Accurate Determination of the Lattice Constant Deviation at Nanoscale by Diffraction Mapping

Bekarevich, R.[1], Mitsuishi, K.[1], Ohnishi, T.[1], Mano, T.[1], Uesugi, F.[1] and Takeguchi, M.[1]

[1] National Institute for Materials Science, Japan

In this study we report the improved scanning diffraction method using two-dimensional (2D) Gaussian fitting for accurate measurement of lattice constant (LC) deviation at thin film interface.

Determination of lattice constant deviation is important issue for material engineering. Conventional methods like X-ray diffraction (XRD) enable us to get all necessary information in macroscale, but there is a lack of simple and reliable methods when we move to nanoscale.

Recently a strain mapping method combining nanosized selected area electron diffraction (NSAD) with a two-dimensional (2D) sample scanning system was proposed [1], but it suffers from the poor accuracy and precision. Scanning NSAD method enables us to detect LC changes from 2D diffraction maps by measuring the inter-spot distances at different locations of the sample. We improved the precision of abovementioned method by accurate determination of the centres of diffraction spots using 2D Gaussian fitting [2].

This work is continuation of our previous study aiming the accuracy and sensitivity evaluation of scanning NSAD method. Herein we determined a LC deviation at thin film interface from diffraction map and compared the results with XRD data.

For sensitivity evaluation we used pulsed-laser-deposited $SrTiO_3$ film on a $SrTiO_3$ substrate. The LC of the film locked to the substrate in horizontal (in-plane) direction, but expanded on ~0.7% in out-of-plane direction (Figure 1). In-plane and out-of-plane LC deviations presented in Figure 2 as 15×15 pixels maps obtained by NSAD, where one pixel is ~12×12 nm^2. It is seen that in in-plane direction the LC is same for film and substrate, but there is a difference in out-of-plane direction. The difference between the LCs of film and substrate is slightly varies from one place to another, but all the values of LC change are lies within 0.4 - 0.45% in out-of-plane direction, what is slightly smaller than data derived from XRD spectrum.

We used thin film of InAlAs grown onto semi-insulating GaAs (111) A substrate to study the mismatches in LC between two layered materials. For this materials the LC difference is 3.5% and 3.6% in out-of-plane and in-plane directions respectively. NSAD technique enabled us to draw the LC deviation maps well correlating to the local structure of the interface area (Figure 3). The LC differences calculated from these maps are 3.3 and 3.5% for out-of-plane and in-plane directions respectively. The measured value of LC deviation is again slightly smaller than expected. Therefore, if we will assume the XRD data as true value, the accuracy of our method is ~0.2 - 0.3%. However, films on the thin lamella used for transmission electron microscopy (TEM) observations are in relaxed state in comparison with bulk material observed by XRD. This feature of TEM sample can explain the difference between XRD and scanning NSAD results.

In summary, we created an accurate, precise and reliable method for detection of LC deviation at nanoscale. It is expected to apply this method for study of quantum wells and battery materials.

Acknowledgements: Part of this work was financially supported by the research project "Advanced Low Carbon Technology Research and Development Program for Specially Promoted Research for Innovative Next Generation Batteries" of the Japan Science and Technology Agency (JST ALCA-SPRING) and by the Ministry of Education, Culture, Sports, Science and Technology (MEXT) program for the Development of Environmental Technology using Nanotechnology.

References:

[1] F. Uesugi, Ultramicroscopy 135, 80-83 (2013).

