New Method to Directly Determine Atomic Positions in Epi-Films

Beamlines: NSLS, X25
APS, ID-7

Technique: Coherent X-Ray Diffraction

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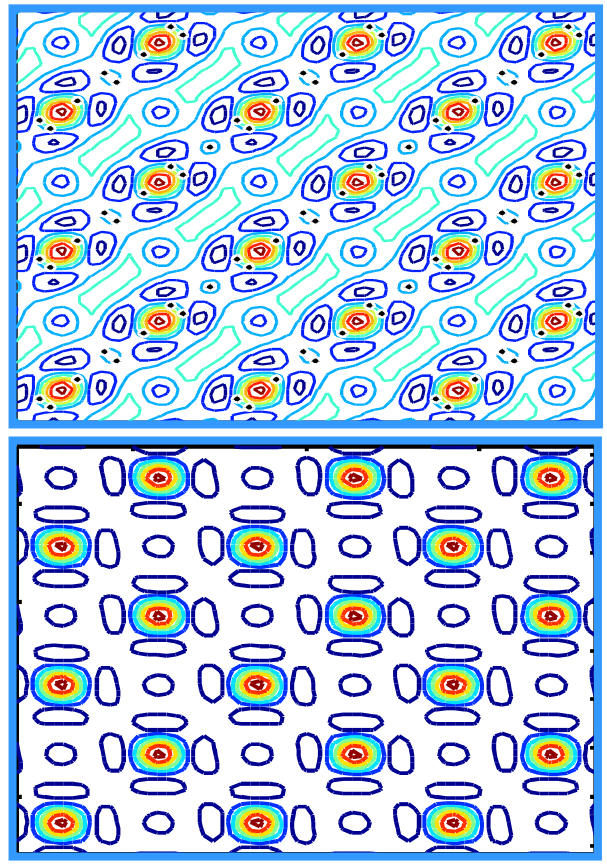
Y. Yacoby, et al. "Direct determination of epitaxial interface structure: Gd_2O_3 passivation of GaAs" *Nature Materials* **1**, 99 (2002).

Motivation: The increasing use of epitaxial thin films in the manufacturing of semiconductor devices makes it essential to understand the atomic structures of these films and how they interface with underlying substrates. Epitaxial films of Gd_2O_3 on GaAs substrates are of technological interest because Gd_2O_3 retains its bulk electronic properties even in films as thin as 10 molecular layers.

Results: A new method was developed to directly determine atomic positions with sub-angstrom resolution. The method, given the acronyn COBRA, involved an analysis of the coherent interference of synchrotron x-rays diffracted along Bragg rods from an epitaxial film-substrate system. When applied to the Gd_2O_3-GaAs system, we obtained electron density maps parallel to the interface indicating that atoms in the first few layers of the epitaxial film as well as the stacking sequence of these layers adjusted to mimic the structure of the atoms in the substrate. We are currently attempting to apply the COBRA technique to the case of a 2D protein crystalline layer bound to a 3D protein crystal.



Electron density map of one of the layers of the Gd_2O_3 epitaxial film close to the GaAs substrate (*upper*) and a layer in the substrate (*lower*).