# Structural analysis of metal oxide quasicrystal thin films

Junji YUHARA

*School of Engineering, Nagoya University,*

*Furo-cho, Chikusa-ku, Nagoya, Aichi 464-8603*

We have studied metal oxide quasicrystal ultra-thin films [1] using massively parallel computer simulations. This year, we focused on the structural analysis of honeycomb structure ultrathin Ce-Ti-O films on Pt(111) [2]. The density functional calculations were conducted using VAPS 5.4.4.

After deposition of 0.5 ML Ce and 0.8 ML Ti on Pt(111)/sapphire(0001), following with annealing in oxygen atmosphere and vacuum, an arrangement of dodecagonal clusters, which consists of triangles and squares marked in white, were locally observed in STM image (Fig. 1). In addition, there are some purple triangles and green trapezoids which have an unequal distance to the clusters marked in white, leading it to be recognized as OQC-related structure.

For the OQC-related structure of the ultrathin Ce-Ti-O film, Ce corresponds to $Ce^{3+}$. Titanium appears as $Ti^{2+}$ ions, as the XPS and XAS spectra indicate. The elemental atomic composition was determined based on the experiment, proposing a low-density model, as shown in Fig. 2. This model's stability and STM simulation are calculated using VASP. Surface atomic density is estimated through XPS and Rutherford backscattering spectroscopy.

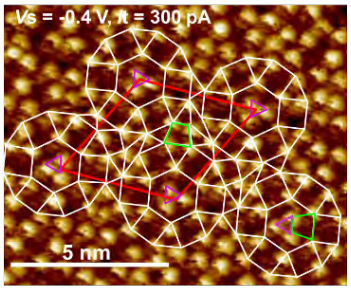


Fig.1: STM image of OQC-related structure of ultra-thin Ce-Ti-O film.

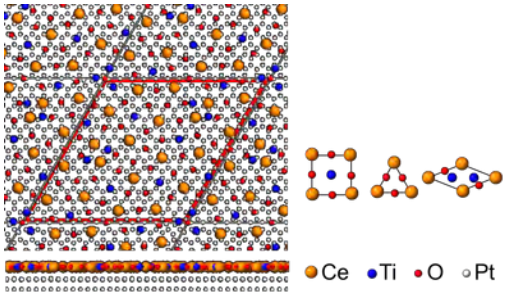


Fig.2: Schematic structural model of OQC-related structure of ultra-thin Ce-Ti-O film.

## References

[1] J. Yuhara, K. Horiba, R. Sugiura, X. Li, T. Yamada, Phys. Rev. Mater. **4**, 103402 (2020)

[2] X. Li, S. Yamada, Y. Yamada, M. Yoshida, Y. Hashimoto, T. Matsushita, W. Ma, E. Gaudry, and J. Yuhara, J. Phys. Chem. C **128**, 20238 (2024)