Realizing Great Pyramid Geometry within Inorganic Nanoscale Pyramid Arrays: A Crystallographic Guidance

Hans Hermann Otto

Materials Science and Crystallography, Clausthal University of Technology,
Clausthal-Zellerfeld, Lower Saxony, Germany

E-mail: hhermann.otto@web.de

Abstract

We propose to realize the growth of nanoscale pyramids of inorganic material that adapt the golden aspect ratio of the Great Pyramid. Suitable for this research is tetragonal TiO_2 (rutile) deposited onto a KBr substrate. Besides pure mathematical respectively philosophical concern physical properties of such pyramidal arrays could be of interest.

1. Introduction

The model of the Great Pyramid as special golden mean based body can inspire the design of non-space-filling pyramidal origami patterns that could have interesting mechanical or optical properties resulting from the intrinsic geometric frustration that causes multi-resonator properties at special frequencies with attention to chiral components. Asymmetric light scattering was recently observed in pyramidal silicon nanoparticles, and applications were proposed [1]. In silicon *PV*'s, an enhancement in the generated short-circuit current of about 40% was described by embedding periodic arrays of square pyramidal-shaped nanoparticles as multi-resonators [2]. The optimum of current gain was observed with a pyramidal aspect ratio of about 2. However, we ask what gain would be possible with an aspect ratio similar to that of the Great Pyramid? We will consider growing of nano-scale pyramids of inorganic materials on selected substrates by methods of physical or chemical vapor deposition. Whereas the formation of pyramids was observed even on materials with a sheet structure such as $MoSe_2$ by a screw dislocation mechanism [3], the deposition of pyramidal islands should be easier when using materials such as TiO_2 in the rutile modification. We explain in the following a guideline for growing experiments to deposit nanoscale 'golden' pyramidal arrays of inorganic material onto a substrate. Besides a more philosophical respectively mathematical concern there may be also a practical importance of geometrical frustrated nano-pyramid arrays.

2. Crystallographic Consideration

If the base length of the Great Pyramid is chosen as $a = 2$, then the Pyramid height yields $h = \sqrt{\phi}$, where big $\phi = \varphi^{-1} = 1 + \varphi$ and $\varphi = \frac{\sqrt{5}-1}{2} = 0.6180339887$ is the golden mean (see **Figure1**).

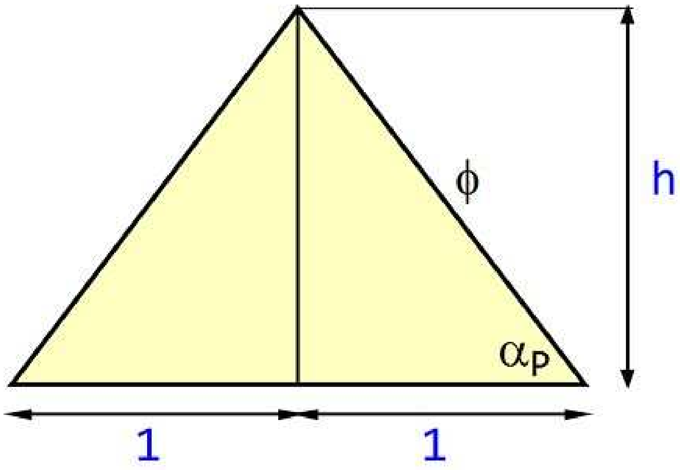

Figure 1. Cut through the middle of a Great Pyramid's face down the apex.
Big ϕ denotes the inverse of φ: $\phi = \varphi^{-1} = 1 + \varphi$ [4].

The aspect ratio as height to base of the Great Pyramid is given by [4] [5] [6]

$$\frac{h}{2} = \frac{\sqrt{\Phi}}{2} = \frac{1}{2\sqrt{\varphi}} = \frac{\tan(\alpha_P)}{2} = 0.636009824 \approx \frac{2}{\pi} = 0.63661977 \quad (1)$$

where $\alpha_P = \arccos(\varphi) = 51.827292°$

When we search for an inorganic material that approximated the Great Pyramid's golden geometry, we will first consider an ideal octahedron that is lying on its edge. A sheet structure composed of such diagonally placed octahedrons deliver the following ideal lattice parameter ratio (see **Figure 2**)

$$\frac{c}{a} = \frac{2}{3} = 0.66667 \quad (2)$$

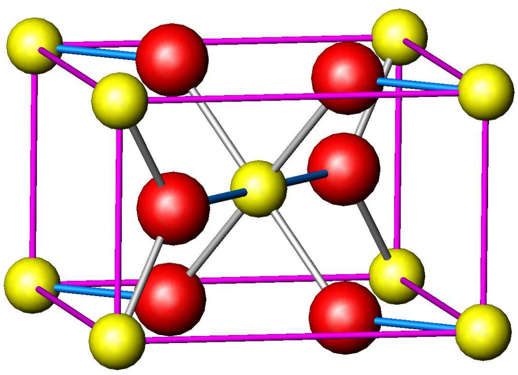

Figure 2. Crystal structure of rutile, tetragonal TiO_2.
Titanium atoms yellow, oxygen atoms red, unit-cell magenta.

