The Kepler Tiling as the Oldest Complex Surface Structure in History: X-Ray Analysis of a Two-Dimensional Oxide Quasicrystal Approximant

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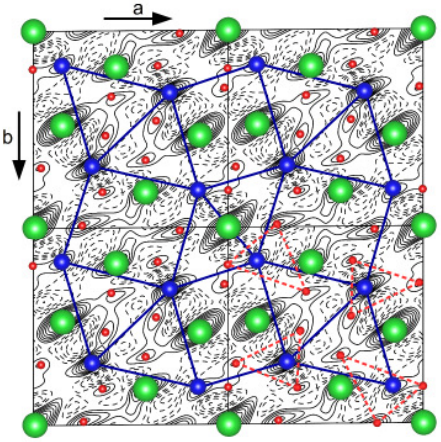
An oxide type of quasicrystal has been discovered which is related to barium titanate (BaTiO3) [1]. The two-dimensional (2D) oxide quasicrystal (OQC) and its periodic approximant (AP) were grown in situ on Pt(111) and were investigated by scanning tunneling microscopy (STM) which provided clear evidence for the presence of different tilings. For both, the OQC and the AP only one kind of protrusion could be observed by STM, which are arranged in a 2D pattern identified as Stampfli-Gähler tiling [2, 3] for the OQC and the Kepler tiling for the AP, respectively. The Kepler tiling was already described in 1619 [4].

We have carried out a surface x-ray diffraction study to analyze the geometric structure of the AP, which also allows developing a model for the OQC structure [5, 6].



2D charge density contour of the AP structure. The Kepler tiling of the Ti atoms is indicated by solid lines

Figure 1 shows the z-projected charge density contour plot calculated based on 43 reflections $|F_{hk0}|$ [5, 6]. Four 2D unit cells with lattice parameter a=13.1 Å, b=12.9 Å, γ=90.5° are shown. Superimposed are the approximate atomic positions derived from the least squares refinement (R=13%). Protrusions observed by STM [1,5] are related to titanium atoms (medium sized blue balls) each of which being surrounded by three oxygen atoms (small, red) approximately forming a triangle. Furthermore, barium atoms (big, green) are located at the origin of the unit cell. Further barium atoms are located in the vicinity near two out of four edges of the squares. The AP's stoichiometry is given by $Ba_4Ti_4O_{10}$.

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