[2] R. Bekarevich et al., Microscopy, https://doi.org/10.1093/jmicro/dfx121

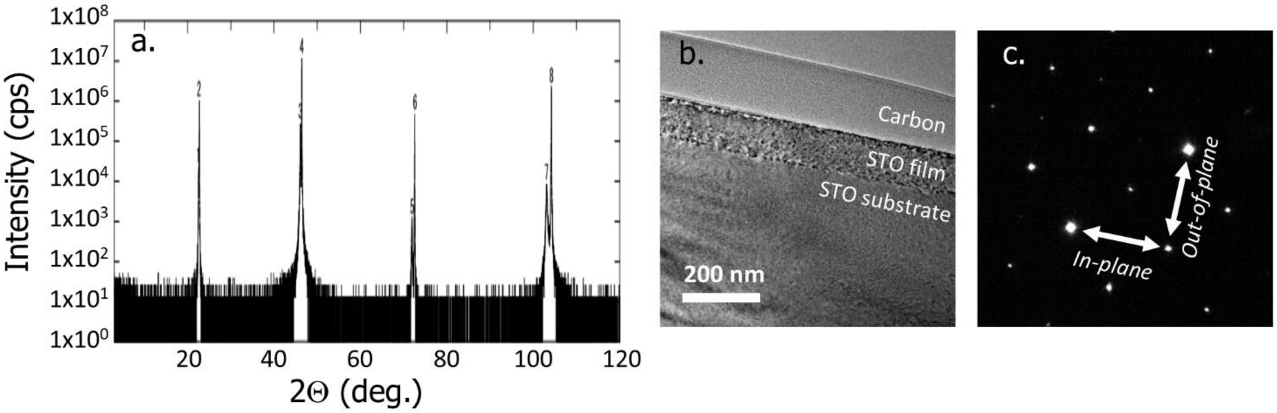

Figure 1. XRD spectrum of SrTiO₃ film on SrTiO₃ substrate (a), corresponding TEM image (b), and typical diffraction pattern (c). The splitted peaks on XRD spectrum indicate the LC mismatches between film and substrate. White arrows on diffraction pattern show the spots used for evaluation of LC changes.

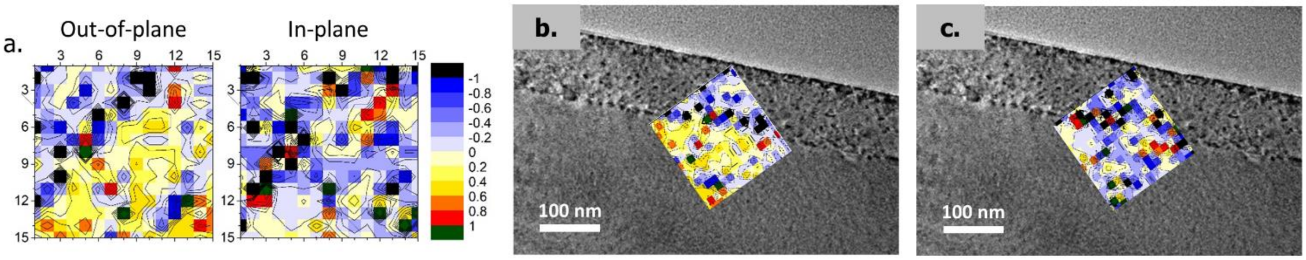

Figure 2. Maps of LC changes in out-of-plane and in plane directions (a) and their projections on TEM image (b, c).

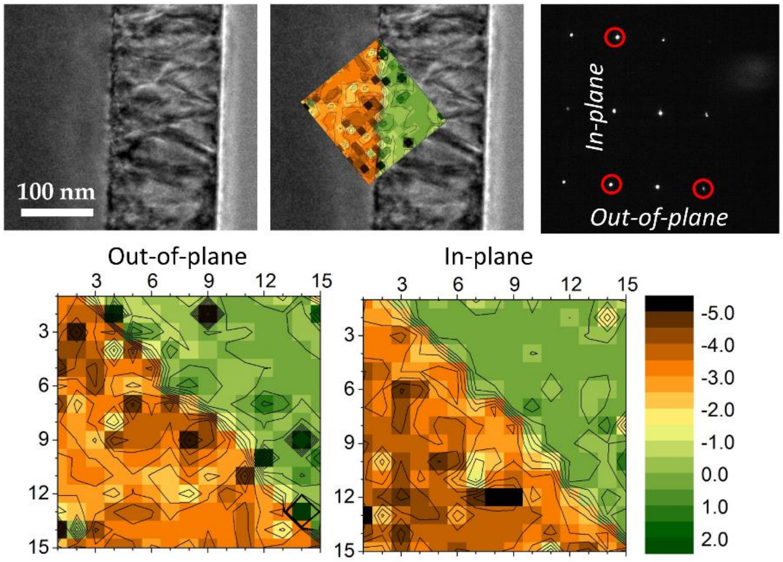

Figure 3.TEM image, typical diffraction pattern, and LC change maps of InAlAs film heteroepitaxialy grown onto GaAs(111)A substrate