Application Report XRD 19

D8 DISCOVER with PILATUS3 R 100K-A 2D RSM of Thin Films

The D8 family of diffraction solutions combined with the DECTRIS PILATUS3 R 100K-A hybrid photon counting (HPC) pixel detector is an innovative 2D x-ray diffraction (XRD^2) solution that is well suited for multipurpose modern materials research characterization. In this report, we present examples of Reciprocal Space Maps (RSM) taken with this detector to characterize thin films.

Introduction

Thin films are layered materials ranging in thickness from fractions of nanometers to several micrometers. Thin films are of major technological interest, since the nanoscopic scale can emphasize or even modify physical behaviors of the corresponding bulk material. Depending on the targeted film properties, different materials and deposition processes (physical or chemical) can be used to produce the desired atomic structure and morphology. For example, a Tungsten coating can be applied in a polycrystalline form for corrosion prevention, whereas a SiGe film may be deposited as a single crystal following the crystalline structure of the substrate (epitaxially) for semiconductor applications. Reciprocal Space Mapping (RSM) with X-ray diffraction (XRD) is a non-destructive technique that can be used to characterize these parameters. Typically, RSMs require a series of many scans that allow the substrate and film diffraction intensity to be mapped in angular space and then optionally converting to reciprocal space for analysis. These types of measurements can be done very easily and much more quickly using a 2D detector.

Measurement

To illustrate this technique, 4 samples were measured: A randomly oriented polycrystalline tungsten film on Si substrate, a preferentially oriented (textured) copper film on Si substrate, an epitaxial GaAs film on a Si substrate, and an epitaxial 30% SiGe on Si substrate. The samples were measured in reflection with a D8 DISCOVER equipped with a Cu target IµS micro-focus source, a parallel beam Montel optic, 300 micron collimator and PILATUS3 detector. The detector was set to a distance of 2.3 cm and 2 frames were collected. Frame 1 had coverage of 36° to 102° 2θ with the sample being rocked from 20° to 70°. Frame 2 had coverage of 66° to 132° 2θ with the sample being rocked from 26° to 104°. Each frame collection took 5 minutes, resulting in a total data collection time of 10 minutes. The high count rate capability of the PILATUS detector prevents saturation effects even with the strong single crystal peak intensities. The resulting 2D scattering was used to generate a RSM and evaluate the films.

Results

The XRD^2 images were imported into DIFFRAC.EVA, where they were merged together using a projection onto a cylindrical coordinate system. By covering a large portion of reciprocal space with a single rocking motion, many reflections are captured within a single frame. The point like high intensity reflections consistently seen in all 4 figures correspond to the single crystal Si substrate.

The 2D RSM of all 4 samples are shown in Figures 1-4. In Figure 1, continuous conic sections are observed at the anticipated locations for the tungsten film. This indicates a random crystallographic orientation of the film. Figure 2 shows the Cu film diffraction rings with intensity variations along each ring indicating texture. Further analysis showed that it exhibited fiber texture that was along the [001] crystallographic direction pointing out of the plane of the film. Figures 3 and 4 show epitaxial films of GaAs on Si and SiGe on Si, respectively. The horizontal alignment of the film reflections relative to the Si substrate reflections indicates the degree of relaxation of the film, which is a measure of how much the lateral lattice parameters of the film have been strained to match the substrate. The 2D RSM of the GaAs film in Figure 3 indicates that it is fully relaxed (no strain) while the SiGe film in Figure 4 is fully strained. In addition, the horizontal broadening of the GaAs reflections indicates a large degree of mosaic spread, while the sharp SiGe reflections indicates the films high crystalline quality.

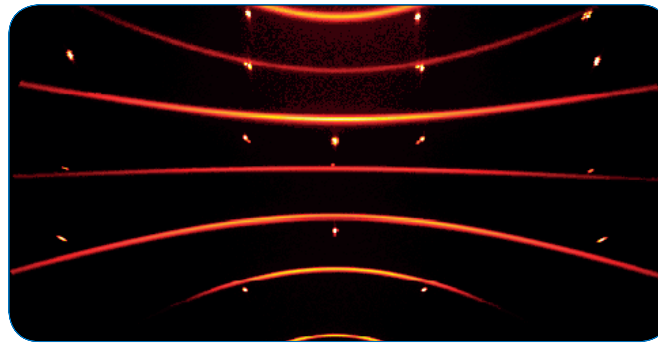

Figure 1: 2D RSM of **randomly oriented W** film on Si

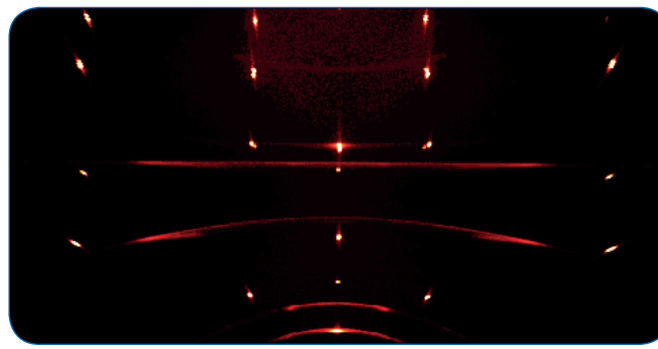

Figure 2: 2D RSM of **fiber textured** Cu film on Si

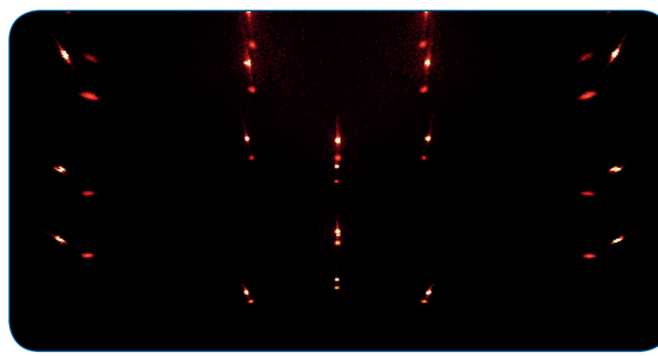

Figure 3: 2D RSM of **relaxed epitaxial** GaAs film on Si

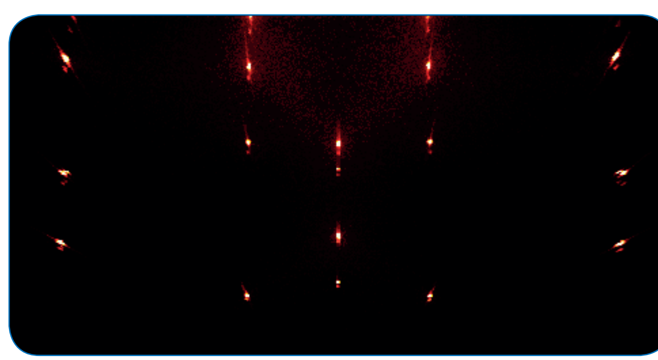

Figure 4: 2D RSM of **strained epitaxial** SiGe film on Si

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