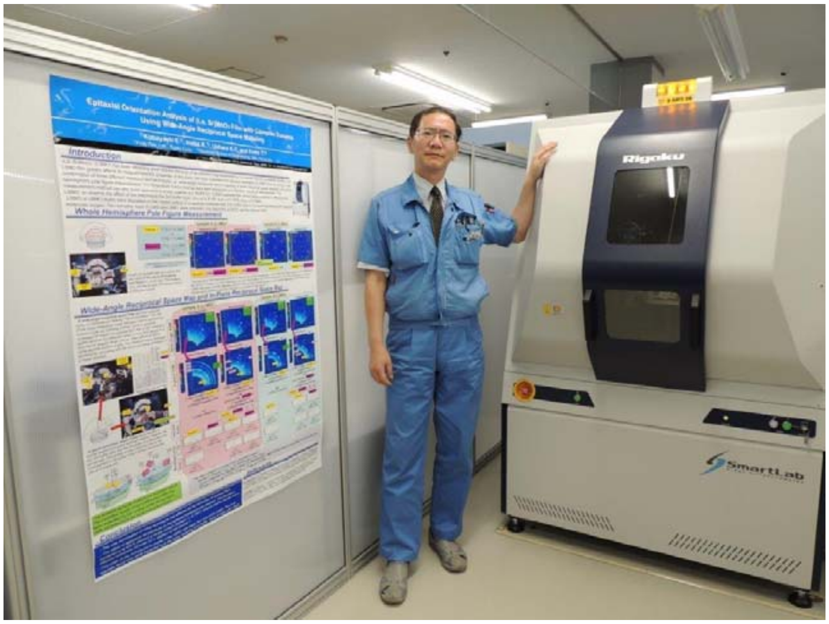
Lab in the Spotlight



This month we are pleased to introduce Dr. Katsuhiko Inaba's paper on HRXRD analysis of thin films. Dr. Inaba manages the Thin Film Characterization group at Rigaku.

The paper has been downloaded over 3300 since it was first published in 2013, and offers helpful hints on the analysis of new functional thin films. It is available via the Open Access journal *Advances in Materials Physics and Chemistry:*

http://www.scirp.org/Journal/PaperInformation.aspx?PaperID=30348

Title: High Resolution X-Ray Diffraction Analyses of (La,Sr) MnO_3/ZnO/Sapphire (0001) Double Heteroepitaxial Films

This article shows the results of XRD analysis of complex orientation relations in (La,Sr)MnO_3 / ZnO double heteroepitaxial layers on Sap(0001) substrates using the SmartLab system.

Various XRD techniques were employed in the analysis, such as out-of-plane 2θ/ω scans, ω rocking curves, pole figure methods, in-plane 2θχ/ϕ scans, ϕ rocking curves, in-plane 2θχ/ϕ–ϕ Reciprocal Space Mapping (RSM) measurements, as well as out-of-plane wide-range RSM using a 2D detector together with CBO-*f* optics. Experimental setups and important issues for performing these measurements are comprehensively explained with an aim toward creating a guide for SmartLab users studying thin film specimens. For this purpose, this article was submitted to an Open Access scientific journal.

As for the materials featured, (La,Sr)MnO_3 manganate has been studied as a colossal magnetoresistance material and as a *p*-type conductive semiconductor. Note that this material used to be called “manganite”, but this is not correct, since the mineral name of “manganite” is dedicated to the material with the chemical formula MnOOH. On the other hand, ZnO is an *n*-type conductive semiconductor widely studied as a transparent conductive oxide (TCO) for thin film transistors (TFT) or window materials of solar cells or displays. The epitaxial integration of (La,Sr)MnO_3 and ZnO will enable the *p-n* heterojunction composed with transparent oxide semiconductor materials.

The great obstacles to this end were the large lattice mismatch between these two materials and the significant difference of their crystallographic structures. These differences hindered a simple and single crystalline epitaxial growth, forming very complicated domains where these materials were grown with certain crystallographic orientation relations between (La,Sr)MnO_3 , ZnO, and the sapphire substrates.

By careful and thorough analysis of XRD data from various XRD techniques, we found that three kinds of orientation relations exist, specifically

1. LSMO (110) phase：$[1\bar{1}0](110)\mathrm{LSMO}//[1\bar{1}00](0001)\mathrm{ZnO}//[11\bar{2}0](0001)\mathrm{Sapphire}$
2. LSMO (001) phase：$[110](001)\mathrm{LSMO}//[1\bar{1}00](0001)\mathrm{ZnO}//[11\bar{2}0](0001)\mathrm{Sapphire}$
3. LSMO (111) phase：$[1\bar{1}0](111)\mathrm{LSMO}//[1\bar{1}00](0001)\mathrm{ZnO}//[11\bar{2}0](0001)\mathrm{Sapphire}$ or
   $[11\bar{2}](111)\mathrm{LSMO}//[1\bar{1}00](0001)\mathrm{ZnO}//[11\bar{2}0](0001)\mathrm{Sapphire}$

Each orientation relation is composed of multiple variants, based on the combination of crystallographic symmetries of its constituents. These orientation relations are summarized in the figure in the end of this note.

We hope this article will be helpful for researchers studying epitaxial thin films by supporting and giving some hints for the approaches to XRD measurements and analysis.