Oxide quasicrystal approximants in the Ba-Ti-O system on Pd(111): A LEED and STM study

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Two-dimensional oxide quasicrystals are found in Ba- or Sr- decorated Ti_2O_3 monolayers supported on Pt(111) substrates [1,2,3]. In these systems, the alkaline earth metal ions form the vertex positions of a dodecagonal triangle-square-rhombus tiling. In this contribution, we report on structure formation in two-dimensional Ba-Ti-O on Pd(111), which possesses a 1% reduced lattice parameter in comparison to Pt(111). We find a series of quasicrystal approximants with varying Ba density. At a stoichiometry of $Ba_{0.67}Ti_2O_3$ we observe a triangle-square tiling, the σ-phase approximant. Higher Ba densities result in patches of this triangle-square tiling with one-dimensional antiphase domain boundaries in between. This way rhombuses are introduced to the tiling. The frequency of the antiphase domain boundaries is adapted to the surplus of Ba [4]. At the nominal composition of the oxide quasicrystal of $Ba_{0.73}Ti_2O_{3.10}$ such antiphase domain boundaries are incorporated in two orthogonal directions, introducing periodic unit cells with a triangle-square-rhombus tiling [5]. The unit cell of the resulting structure is orthorhombic with dimensions of (2.6x6.4)nm² inclining an angle of 92.5°. By applying the tiling decoration scheme of oxide quasicrystals to this structure [2,6], the complex Ti_nO_n ring structure with its different ring sizes of n=4,7,10 hosting the Ba atoms can be unraveled as shown in Figure 1. It turns out that this orthorhombic phase forms at 73% coverage of all Ti_nO_n rings with Ba and it contains 40 Ba, 110 Ti and 170 oxygen atoms. The complex diffraction pattern of this phase will be discussed in the light of its subtle differences to the diffraction of a dodecagonal structure.

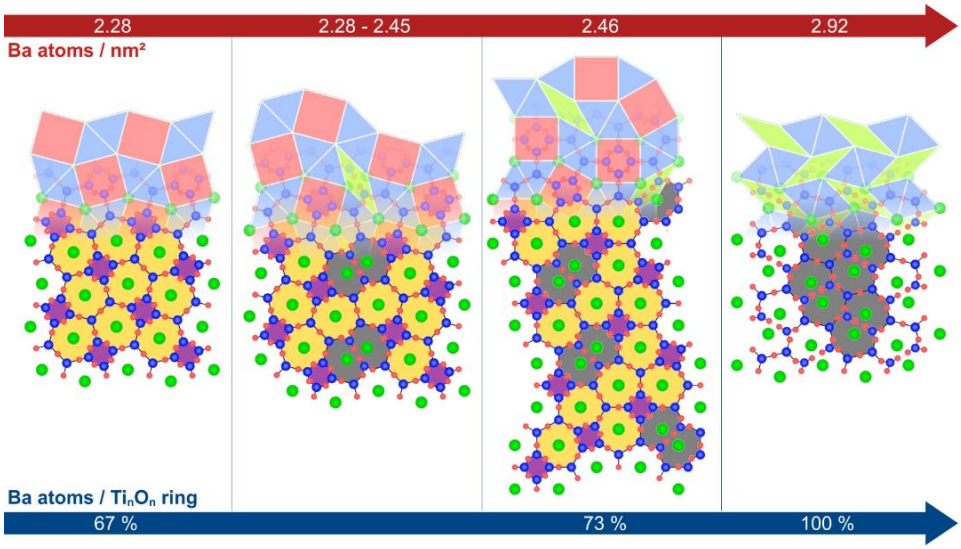

Fig. 1. Phase diagram of monolayer $Ba_xTi_2O_3$ on Pd(111) depending on their Ba density (top axis) and relative Ti_nO_n ring occupation (bottom axis) [5].

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