Pacific Northwest Consortium CAT

COherent Bragg Rod Analysis (COBRA)

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1) Introduction.

We have devised a new x-ray method for the direct determination of epitaxial structures. Examples include: reconstructed crystal surfaces, epitaxial thin-films, their interface with the substrate and layered heterostructures, crystalline-amorphous interfaces (Si-SiO_2) and proteins crystallized on a substrate. The high brightness and coherence of the APS undulator radiation enable interference measurements along the characteristic Bragg rods, preserving the *phase* of the scattered x-rays. Using a highly efficient numerical procedure, the complex structure factors (CSF) of the film and the interfacial region are extracted from these interference measurements along the substrate defined Bragg rods. Fourier transformation of the CSF then provides a complete three-dimensional map of the electron density revealing the structure of epilayers even far from the interface, as well as distortions in the underlying substrate. Here we describe the use of this novel technique to study the structure of a thin Gd_2O_3 passivation layer on GaAs.

2) The method:

The method consists of the following steps:

- Measure diffraction intensity along the Bragg rods.
- Consider the electron density as composed of two parts: A known part such as the ideal substrate or a crude model of the system and a second unknown part that together with known add up to the real system.
- Assumption: The complex scattering factor (CSF) U(k) of the unknown part varies along the Bragg rod more slowly than that of the known part S(k). The known part of the electron density is chosen in such a way so as to satisfy this assumption.
- Calculate the CSF of the unknown part at every point along the Bragg rod using two simple equations:

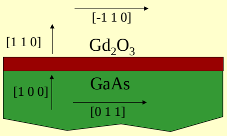
$U(k)+S(k_-)=|T(k_-)|$

$u(k)+S(k_+)=|T(k_+)|$

Here: k_- and k_+ are two points one below and one above k; |T| is the measured diffraction intensity.

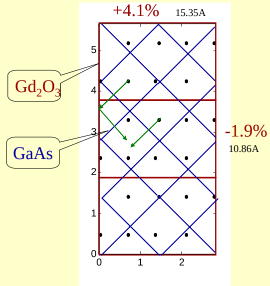
- Fourier transform the CSF into real space to obtain the three dimensional electron density.

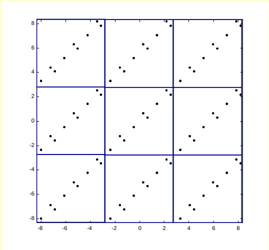
3) The GaAs-Gd_2O_3 system



Gd_2O_3 grows on GaAs as a single crystal single domain film. The Gd atoms are approximately located on planes parallel to the interface.

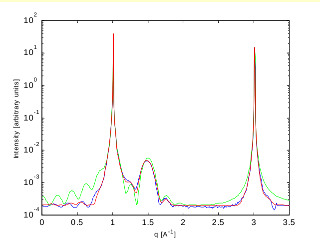
4) The GaAs and Gd_2O_3 2D unit cells





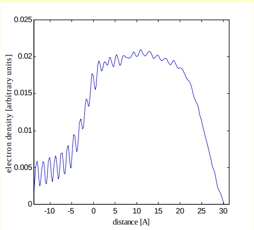
At planes parallel to the interface three Gd_2O_3 cells approximately match 4 GaAs face diagonals and one Gd_2O_3 face diagonal matches 2 GaAs face diagonals. The electron density that we obtain from the measurements along the GaAs Bragg rods corresponds to a GaAs 2D unit cell with all atoms translated into this cell by in-plane unit cell vectors. The result is shown on the right.

5) Experimental results



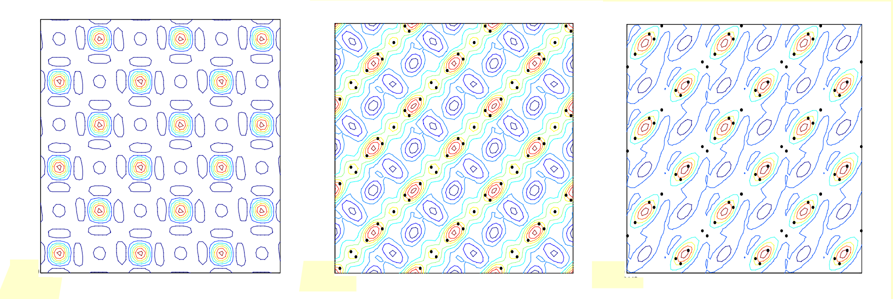
The diffraction intensity along the [h 1 -1] Bragg rod. This is one of the 13 symmetry inequivalent Bragg rods measured. Experimental curve - blue; 9 parameter model - green; result using 'COBRA' - red. Similar quality results are simultaneously obtained for all 13 rods.

6) Layer electron density



The electron density as a function of distance from the nominal interface. Notice the gradual rise and fall in electron density showing the interface and surface roughness regions. The large oscillations show the Ga and As monolayers. The fact that the oscillations on the Gd_2O_3 side are small indicates the presence of large disorder.

7) In-plane electron density



Examples of in plane electron density maps. Left Ga or As plane; Middle and right, layers14 and 15. Each map consists of 3X3 GaAs unit cells. The black dots represent the positions of the Gd atoms after translation into one GaAs 2D unit cell.

Analysis of the electron density maps shows that the structure of the Gd oxide film is quite different from the structure of the Gd oxide three dimensional crystal.

8) Conclusion: **COBRA is a powerful new method to determine the structure of epitaxial systems.**