Such structure is realized in the tetragonal TiO_2 modification of rutile. However, the edge-sharing of octahedrons causes strong periodic bonding down the chain axis *c*, leading to a remarkable reduction of the *c* to *a* ratio (lattice parameters from PDF card #00-021-1276)

$$\frac{c}{a} = \frac{2.9587}{4.5937} = 0.6441 \quad (3)$$

In this way, we approach the aspect ratio of the Great Pyramid. Better adapted to the aspect ratio of the Great Pyramid is the lattice parameter ratio of stishovite, the rutile modification of SiO_2 (high pressure modification)

$$\frac{c}{a} = \frac{2.6651}{4.1772} = 0.63801 \quad (4)$$

Whereas stishovite as high pressure phase is hardly accessible, we recommend research on rutile as interesting electronic material.
The habitus of the mineral rutile is dominated by three morphological forms, {101}, {100} and {110}. The pyramid (bi-pyramid) {101} is the form we were interested in. Although crystals with strong bonding strength in *c* direction tend to grow in form of rods or needles, we can expect at the beginning of material deposition pyramidal growth without surfactant support. So it is recommended to try the growing of TiO_2 micro-pyramids or nano-pyramids.
For TiO_2 deposition we should use a KBr (100)-substrate. KBr crystallizes in the face-centered cubic halite structure with a lattice parameter of *a* = 6.597 Å (see **Figure 3**).

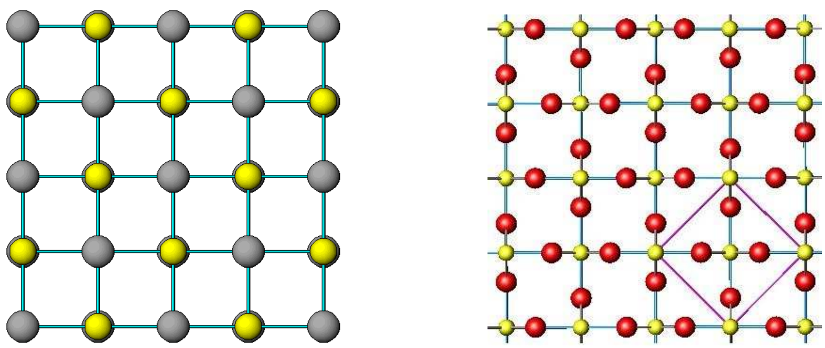

Figure 3. Left: projection of KBr crystal substrate down [001], right: TiO_2 rutile down [001], unit-cell (magenta) rotated in diagonal position to match the growing direction onto the substrate.

The separation of $\frac{a}{\sqrt{2}} = 4.665$ Å is only slightly larger as the lattice parameter for rutile of *a* = 4.5937 Å. The resulting strain is wanted. It causes an increase of the lattice parameter *a* respectively a reduction of the lattice parameter *c* for the deposited rutile. In this way we can indeed reach a ratio of the strained lattice parameters that is adapted to the golden mean aspect ratio of the Great Pyramid by retaining the original unit-cell volume of rutile

$$\frac{c}{a} = \frac{2.934}{4.613} = 0.63603 \quad (5)$$

A (100)-cut crystal substrate of KBr with dimension 10mm x 10mm x 2mm can be obtained from the manufacturer *MSE Supplies LLC*. However, by the use of a $KBr_{1-x}Cl_x$ mixed crystal substrate one can perfectly align the lattice parameters of substrate and growing rutile crystal. Lattice parameters of $KBr_{1-x}Cl_x$ mixed crystals are given in reference [7]. A $KBr_{0.8}Cl_{0.2}$ crystal substrate with a lattice parameter of about 6.528 Å would give a diagonal distance of 4.613 Å and matches the strained rutile lattice parameter given in relation (5).
However, in order to adapt an aspect ratio of about 2 as was pointed out in reference [2], the pyramidal half-octahedral form with *Miller* indices {h0l} = {301} must be grown. In this case the shape has to be controlled by the use of appropriate surfactants.

Once such pyramidal arrays have been successfully deposited, substrates other than KBr will also be found, e.g. artificially made micro-square structures in a gold foil, but in this case the strain effect is not given.

3. Physical Consideration

The application prospect of such rutile-based nano-pyramidal arrays as anode material for Li-ion batteries (LIBs) depends on the electric conductivity. We expect indeed an enhanced electric conductivity of such arrays in contrast to other deposited TiO_2-based anode sheets.
Moreover, in nano-scaled pyramids the displacement of extern energy fields should be considered as explained by the *Casimir* effect [7]. The *Casimir* effect is the dominant interaction between nano-scale objects, where the omnipresent quantum electromagnetic vacuum energy in parts is displaced between, for instance, two perfectly conducting parallel plates. On the other hand, electromagnetic energy in the optical range can be concentrated in the pyramids. The refractivity indices of rutile are large with $n_\omega = 2.61$ and $n_\varepsilon = 2.90$ compared to that of diamond with $n = 2.42$.

4. Conclusion

The realization of an array of inorganic micro- respectively nano-pyramids with the aspect ratio of the Great Pyramid seems to be practicable by vapor deposition of rutile-type TiO_2 onto a (100)-cut KBr substrate. It is expected that the strain between substrate and deposited TiO_2 shifts the lattice parameters of TiO_2 towards the wanted aspect ratio of the Great Pyramid. Enhanced electric conductivity of such arrays for use as anode material for LIB's is also expected. The effect of the *Casimir* force on nano-pyramids of this special geometry may also be of fundamental interest.

Conflicts of Interests

The author declares no conflicts of interest regarding the publication of this paper.

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