ORIGAMI OF A PEROVSKITE STRUCTURE

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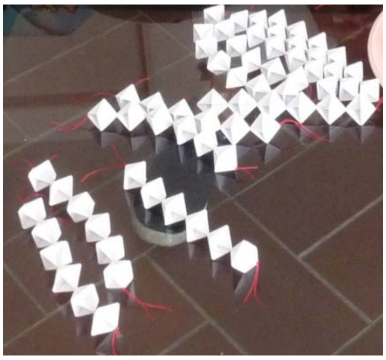
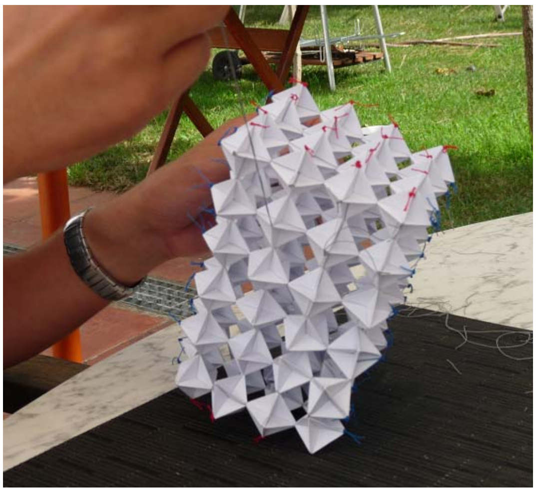
Here we show how to construct an origami of corner sharing octahedra that reproduces the octahedron tilts described by Glazer[1]. This origami is able to reproduce most of the phases that you can obtain from a cubic perovskite by tilting the octahedra as well as to reproduce domain walls and apply stress and observe how the octahedra act in response. Also it is possible to construct models with different octahedron sizes reproducing ordered perovskites or defect supercells.



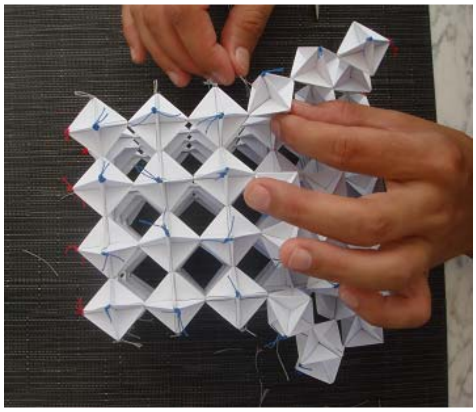
The perovskite structure ABO_3 consist on corner-sharing octahedra with six oxygen atoms at its vertices and *B* cation in the center. Typically the *A* cation has small ionic radius compared to the space left in between octahedra so the structure is deformed by tilting the octahedra with respect to each other to contract the structure and fill the empty space.

As the number of constrains is exactly the same of the number of degrees of freedom minus 6, the structure is critically rigid. It is a very hard problem to simulate numerically as no general algorithms exist to solve them exactly.



In order to study the collective rotations of corner-sharing octahedra as in the perovskite structure we constructed a model with folded paper (origami) octahedra and then join them together by sewing their vertices with a thin thread so they have some freedom to allow rotation and tilting. In this report we explain you how to make it.

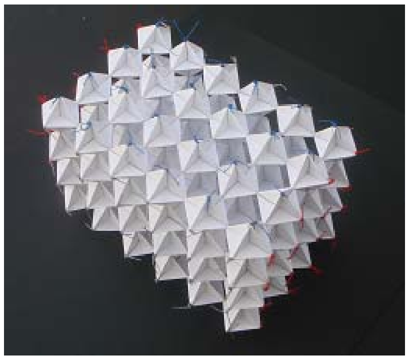
You have to construct a certain amount of octahedra by standard origami techniques [2]. In this case we made 96 identical octahedra which allow us to construct a 6x4x4 octahedron model.



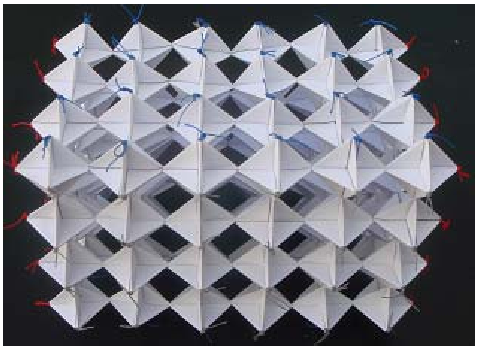
Once you have all the octahedra you start sewing them by using a conventional needle and a conventional thread.

First, we decided to make lines of 6 octahedra each. By the help of a little bead or any stopper you tight them by a knot.

Then you sew 4 of these lines together to obtain a planar 6x4 octahedra layer.



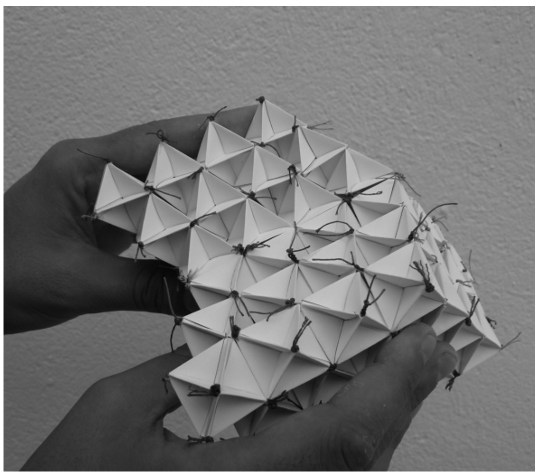
Finally, you sew the 4 planes together to obtain the 6x4x4 model. In this last step, as the model gets 3D it is more difficult to sew together so it is recommended to leave some extra wire that allows to separate the octahedra, as you need space to manipulate the needle. Once you have everything connected you can tight the knots and the octahedra together.



Once you have the model constructed you can start playing with it.

The total hand work is around 2 days of office/lab time once you get used.

This model is very useful to test if a certain domain wall can be formed without deformation of octahedra or to check if a certain stress will rotate the octahedra or expand the lattice size in a certain way. It is observed that the structure can be modified by applying stress just at certain directions, and some times it has to be a shear stress in a particular plane, so it is not that obvious which kind of stresses will produce octahedron rotations and which ones will increase bonding distances in real systems.



Also we have observed that impurities will produce local rotations of octahedra in order to accommodate different impurities with larger or lower ionic radius suggesting that some phase observed at certain degree of cation substitution in some double perovskites may be caused by percolation of local octahedron rotations and distortions.

We believe that this model may be useful for the people working in perovskites.

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[1]. Classification of Tilted Octahedral in Perovskites. *A.M Glazer, Act.Cryst (1972) B28, 3384*

[2]. Octahedron from 6 squares. Youtube http://www.youtube.com/watch?v=NnX8YuEkRBI