

MS21-1-2 Quasicrystalline ultrathin oxide films : model structures and properties
#MS21-1-2

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Abstract

Recently, the discovery of the quasiperiodic order in ultra-thin perovskite films reinvigorated the field of 2-dimensional oxides on metals, and raised the question of the reasons behind the emergence of the quasiperiodic order in these systems [1]. In this talk, we focus on a theoretical approach based on Density Functional Theory to investigate quasicrystalline ultrathin oxide films grown on metallic single crystal substrates [2]. The crystalline structure of these 2D phases can be described by specific tilings using a few elementary tiles (squares, triangles and rhombuses) [3] as observed by Scanning Tunnelling Microscopy (STM). Calculations point the exothermic formation of these systems, which interact quite strongly with the underlying metal support, but more weakly than less complex structures. The optimization of the atomic positions shows a significant relaxation in the direction perpendicular to the surface, which could alleviate the strain due to the lattice mismatch between the substrate and the oxide layer. The interaction between the film and the underlying metal is ensured by hybridization of electronic states and by charge transfer from the oxide layer to the underlying metal. The calculated STM images are in perfect agreement with the experimental images, which confirm both the atomic structure model and the two-dimensional character of the oxide formed. Compared to the initial perovskite structure, the 2D oxide films obtained after reduction are under stoichiometric both in oxygen and in strontium. Electronic effects are found important parameters that influence the formation of quasicrystalline ultra-thin oxides. Up to now, experimentalists have mainly focused on BaTiO₃/Pt and SrTiO₃/Pt, because of the small size mismatch with Pt. We strongly believe that many complex 2D oxide quasiperiodic or approximant systems remain to be discovered.

References

- [1] T. T. Dorini et al., Two-dimensional oxide quasicrystal approximants with tunable electronic and magnetic properties, *Nanoscale*, 13, 10771 (2021)
- [2] C. Ruano Merchan et al., Two-dimensional square and hexagonal oxide quasicrystal approximants in SrTiO₃ films grown on Pt(111)/Al₂O₃ (0001), *Phys. Chem. Chem. Phys.*, 24, 7253 (2022)
- [3] E. Cockayne et al., Structure of Periodic Crystals and Quasicrystals in Ultrathin Films of Ba-Ti-O, *Phys. Rev. B*, 93, 020101 (2016)

Structural model of a 2D quasicrystal approximant

