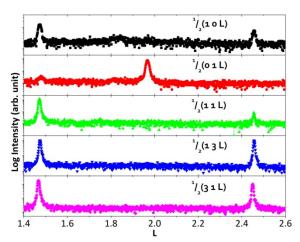
Octahedral Tilting in SrRuO₃ Films Studied by Half-Order Reflexions

Wenlai Lu¹, Ping Yang², Gan Moog Chow¹ Jingsheng Chen¹

- 1. Department of Materials Science and Engineering, National University of Singapore, Singapore 117576, Singapore
- 2. Singapore Synchrotron Light Source (SSLS), National University of Singapore, 5 Research Link, Singapore 117603, Singapore

Octahedral tilting has been of great interest since it is intimately linked to the electronic structure and thus the physical properties of ABO_3 perovskite oxides. Recently, there are reports on the modification of octahedral tilting in $SrRuO_3$ films either by strain engineering [1] or by varying film thickness [2]. Despite the extensive studies on the crystal structures of $SrRuO_3$ films, direct evidence for the accurate octahedral tilt system is missing.

In our study, half-order reflexions have been employed to investigate the octahedral tilting in SrRuO₃ films. According to Glazer [3], there are basically two types of tilt: tilts where octahedra rotate in-phase along one axis, denoted by the superscript +, and tilts where the octahedra are rotated out-of-phase,



denoted with the superscript -. The in-phase and out-of-phase tilt about a particular axis can be easily distinguished by the presence of odd-odd-even type and odd-odd-odd type peaks. As shown in Figure 1, the presence of 1/2103 and 1/2105 peaks implies that there are in-phase tilts about [010] axis, denoted by b⁺. The absence of 1/2013,

1/2015 peaks and existence of 1/2113, 1/2115 peaks indicates that the rotations about a axis are out-of-phase, denoted by a⁻. Similarly, there are purely – tilts about c axis, indicated by the absence of 1/2132, 1/2312 and the presence of 1/2133 peak. Considering the equality of lattice parameters a_c and b_c based on the pseudocubic cell, the tilt system is immediately determined to be $a^-a^+c^-$, which is consistent with the tilt system inferred from the lattice parameter measurements as reported previously [1].

These results show that the measurement of half-order peaks is a straightforward approach for determining the octahedral tilt system and can be applied to other perovskites.

Acknowledgment The author would like to thank Shanghai Synchrotron Radiation Facility (SSRF) for the support.

^[1] A. Vailionis, H. Boschker, W. Siemons, E. P. Houwman, D. H. A. Blank, G. Rijnders and G. Koster, Phys. Rev. B **83**, 064101 (2011).

^[2]Seo Hyoung Chang, Young Jun Chang, S. Y. Jang, D. W. Jeong, C. U. Jung, Y.-J. Kim, J.-S. Chung and T. W. Noh, Phys. Rev. B 84, 104101 (2011)

^[3]A. M. Glazer, Acta Cryst. A 31, 756 (1975)