics and advanced metallization systems are now routinely characterized by this approach, and the recent integration of X-ray systems into fab-compatible process metrology tools suggests that the importance of X-ray reflectometry will continue to grow in time. Unfortunately, the results obtained from a high resolution X-ray analysis are often compromised by the combined effects of limitations in hardware, software, the sample, and the experimental technique. For example, all X-ray experiments are subject to the effects of noise that generates a minimum threshold for the expected goodness of fit between the experimental data and a curve that is calculated from an assumed model structure. Various experimental aberrations such as (but certainly not limited to) displacement of the sample from the instrument rotation axis and misalignments of the sample and detector rotation axes can distort the measured X-ray reflectivity profile. Finally, there is the question of the uniqueness of an assumed model structure: how complex must an assumed structure be before a to the experimental data set is considered to be statistically reliable?

This talk will discuss some basic principles of high resolution X-ray reflectometry and will describe a number of the issues that limit their accuracy and precision. We will describe the design, construction and performance of a novel high resolution X-ray reflectometer that incorporates several features that have been specifically incorporated to improve its capabilities for precision angle metrology. The system consists of two coaxial goniometers that are located on a precision platform that provides independent adjustment of the alignment of the rotation axes within known tolerances. Thermal effects (both thermal expansion and the generation of thermal gradients by the goniometer drive motors) have been accounted for in our design. The goniometers have state-of-the-art angle encoders directly fitted to the moving circles to measure the angle settings of the both the \( \omega \) and the \( 2\theta \) axes with full-circle closure calibration. A program has been initiated to examine the cross-coupling of experimental aberrations in X-ray reflectometer measurements and the effects of these errors on structural determinations. The effects of noise on these physical factors and their combined effect on the determination of the true structure of a thin film semiconductor structure will be discussed.