GUIDE TO DEPOSIT ITEMS FOR

Tilts and tetrahedra: the origin of the anisotropy of feldspars

Ross J. Angel*, Lindsay M. Sochalski-Kolbus,

Crystallography Laboratory, Department of Geosciences, Virginia Polytechnic Institute and State University, Blacksburg, Virginia 24061, U.S.A.

Mario Tribaudino

Dipartimento di Scienze della Terra, Università di Parma, Viale G.P. Usberti 157/A, I-43100 Parma, Italy

*Email: rossjohnangel@gmail.com

*Current address: Dipartimento di Geoscienze, Via G. Gradenigo 6, I-35131 Padova, Italy

INTRODUCTION

This document is a very brief guide to the movies deposited as additional material to the manuscript. The movies are loops showing the tilt systems of feldspars. The original movies were generated in Crystalmaker (www.crystalmaker.com) from a series of *cif*'s of the structures generated with exactly regular and rigid tetrahedra.

The movies are "wmv" = "Windows media audio/video" files that can be viewed with Windows Media Player. You are welcome to download and use the videos for non-commercial and teaching purposes, provided appropriate acknowledgement of the source and reference to the published paper is given. If you have problems viewing the movies with an appropriate media player, try viewing them on the website www.rossangel.net.

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feldspar_4ring.jpg: The key to understanding the feldspar structure is the basic building unit of the tetrahedral framework, which is the ring of 4 tetrahedra shown in this jpeg. It can undergo four different tilts of the tetrahedra that we show in the movies. These four tilt systems do not deform the tetrahedra, and we have simulated them with perfect regular tetrahedra in the monoclinic structure to calculate how the unit-cell parameters and volume change with the tilts. Similar tilts can occur in any ring of an even number of corner-shared tetrahedra, and are the basis of the structural evolution of not just feldspars but all structures made up of frameworks of tetrahedra. Therefore the techniques and ideas shown here can be easily extended to explain the behavior of framework structures such as feldspathoids and zeolites. This is work on progress!

To make the movies easier to follow, the T1 tetrahedra are shown in yellow, and the symmetrically distinct T2 tetrahedra are shown in green.

Tilt1_ring.wmv: Tilt #1 is a tilt of the T1 tetrahedra around the Ob-Od edge. The movie shows a range of tilts from -20deg (outward tilt), through the un-tilted position, and on towards a +20deg inward tilt. Real feldspars normally have small positive (inward) tilts on average, which only vary between 0 and 5deg.

Tilt2_ring.wmv: Tilt #2 is a tilt of the T2 tetrahedra around the Ob-Od edge in a similar manner to the #1 tilt. The movie only shows the tilts from the un-tilted structure to positive tilts, because in feldspars negative values of tilt #2 lead to very short distances between oxygen atoms. Real feldspars exhibit a large range of positive tilts.

Tilt3_ring.wmv: Unlike the first two tilts, tilt #3 is a cooperative torsion of both the T1 and the T2 tetrahedra. The movie shows a range of tilts from the un-tilted position up to +30deg. Real feldspars exhibit a wide range of large positive tilts, which are strongly coupled with tilt #2.

Tilt4_ring.wmv: Tilt #4 is a simple shear of the 4-ring. Alkali feldspars show very little change in this tilt at crustal pressures, but there is significant change at pressures above 5 GPa and in the plagioclase feldspars. The movie shows tilts from -20 to +20 deg.

Tilt2_view001.wmv: Of the four possible tilt systems only two, #2 and #3 result in large changes in unit-cell volume. These are the two tilts that account for the structural changes in alkali feldspars at low pressures. This movie is the #2 tilt viewed down [001]. The b-axis runs vertically, and the (100) plane normal runs horizontally. The (010) mirror plane of the monoclinic structure runs horizontally across the middle, and reflects the top half of the structure in to the bottom half. At one end of the movie loop you can see that the oxygen pairs across the mirror plane are very close together. Oxygen-oxygen repulsion is why the #2 tilt only takes positive values in all feldspars. By following the motion of the oxygen atoms at the corners of the tetrahedra you can easily see why this tilt gives rise to large changes in all of the unit-cell parameters and a large change in volume.

Tilt3_view001.wmv: This is the #3 tilt shown in the same orientation as tilt #2 in *Tilt2_view001.wmv*. Compare the this movie with the one of tilt2 carefully and you can see why both tilts lead to large changes in d(100) across the pictures, because of the motion of the apical Oc oxygens on the tops of the yellow T1 tetrahedra, which force the neighbouring rings along (100) apart. But this tilt #3 is a torsion which does not lead to the large rotations of the T2 tetrahedra seen with tilt #2 (above). Therefore the change in the vertical dimension in these movies (the b axis) decreases with tilt #3 but increases with tilt #2. So, different tilts of the 4-ring lead to different changes in the cell parameters of feldspars and different anisotropy of expansion and compression because the different tilts move the oxygens that connect adjacent 4-rings in different ways.

Tilts2and3_view010.wmv: Large volume changes can only be accommodated in feldspars by tilts 2 and 3; this is because of the way in which the rings are linked together. Further analysis shows that the values of the tilts in feldspars maximise the shortest non-bonded O-O distances within the structure. For details see the paper! The enormous anisotropy of feldspars is the result of this combination of tilts 2 and 3, as can be seen in this movie. The movie shows the structural changes from Li-feldspar to Rb-feldspar. When both tilts operate together, you can see that d(100) (across the page) expands and contracts enormously, while the vertical direction (c-axis) hardly changes because the strain due to tilt #2 is almost cancelled by that due to tilt #3. The anisotropy is therefore a result of the framework topology and not a product of interaction with the extra-framework cations (seen here as purple spheres).